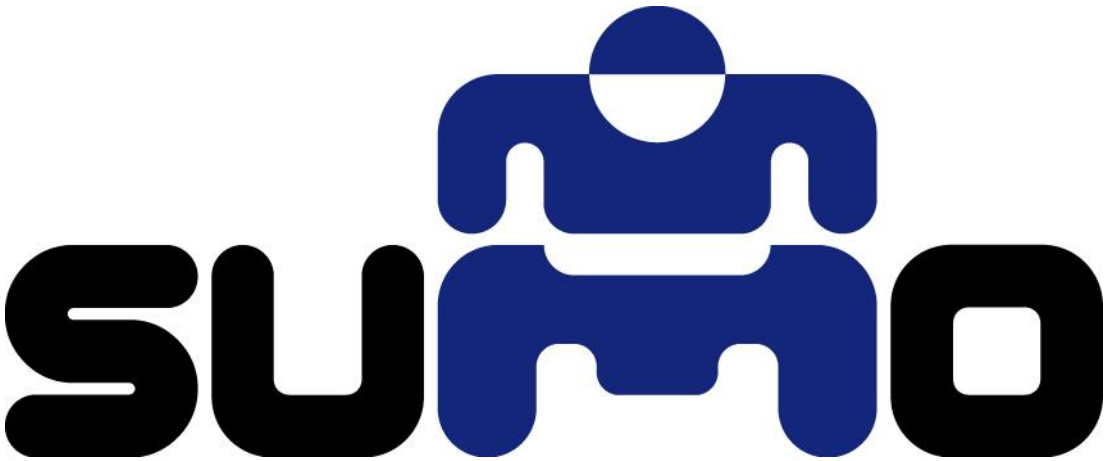
Sumo22.1 documentation



BY

Dynamita, www.dynamita.com, Sigale, France

Sumo *is a third-generation wastewater process simulation software. It was put together by a dedicated team with professionalism and thousands of days of tender loving care. Enjoy, and please let us know if you find somewhere it is coming short of your expectations. We will do our best to improve it.*

Imre Takács, on behalf of the whole Dynamita team

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Released: September, 2022

Last updated: April, 2024

Introduction

This document is the detailed documentation of the wastewater simulation software Sumo22.1. The following chapters are screenshots of the wiki page of Sumo22.1 from April of 2024. The following link is continuously updated to the latest released version of Sumo:

Dynamita's Sumo Wiki page

The Technical reference chapters are focusing on the process models and units describing the processes in detail and showing all the available functions for building your project using the standard library.

The Advanced User topics provide information for users to make every day's work more efficient, meanwhile the Developers topics are useful for users developing custom models and writing custom code.

The Digital Twin Toolkit chapter gives a programming overview of the possibilities of Sumolator.

What's new

This document summarizes the new features and improvements in Sumo releases compared to previous versions.

Sumo 22.1

New process model features

Nitrification inhibition in HPO model improvements

New and improved process units

- New ”fixed DO” aeration option in bioreactors (simulations are faster but the fixed DO model does not consider blower limitations or DO carry over)
- Minimum air flow requirement introduced (in case mixing is to be maintained in anoxic zones by airflow)
- Catchments and Rivers extended with sewer and river flow dividers, urban catchment extended with removal fractions for outgoing mass flows
- Minor fixes in THP, Primary settler, Pond and Granular SBR models

Tools

Easier switch controller setup (using a direct parameter to set up the effective range/strictness of the switch, instead of slope)

New interface features

- Faster navigation among output tabs, dropdown list for selection
- Faster loading and display of dynamic input tables
- Improved custom code handling (“Save for support” command changed to “Save with custom code”; the user can specify which custom process code files to ship with the project when saving and which ones to import when opening)
- Improved Add-on installer (available from the menu)
- Model continuity checker included (available from the menu)

Sumo 22

New process model features

Sumo 22 contains major additions and improvements:

- A module to perform scope 1 and 2 **Carbon Footprint** calculations and database
- **Integrated Urban Water System** (IUWS) library – enabling user to handle sewers, plant, river in the same configuration
- Faster, more realistic, and stable bio-P model (PAOs and GAOs as **carbon storing organisms**, CASTOs)
- Improved **dynamic alpha** model – more accurate OTR prediction
- **Aluminum** addition

New and improved process units

- Reverse Osmosis
- 3rd generation **pond** model with algae state variable
- More **chemical dose** options
- **Primary effluent** input and tool with typical fractions
- **Preferential inorganic removal** in primaries
- **SVI-based settling** parameter input option in layered clarifiers
- **Flexible SBR** – any cycle/phase setup can be entered
- Improved **P recovery** unit
- A number of new **examples** are also provided
- Significant **MABR** improvements

Tools

- Much improved and battle-hardened **Digital Twin Toolkit** (for additional fee)
- Online raw data cleaning (dDesk, dDock from Primodal - separate products that can be interfaced with Sumo)

New Sumo tools

- Primary effluent fractionation tool
- Industrial COD fraction converter
- Switch controller
- Vesilind settling tool

Documentation

- Updated **Manuals**

- **Technical Reference**
- **Dynamita Wiki** - In addition to the pdf versions of Manuals
- **XML debugger** description in Wiki – useful interactive debug feature for custom code

New interface features

- Professionally redesigned **graphics**
- Automated **mass flow** displays on pipes
- New **Calculators**: Sum, Ratio and Advanced ratio
- New **Statistic tools**: Run-based and cycle-based Totalizers, Noise
- **Mapping tool**: target parameter will dynamically follow source
- Factory library should not be edited – **custom code** should go to My Process Code
- Sumo 22 is **compatible** with Sumo 21 configurations in most cases (depending on the level of customization)
- Sumo 22 will be available in the Korean, Chinese, Japanese, Spanish, German, Turkish and Vietnamese **languages** after the initial English release
- There are several usability improvements and fixes

Add-ons available for this release

- Realistic simulation of **carrier movement** in an MBBR plug-flow zone (mobile carrier) and the Wanner-Reichert biofilm model
- **Sewer trunk** and odor model (iron and nitrate addition for odor control)

The Add-ons are available from the Products page.

Known issues with Sumo 22.0.0

- Don't use “Overwrite all initial conditions with current values” from the Advanced menu on projects built with biofilm units → **Fixed in 22.1.0**
- For Boolean parameter inputs (e.g. SRT control), text entries are not accepted. Just type 0 for FALSE and 1 for TRUE → **Fixed in 22.1.0**
- When modeling HPO systems, the low pH limit needs to be raised to inhibit nitrification, as there is a lot of bicarbonate (substrate) available even at lower pH values → **Fixed in 22.1.0**

Sumo 21

New process model features

Sumo 21 contains major additions and improvements:

- Energy (pumps, blowers, CHP, biogas tank, fixed consumers…)

- Cost (electricity, chemicals, product sales, disposal fees)
- Faster, more realistic and stable bio-P model (PAOs and GAOs as carbon storing organisms)
- Greenhouse gas model
- Dynamically predicted alpha factor depending on loading
- Prediction of sludge dewaterability
- AOR calculation

New process units

- UASB
- BAF
- HPO
- Pond – lagoon
- P recovery units
- Sludge input units
- Advanced oxidation unit
- A number of new **examples** are also provided

Tools

Digital Twin Toolkit (for additional fee) connecting to plant hardware, realtime run, cloud-based run, distributed computing, custom interface option, etc.

New Sumo tools

- Aeration (SOTE) Tool
- Industrial COD fraction converter
- PD Blower Tool
- Turbo Blower Tool
- CF Pump Tool
- Power Tariff Tool
- Noise generator
- Totalizer

Documentation

Extended Sumo FAQ, User Manual, Quick Tutorial, The Book of SumoSlang and new Technical Reference

New interface features

- **Numerical solvers** were much improved (all corners: pH, loops, steady-state, dynamics)

- **Controllers** can be used in PFR units connecting to individual zones
- Sumo 21 is **compatible** with Sumo 19 configurations in most cases (depending on the level of customization)
- Sumo continues to be open process source based, but can be delivered **with encrypted process library** (i.e. in case a user provides a proprietary model to clients)
- Sumo 21 will be available in the Korean, Chinese, Japanese, Spanish, German and Turkish languages
- There are several usability improvements and fixes

Add-ons available for this release

- Realistic simulation of **carrier movement** in an MBBR plug-flow zone (mobile carrier) and the Wanner-Reichert biofilm model
- **Sewer trunk** and odor model (iron and nitrate addition for odor control)

The Add-ons are available from the Products page.

Known issues with Sumo 21.0.2

- If a model, implemented in Sumo 19, containing SRT controller(s) is loaded into Sumo21, the SRT controller has to be manually activated

Sumo 19

New process model features

Sumo 19 contains whole-plant **biokinetic models** with major improvements:

- Calibrated for carbon capture in high rate processes (A-stages as low as 3-hour SRT)
- New bio-P model for much wider application range (S2EBPR, deep ORP conditions)
- Detailed sulfur reactions and sulfur-iron interactions in whole plant models
- Aluminium, iron and polymer addition

Aeration calculations were significantly extended to include several types of fine and course bubble equipment as well as mechanical aeration. Surface DO intrusion in taken into account in all (e.g. anoxic) reactors

New process units

- Trickling filters
- Aerobic granular sludge
- MABR
- BOD influent
- Sand filter
- DAF

- Grease trap
- Plug-flow reactors with unlimited number of zones, feed, recycle and internal recycle options
- Extended chemicals for pH control and flocculation
- A number of new **examples** are provided

New utilities

- The **steady-state** solver has been corrected and finalized (Never-To-Fail© Dynamita exclusive)
- **Controllers** are now included in the Sumo 19 base package: Timer based on-off, ratio feed-forward, deadband, P, PI, PID, cascade, SRT and DO controllers
- New **tools** are included: Scenarios (save several operating conditions in the same file), moving average, aeration tool
- SBRs calculate reactor **SRT** automatically
- Extended Sumo **FAQ, Manual, Quick Tutorial**, The Book of SumoSlang and Technical Reference
- ExcelIO – Customizable operator interface – Your own plant model for operational scenarios

New interface features

Scenarios can be created within one simulation – i.e. winter and summer conditions both can be saved in the same configuration and run by selecting the required condition. There is no need to create copies of the same configuration containing different sets of parameters, therefore updating the plant model becomes centralized and much easier to manage.

Saving state variables: Any simulation condition can be named, saved, and reloaded later. Concentrations can be copied from one effluent to an influent (i.e. sidestream model to mainstream model) or to a reactor content.

Sumo 19 is **compatible** with Sumo16 configurations in most cases (depending on the level of customization).

Sumo continues to be open process source based, but from Sumo19 can be delivered **with encrypted process library** (i.e. in case a user provides a proprietary model to clients).

Sumo 19 will be available in the Korean, Chinese, Japanese, Spanish and Turkish languages.

There are several usability improvements and fixes.

Add-ons available for this release

- Realistic simulation of **carrier movement** in an MBBR plug-flow zone (mobile carrier) and the Wanner-Reichert biofilm model
- **Sewer trunk** and odor model (iron and nitrate addition for odor control)
- **Sensitivity analysis** (using Python scripts – Python knowledge required)

The Add-ons are available from the Products page.

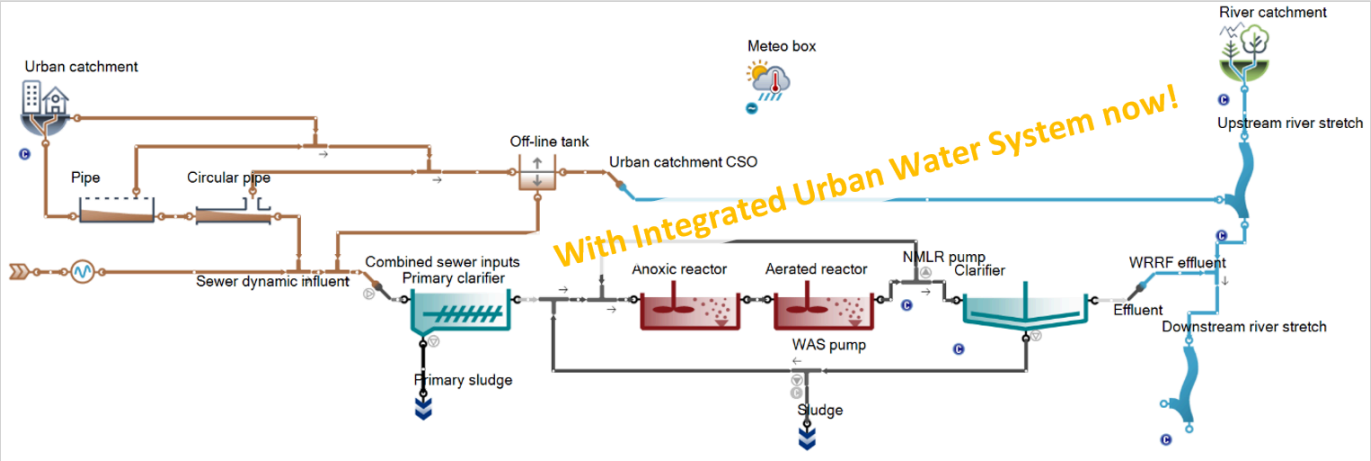
Known issues with Sumo 19.2

- Configurations developed in Sumo 16 should update automatically and will work in the release version – if this is not the case, we provide an update service for our customers. Predictions may change slightly as the models have been improved since the release of Sumo 16.
- Dynamic data tables must always have an entry at t = 0.
- Not all features of the software are covered by prebuilt examples. Please contact us if you need a specific example configuration.
- As with any complex software, it is good practice to save often. In case of unexpected behavior please contact us . It often helps to Exit Sumo, restart it and reload the model. Sumo will inform you if an Autosave (saved every five minutes by default) is available.

Why choose Sumo22

The Sumo© full featured - Wastewater Process Simulator

The new Sumo22[1] is out with significant improvements. Comes with IUWS (urban catchment and river models), scope 1 and 2 Carbon Foot Print, primary effluent input, RO, new pond model, flexible SBR, SVI input, updated industry-leading bio-P and dynamic alpha prediction. Fast Never-To-Fail© steady-state solver, easy scenario handling, and a ton of other new features.



- **Most extensive *calibrated model library* for traditional and advanced wastewater resource recovery processes, GHG, carbon footprint, integrated urban water system**
- ***Supported* by the largest[2] wastewater simulation company round the clock**
- **Sumo is the only *open process source* commercial simulator[2] (coded in Excel tabular format in SumoSlang™)**
- **Virtually *unlimited* activated sludge/anaerobic digester/sidestream treatment *configurations* available[3]**
- **Only simulator that allows complete flexibility to *build your own models* or modify any models in Sumo**
- **Integrated *steady-state* and *dynamic* simulations, 2-way link to Excel or other programs, popups, sticky notes, undo, Book of SumoSlang, extended documentation. Available soon in Korean, Chinese, Japanese, Spanish, Turkish, German and Vietnamese languages**
- ***Fast! Very fast!* Ask for more details: www.dynamita.com or info@dynamita.com**

Technical specifications

Biokinetic/chemical models	Process units/configurations	Strong points
Sumo models (Dynamita in-house researched/developed)	Easy, flexible influent specification	Easiest software to get up to speed with

- Sludge production and oxygen uptake
- One step nitrification/denitrification
- Two step nitrification/denitrification, anammox
- High-rate process, flocculation
- Industry leading Bio-P with PAOs GAOs (for S2EBPR as well)
- Fermentation, anaerobic digestion
- Sulfur oxidation/reduction/precipitation
- Chemical P removal (iron/alum)
- Struvite and other precipitates, nutrient recovery
- Greenhouse gases
- Methanol dosing
- Aeration
- pH, alkalinity
- Gas transfer, stripping
- Controllers (DO, SRT, timer, on-off, ratio, PID)
- Dynamic alpha prediction
- Sludge dewaterability prediction

Museum models

- ASM1
- ASM2d (original or with TUD bio-P)
- ASM3 (w/wo bio-P)
- Barker-Dold
- ADM1

Other models

- UCTPHO+ (UCT)

Your own models

- Model editor/automated mass balance check
- Dedicated process engineering/research support

Reactors

- All types of activated sludge reactors (CSTRs, PFRs, oxidation ditches, SBRs etc.)
- Fermenters
- Anaerobic digesters
- Sidestream reactors
- MBBR, IFAS, TF, Mobile Carrier
- Aerobic Granular Sludge
- MABR, MBR
- BAF, UASB
- Pond/lagoon

Phase separators

- Primary, secondary settlers
- Reverse osmosis, Thickeners, centrifuges, cyclone, dewatering, filters etc.

Other units

- Thermal hydrolysis and advanced oxidation processes
- DO, MLSS, SRT, pH, ORP control

Flow control elements

- Pumps, bypass weirs, channels, EQ basin
- Flow combiners/dividers

Tools

- Sum, ratio, totalizers, noise, mapping…

Configurations

- GUI Windows 10, 11 based (compiled models are platform independent)
- Runs on Mac within Parallels or Windows
- Unique, user-friendly task-flow based software design, undo, Excel report
- Mass flow displays/annotation directly on drawing board. Publication ready
- Expert support in process software
- Training courses, technology transfer
- Sumo team co-authored books (WERF Influent Characterization Manual, Good Modelling Practice Guidelines, various MOPs)
- Industry standard layered settling model for all types of settlers, clarifiers, thickeners with compression
- Open API connection to 3rd party apps Excel toolkit complementing Sumo
- Dynamita Influent Tools
- Dynamita High F/M Tool (Autotrophic growth rate evaluator)
- Dynamita OUR tool
- Dynamita Influent Active Biomass Tool
- Dynamita DSRT Tool (Do you know your sludge age?)
- Dynamita K_La Tool

▸ SumoSlang – built-in intuitive simulation language for any dynamic or algebraic model Energy, cost and CFP calculation layer on top of process layer Add-ons ▸ Carrier movement in PFRs and in plant (e.g., kenaf) ▸ Sewer (including odour) model	▸ Unlimited complexity (largest, most complex plants in the world have been modelled) ▸ Typical example plants (A2O, MLE, SBRs, AS+Digester, whole plant with sidestream treatment, IUWS, etc.) provided with software ▸ Mainstream deammonification ▸ AB process ▸ Thermal hydrolysis + digestion ▸ and many others	▸ Dynamita Pump and Blower Tools Offices ▸ Western Europe (France, Austria) ▸ North America (Canada) ▸ Eastern Europe (Hungary) Representatives ▸ Korea, Japan, China, Spain, Australia

Pricing

Single license with controllers 2300 €[4] **pa including support**

Volume discounts, educational, research and network licenses are available as annual lease or outright purchase.

Training at your location or in Dynamita offices available.

Ask for a detailed pricelist: info@dynamita.com

[1]Sumo19 and Sumo21 remain operational and do not need to be uninstalled

[2]To our best knowledge

[3]If we don't have it, we build it. Timeline and development cost (if any) is case specific

[4]We reserve the right to change pricing without notice

Sumo© is used worldwide.

Municipalities: DCWater, Washington DC, USA; Hampton Road Sanitation District, Norfolk, USA, Clean Water Services, Portland, USA, City of Meridian, Idaho, USA; City of Boulder, USA; First Utility District of Knox County, USA; Great Lake Water Authority, USA; Trinity River Authority, USA; City of Kunming, China, WaterCare, Auckland; New Zealand, Aurecon, New Zealand;

Consultants: CH2M, USA; AECOM, USA; ARAconsult, Austria; UTB, Hungary; Friedrichbüro, Germany; EnviTreat, USA; Ramboll, Finland; InnoWater, Hungary; Black and Veatch, USA; HDR, USA; Stantec, USA; Brown and Caldwell, USA; RF Wastewater, USA; SUEZ (CESMAE), France; Atkins, USA; Carollo, USA; Hazen and Sawyer, USA; Trojan Technologies, USA; AquaConsult Baltic, USA; InCTRL, Canada; BioPolus, Hungary; Veolia USA/France/Sweden; R.M. Towill, USA; OptVantage, New Zealand; Headworks International, USA, Volkert & Associates, Inc. USA; HKF Technology, USA, SWECO Nederland B.V., The Netherlands; HEPS Co., Korea; Kinnear Engineering, USA; Holinger, Switzerland, BG Ingénieurs Conseils SA, Switzerland; Hunziker Betatech, Switzerland; Jiacheng Environmental Protection&Engineering, China; Kiewit Corporation, China; GMB Civiel, The Netherlands; Olsson, USA; Binnies, UK; Sapoval, France; Çevtaş, Turkey;

Universities: VirginiaTech, University of Michigan, Aalto, INSA University of Colorado, TUD (Delft), EAWAG/ETHZ, Università Degli Studenti Firenze, University of Antwerpen, University of Tartu, Technishe Universität Darmstadt, Northeastern University, University of Kansas, INRA, University of Queensland, University of California, Rice University, Universitat de Girona, LIST Luxembourg, University of Washington, Northwestern University, Federal University of Ceara, Lappeenranta University of Technology, BOKU Wien, Harbin Institute of Technology, China; Tshingua University, China; Lunds Universitet, Sweden; Brunel University, UK; Cranfield University, UK; Georgia Institute of Technology, USA;

and others outside these categories such as Transcend Software, USA; CAMBI, Norway; UNESCO, Paris; World Water Works, USA; Tanuki Software, Japan; Kurita Water, Japan;

(partial client list, 2022)

FAQ

In this document we collected the most frequently asked questions and answers related to the use of Sumo.

Installation, licensing, interfacing

Q: What kind of hardware does Sumo require?

A: Sumo will run on any PC (Windows 10+ suggested) or Mac using a Windows emulator like Parallels. For larger jobs ample memory (16Gb or more) and fast multicore processors are recommended.

Q: How do I use the hardlock (delivered with mobile licenses)?

A: Plug the USB hardlock into any computer that has Sumo installed, and at the licensing page in Sumo select “Use Hardlock”. Sumo will work as long as the key is inserted and the license is valid. The key can be moved to any computer which has Sumo installed.
The XXX.XX.X ID on the keyring is a client.producttype.product# identifier from our database. You will need to refer to this if you have a problem or at renewal.

Q: Can I operate my model from other packages or link to other software?

A: Yes, using the Digital Twin Toolkit (sold separately).

Modeling scope

Q: What is the most important first step in modelling?

A: Proper influent fractionation is the most important step - please use the Influent Tool in Input Setup - selecting the influent - bottom middle.

Q: Can Sumo be used for simulation of industrial wastewater treatment?

A: Sumo’s library of models can be used for many different industries (e.g. food industry) directly, however influent fractions and model parameters will have to be adjusted as the default parameter set is for municipal wastewater. Certain industries with toxic, inhibitory wastewater or special components will require modifications to the models. This is possible for the user to do since Sumo is open source, and Dynamita also offers this service.

Q: Are the Sumo models whole-plant models?

A: Yes, the six home grown Sumo models describe behavior in the whole plant, aerobic, anoxic, anaerobic, digestion, sidestream environments. The kinetic rates are applied everywhere except in non-reactive units (for example volumeless separators)

Q: Is there literature I should read?

A: The IWA STR#1 (ASM1 model), the WERF Wastewater Characterization and the IWA STR#22 Guidelines for Using Activated Sludge Models are recommended. Please contact us for information how to locate them.

Working with Sumo

Q: How do I choose how much detail I need in my Process Units?

A: Each Process Unit has several (more or less complex) model implementations in Configure - bottom left pane.

Q: Can I set input parameters (e.g. volumes) for several reactors at the same time?

A: You can select several units by drawing a rectangle around them and change a common variable (e.g. volume) at the same time if the value is the same.

Q: Can I copy process units? Will they preserve their input parameters?

A: You can copy process units, whole plants with all parameters - even into a different Sumo Configuration. The Process Unit or plant will be copied with all input parameters.

Q: Why are my pipes different shades of grey?

A: Pipe colours indicate TSS concentration - effluent should be light grey.

Q: Can I rearrange columns and rows in an output table?

A: Yes, both are feasible. Columns can be reorganized by dragging the column header and dropping it to the desired slot. Rows can be rearranged similarly: first highlight the row(s) to be moved with the mouse, then drag and move the pointer out to the bottom left screen panel for a moment, and finally drop the rows to the desired new place.

Q: What are “Fast” and “Accurate” Simulation modes?

A: Numerical solvers (steady-state and dynamic) are quite complex and use different approaches in Sumo. Depending on model complexity, different settings may be more useful.
• Fast: “Most of the time” the model will run faster and be sufficiently accurate (except very large models)
• Accurate: “Most of the time” the model will run somewhat slower but will present very accurate results. We found biofilms run usually faster in Accurate mode.
Think of the two buttons as “Mode1” and “Mode2” - it is easy to try which one is best for a specific configuration.

Q: Is there Undo in Sumo?

A: Yes, there is Undo - just like in Excel, CTRL-Z, to unlimited level.

Troubleshooting

Q: Why is my DO input CSTR not keeping the DO setpoint?

A1: The DO setpoint will not be met if the blower capacity (maximum airflow) is insufficient.
A2: If the DO setpoint is zero, it may not be met due to DO recycles or surface DO intrusion.

Q: I have too little (or too much) MLSS in my model. How do I fix it?

A: There can be several reasons for this, most of the time problems with data.

1) RAS flow measurement off - lower than real RAS flow results in higher model RAS solids and more wasted mass than in reality. Make a solids mass balance around the clarifier.

2) WAS flow measurement too high - intermittent wastage, rat-holeing? Sample taken at beginning of wastage has much higher concentration than later…

3) WAS-RAS slides measurement wrong - difficult to get representative sample

4) Influent fractions wrong - too high biodegradable material fraction in TSS leads to too low sludge production (more goes to CO2)

5) SRT too low in model compared to reality

6) Influent xCOD/VSS measurement incorrect - too high value will lead to too low solids

7) Average values not cleaned up, containing disturbances. Need to make dry weather average for steady-state runs.

8) Too short or inconsistent period for average data (plant in transient mode)

9) Effluent too high - losing solids in the model through effluent.

We would look at model stoichiometry and kinetics only after all this was covered.

Q: My model is very slow – how do I speed it up?

A: Slow or stalled model runs are most often caused by:

1. Incorrect inputs to the model, if you are using standard library models. Please doublecheck all flows, volumes, any parameters that you changed.
2. Model formulation problems if you developed your own model. We can help for a small fee.
3. If input flow is intermittent to (a part of) the plant, it is a good practice to leave a small minimum flow to the part that is switched off. Controllers controlling flows (e.g. MLSS controller) should have a small WAS flow even when MLSS is lower than the setpoint.

Q: How can I approach you with a support question?

A: Please contact support@dynamita.com with your support questions and send your configuration in email (.msumo) format (File menu > Export to email) with the description of the error and the steps to reproduce it.

Advanced features

Q: Custom code: Where do I insert my own models into Sumo?

A: In the install location there is a "Process Code" folder - this is the standard Sumo library, and must not be changed. Custom code has to be inserted into the proper place in “My Process Code”

Sumo Quick Tutorial

Short and easy introduction to using Sumo

Dynamita, www.dynamita.com , Sigale, France

Sumo *is a third generation wastewater process simulation software. It was put together by a dedicated team with professionalism and thousands of days of tender loving care. Enjoy, and please let us know if you find somewhere it is coming short of your expectations. We will do our best to improve it.*

Imre Takács, on behalf of the whole Dynamita team

Sigale-Toulouse-Budapest-Toronto-Innsbruck

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Install Sumo

The following steps will help to guide you through the installation of Sumo.

Prepare Microsoft Windows for Sumo

Operating system

Make sure your computer is operating Microsoft Windows 7 or later. Sumo supports touch screen computers running Windows 8/8.1 and Windows 10.

Sumo can be used on a Mac with Windows installed or through an emulator like “Parallels”.

Microsoft Office

Sumo requires Microsoft Excel 2007 or later installed.

.NET

Please make sure that your computer is running the Microsoft .NET 4.7.2 framework. You can check it in the list of installed applications (Control Panel / Programs / Programs and Features). If the .NET framework’s 4.7.2 version is not installed, please download and install it from the following location:

https://dotnet.microsoft.com/download/dotnet-framework/net472

Windows 10 comes with the required .NET environment. On other operating systems, if you have it already installed on your computer, the downloaded installer will exit or inform you. Proceed to the next step.

Installation of Sumo

You have received a link to the Sumo installer (or in rare cases the install file on a USB key). This is one file and contains everything necessary to install Sumo once Windows is prepared. Download it through the link

provided to your computer. From the USB key you can install directly if desired, it is not required to copy the file to the computer.

Install Sumo by starting the install package and follow the instructions. Administrator rights may be required during installation. For workstations, we recommend choosing the “Install for myself only” option.

Obtaining a license

Obtaining a license is a two-step process.

1. After install, start Sumo from the Windows Start menu. Sumo will display a message providing multiple options. If you don’t have the license file yet, Select “I need a new license”. Sumo will display two additional buttons to show information about your hardware (Machine Identifier Code) and to copy this information directly to the Windows clipboard. Please paste this code into an email and send it to support@dynamita.com. Dynamita will provide a license file for you according to our agreement.
2. Copy the license file Dynamita provided to a folder on your computer, start Sumo, choose the “I have a license” option, click “Select license file” and navigate to load the license file. As long as the license file is not deleted or moved and it is valid, this validation does not have to be repeated. Other options, like using a license server or a hardlock, are also available.

How to build a plant

Start Sumo from the Desktop icon. Sumo will start with showing the Welcome Screen, as illustrated in Figure 1. Below the Menu Bar, you will see the Task Bar that guides you through the project workflow, all the way from configuration to simulation. The main window is split into four panels with various functionalities.

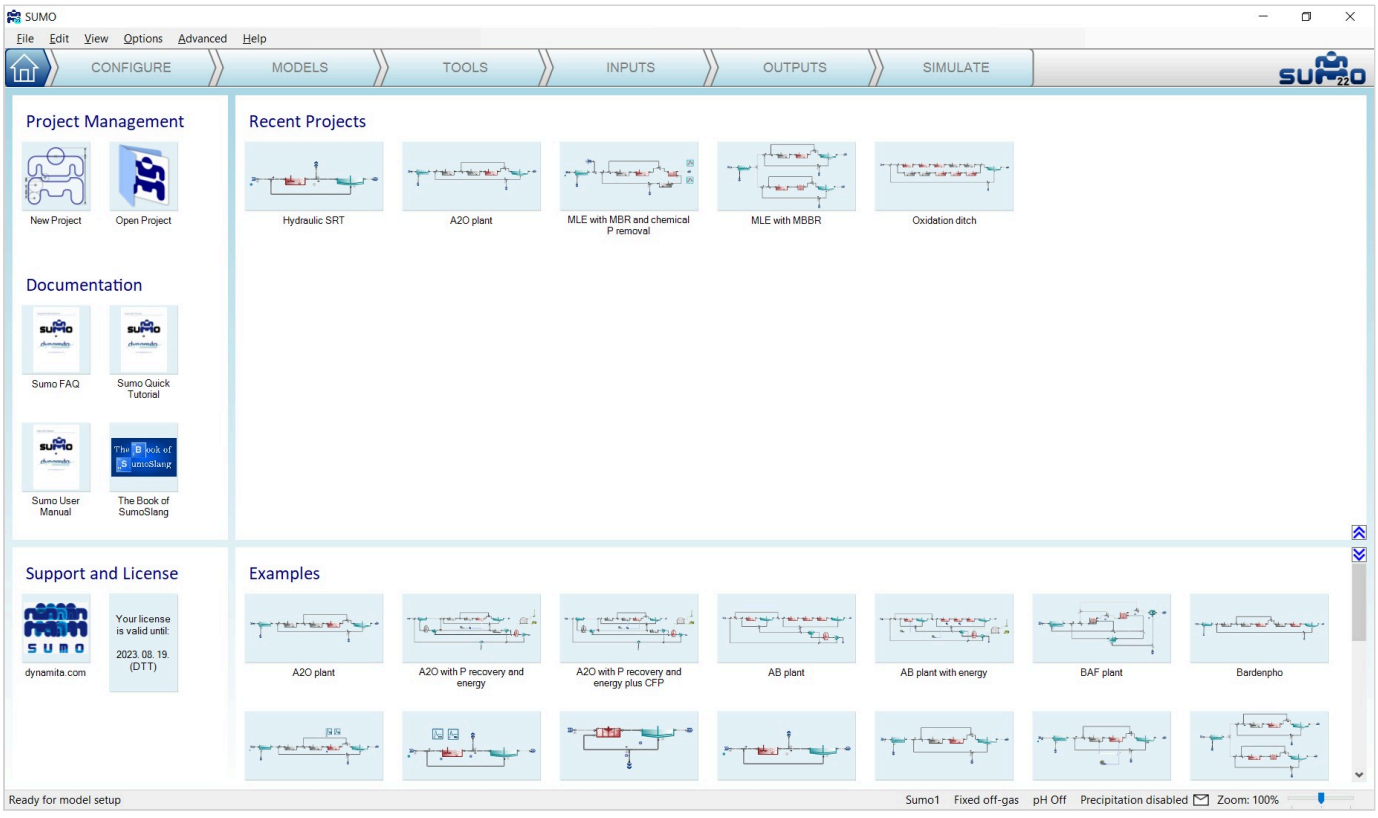


Figure 1 – Sumo21 startup screen

Configure

Click on the *Configure* tab. In this introduction, we will build a simple AO configuration using the *Flow elements*, *Bioreactors* and *Separators* categories from the element list of the top left screen panel. Select the desired process unit by opening the category and dragging the process unit to the drawing board. To drop the selected unit, just release the mouse button (Figure 2).

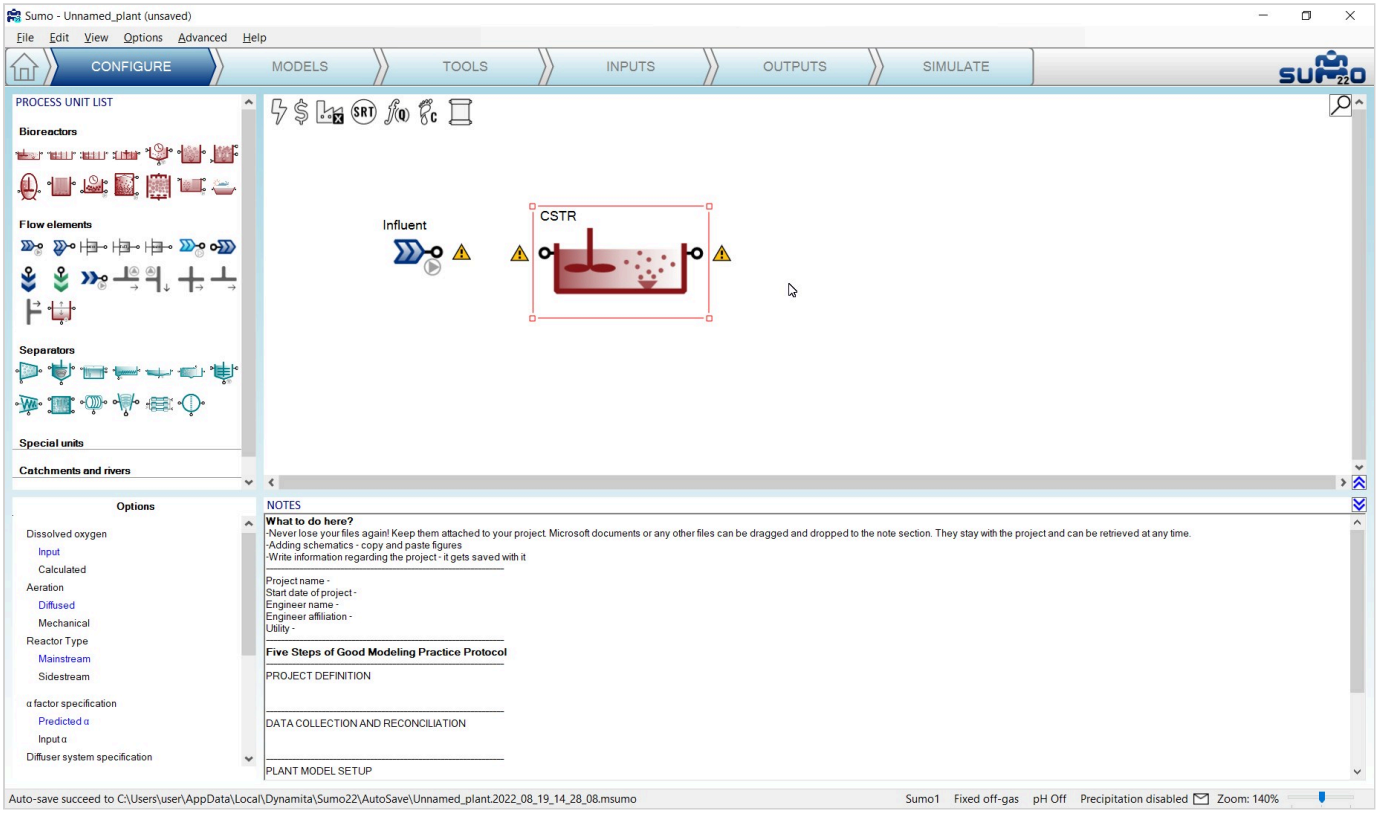


Figure 2 - Building the plant layout

The units can be connected with pipes by simply positioning their outflow connection (port) on top of an input port of another process unit (Figure 3), or by positioning the mouse on an output port of a process unit, pressing the left mouse button, then moving the mouse – and this way drag the pipe – to an input port of another process unit (Figure 4). Existing pipes can be removed by right-clicking on them and selecting *Disconnect pipe* from the pop-up menu.

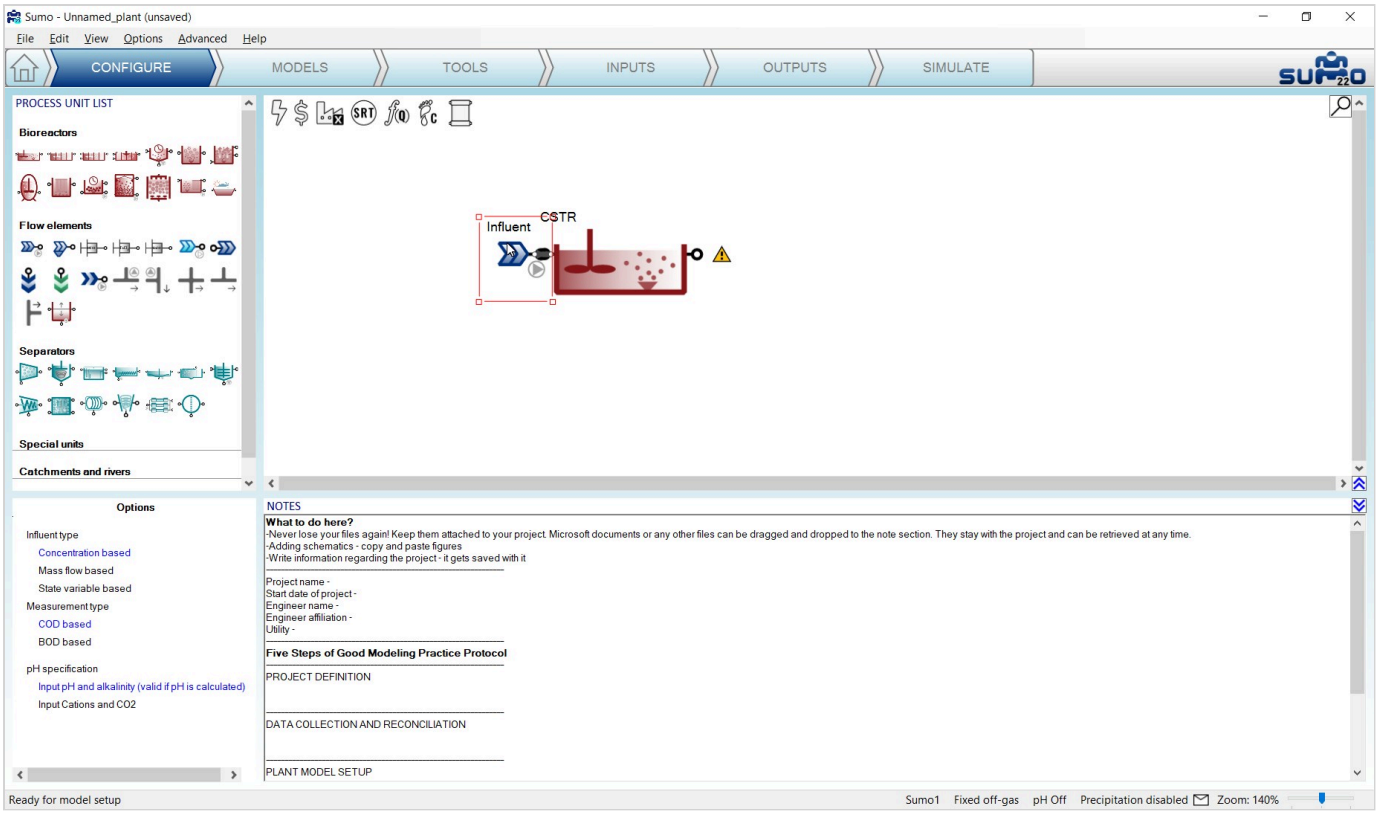


Figure 3 - Pipe created by touching process units

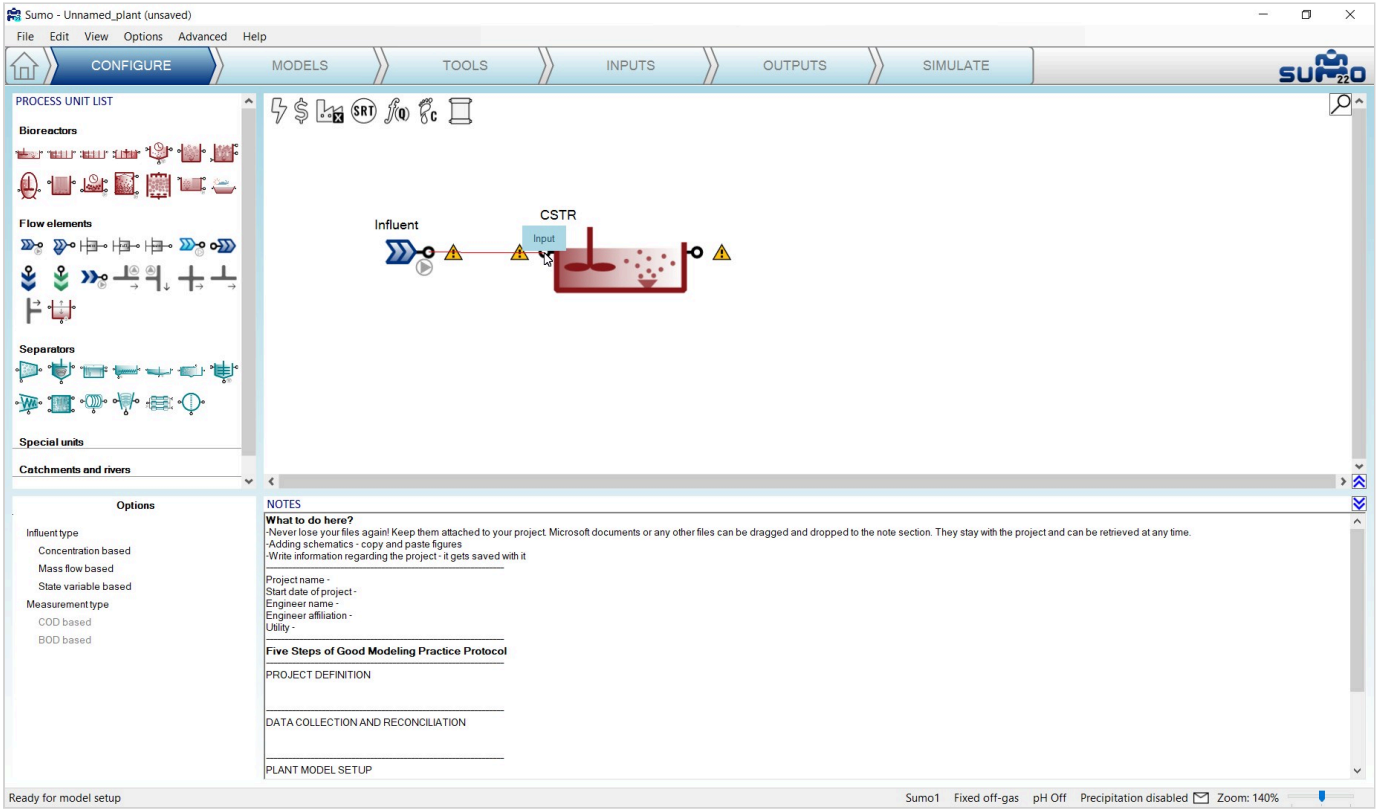


Figure 4 - Pipe created the conventional way

Build the plant configuration and connect the pipes as shown in Figure 5.

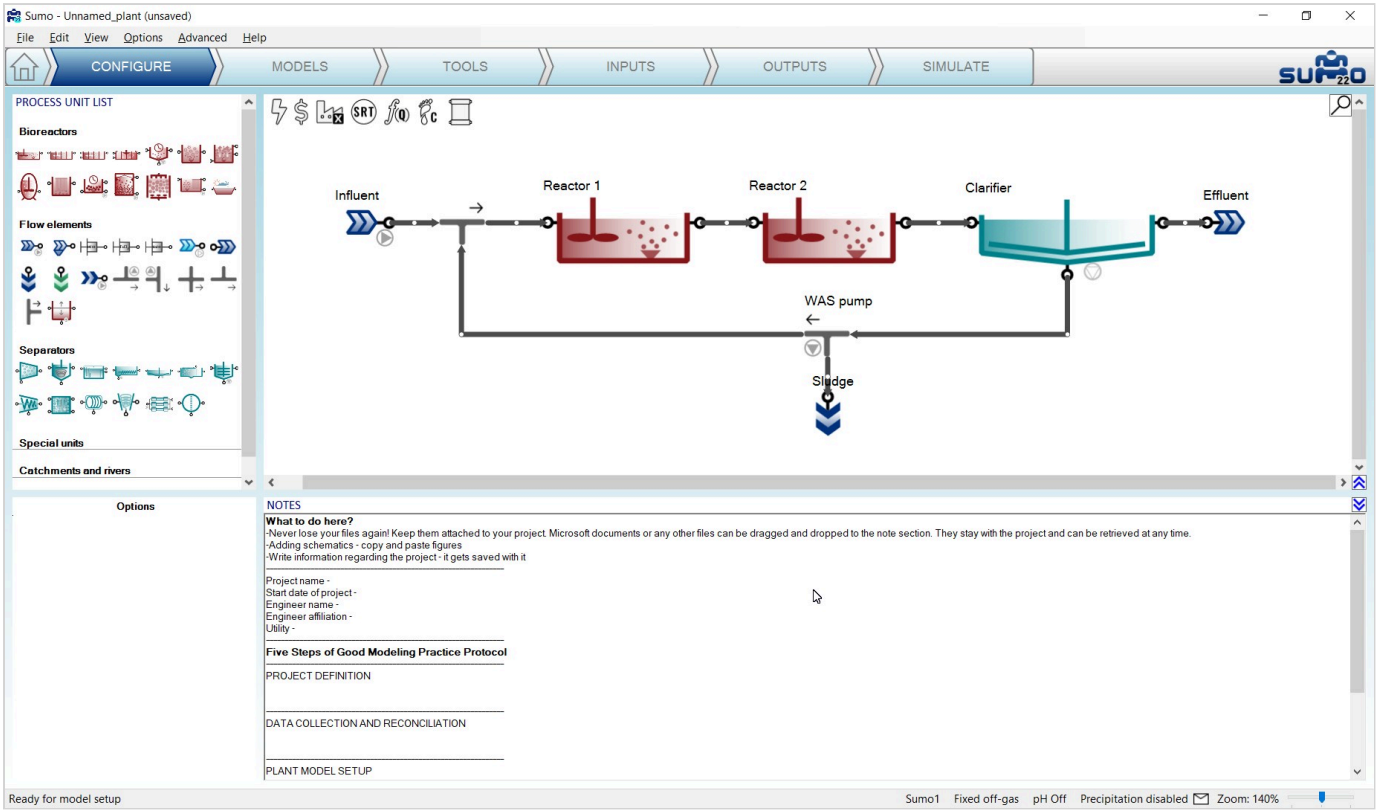


Figure 5 - The example layout

Rename or transform (rotate, mirror) the process units using the right-click pop-up menu. The pipes can be renamed as well, but this is usually not important – the pipe names are hidden by default (this can be changed in the *View* menu on the top). The visibility of process unit names can be controlled on a one-by-one basis.

Note: the above settings can only be modified in *Configuration* mode, but you can return and perform them at any point during your work. Changing the process unit names will not result in recompilation of the project model.

Models

In this tutorial, the setup of model parameters will be left at the default values.

Tools

Proceeding to the *Tools* tab, complex plantwide calculations can be defined ("plantwide" means that the calculations are based on variables contained in several process units around the plant). Various calculations can be added to the simulation, ranging from SRT calculation to different types of controllers. In this example,

a plant SRT calculation will be added by clicking on the *Sludge Retention Time* button in the top left screen panel.

The SRT calculation is set up the following way: drag reactors which contain sludge mass to the numerator and drag the wastage pump – and if desired, the effluent – in the denominator, as shown by Figure 6.

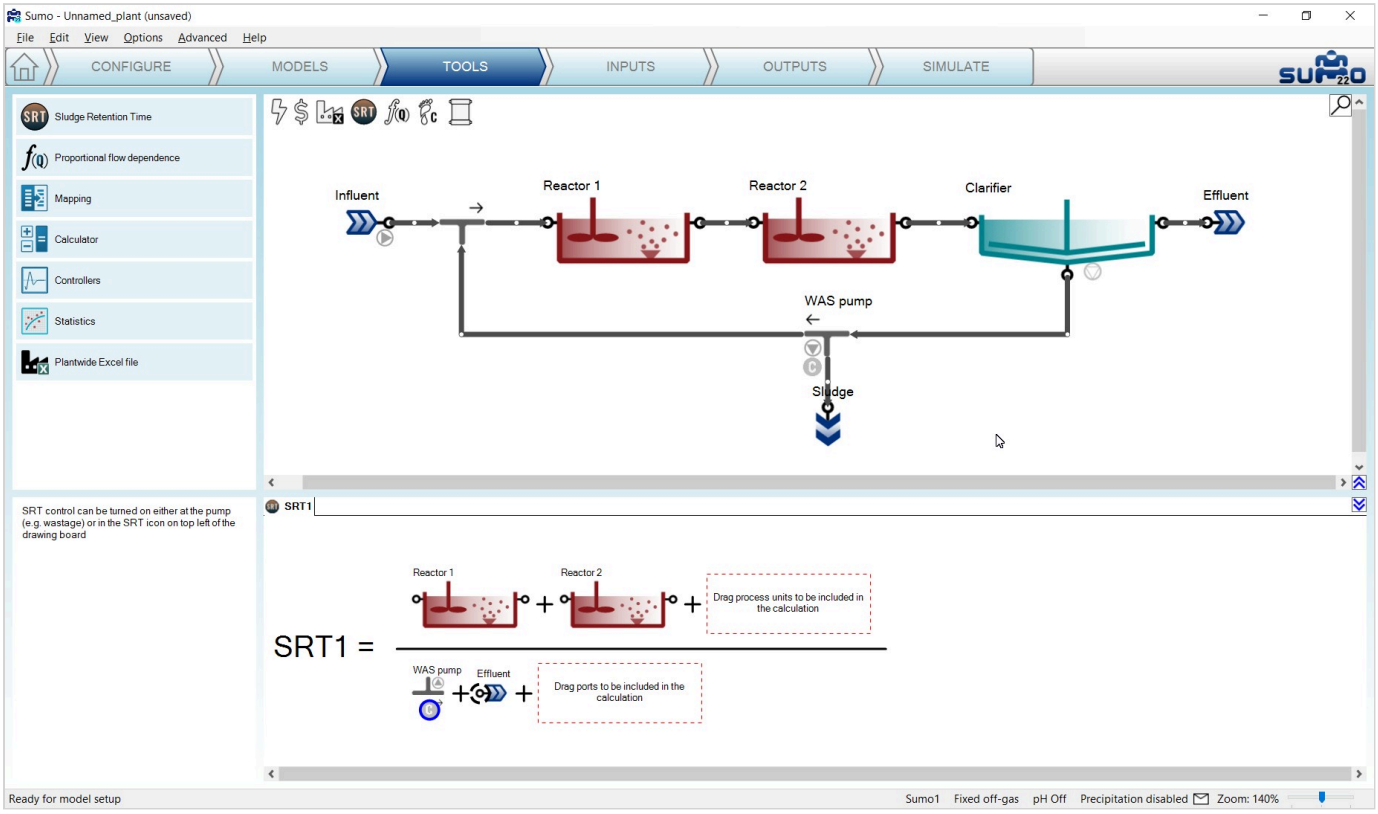


Figure 6 - SRT calculation setup

Target SRT can be defined as well, by assigning a proper controlled port. These ports, such as the WAS pump in our example, are indicated by a “C” sign within a blue circle. A certain pump can only be used to control one SRT.

Inputs

Choosing the *Inputs* task, the blue workflow tab above the drawing board automatically splits into *Constants* and *Dynamics*. Meanwhile, the model starts to be built. For the initial plant setup, we will only need the *Constants*, as shown on Figure 7.

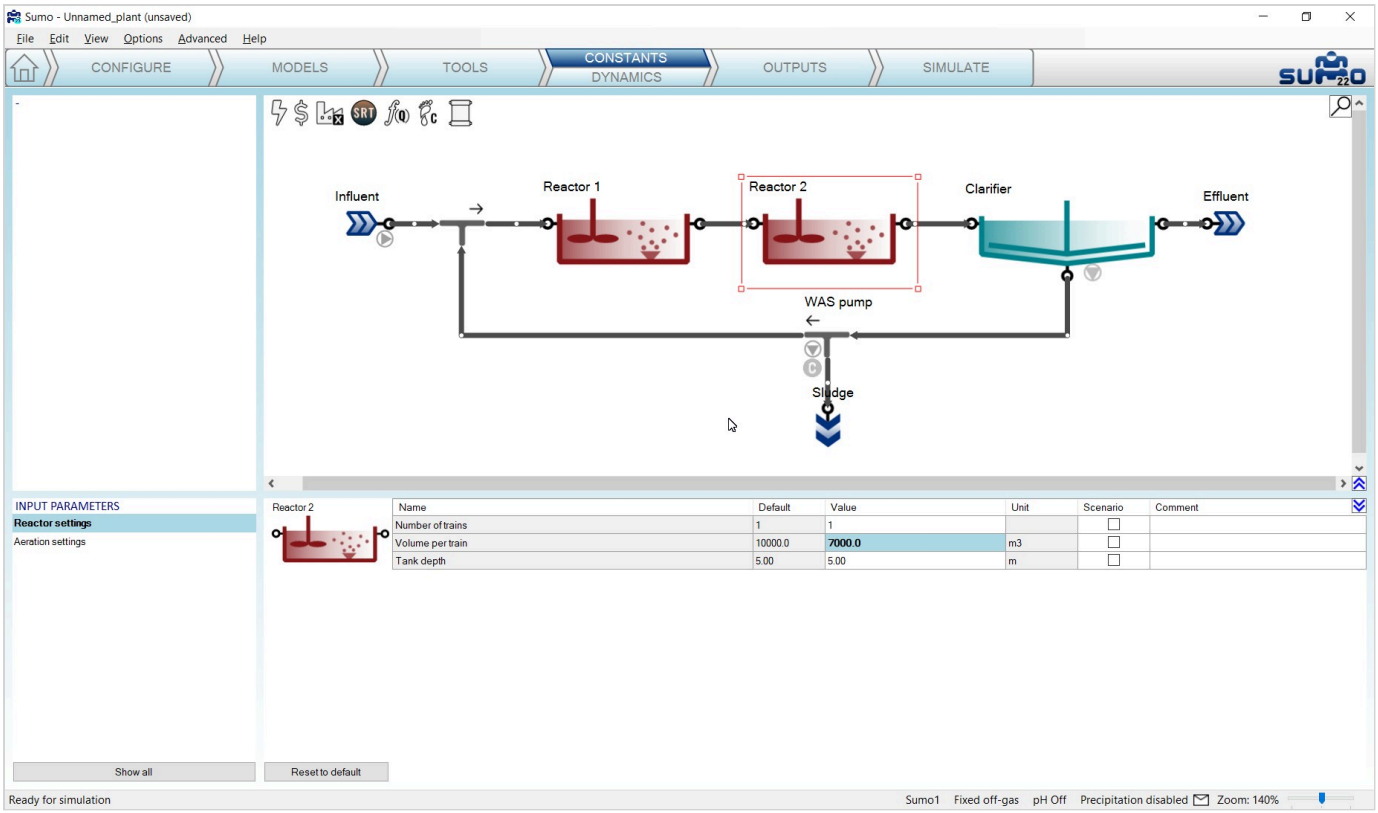


Figure 7 - Constant Input setup example

In this simple configuration, we only need to set a few values to build a realistic plant model, first for typical dry weather operation. Use the values from Table 1 for this example (we will only modify the reactor volumes, the influent, clarifier and wastage pump settings will be left at default values).

Table 1 – Input setup for simple AS plant

Process Unit	Parameter group	Parameter	Value	Unit
Reactor 1	Reactor settings	Volume per train	3000	m^3
Reactor 2	Reactor settings	Volume per train	7000	m^3

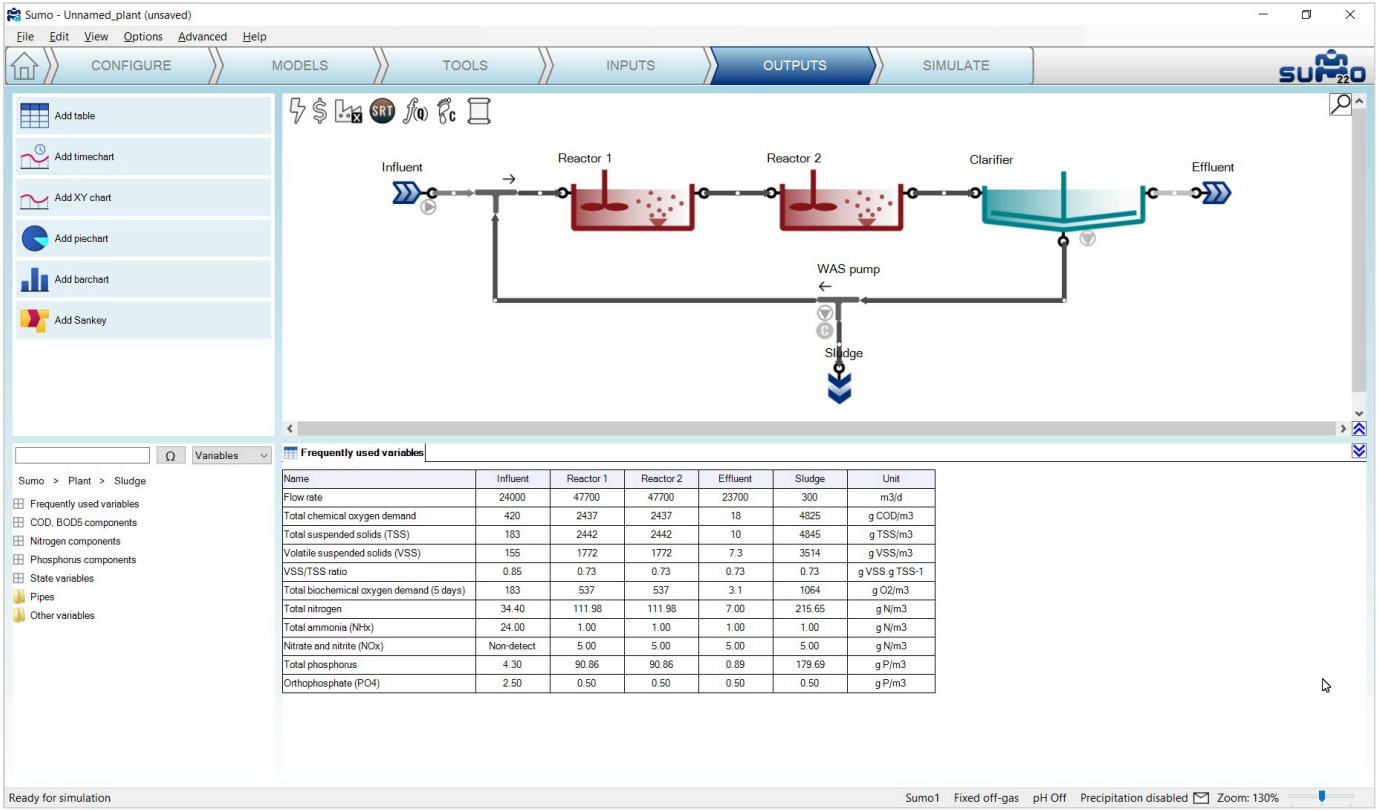
Enter these values by selecting the respective process unit on the drawing board and the parameter group in the *Input parameters* menu (bottom left panel) – the values can be edited in the bottom right panel (Figure 7). Each value that is different from the default will be highlighted with bold letter type. There is also a similar indication in the *Input parameters* menu for parameter groups that contain non-default values.

The input setup of this wastewater treatment plant model is now ready. Meanwhile the model has compiled as well (status bar message: “Ready for simulation”).

Outputs

This task can be used to specify which variables and in what format should be displayed and/or saved during the simulation phase.

For this example, add a **table** with the *Frequently used variables* of the Influent, Reactors, Effluent and Sludge (Figure 8); an MLSS **timechart** (Figure 9), Effluent N **timechart** (Figure 10) and a COD/BOD **barchart** (Figure 11). Select process units on the drawing board, then drag and drop variables (or variable groups) from the bottom left panel. You can also drag and drop process units to add new columns to an already existing table/barchart.



Name	Influent	Reactor 1	Reactor 2	Effluent	Sludge	Unit
Flow rate	24000	47700	47700	23700	300	m3/d
Total chemical oxygen demand	420	2437	2437	18	4825	g COD/m3
Total suspended solids (TSS)	183	2442	2442	10	4845	g TSS/m3
Volatile suspended solids (VSS)	155	1772	1772	7.3	3514	g VSS/m3
VSS/TSS ratio	0.85	0.73	0.73	0.73	0.73	g VSS.g TSS-1
Total biochemical oxygen demand (5 days)	183	537	537	3.1	1064	g O2/m3
Total nitrogen	34.40	111.98	111.98	7.00	215.65	g N/m3
Total ammonia (NHx)	24.00	1.00	1.00	1.00	1.00	g N/m3
Nitrate and nitrite (NOx)	Non-detect	5.00	5.00	5.00	5.00	g N/m3
Total phosphorus	4.30	90.86	90.86	0.89	179.69	g P/m3
Orthophosphate (PO4)	2.50	0.50	0.50	0.50	0.50	g P/m3

Figure 8 - Summary table setup

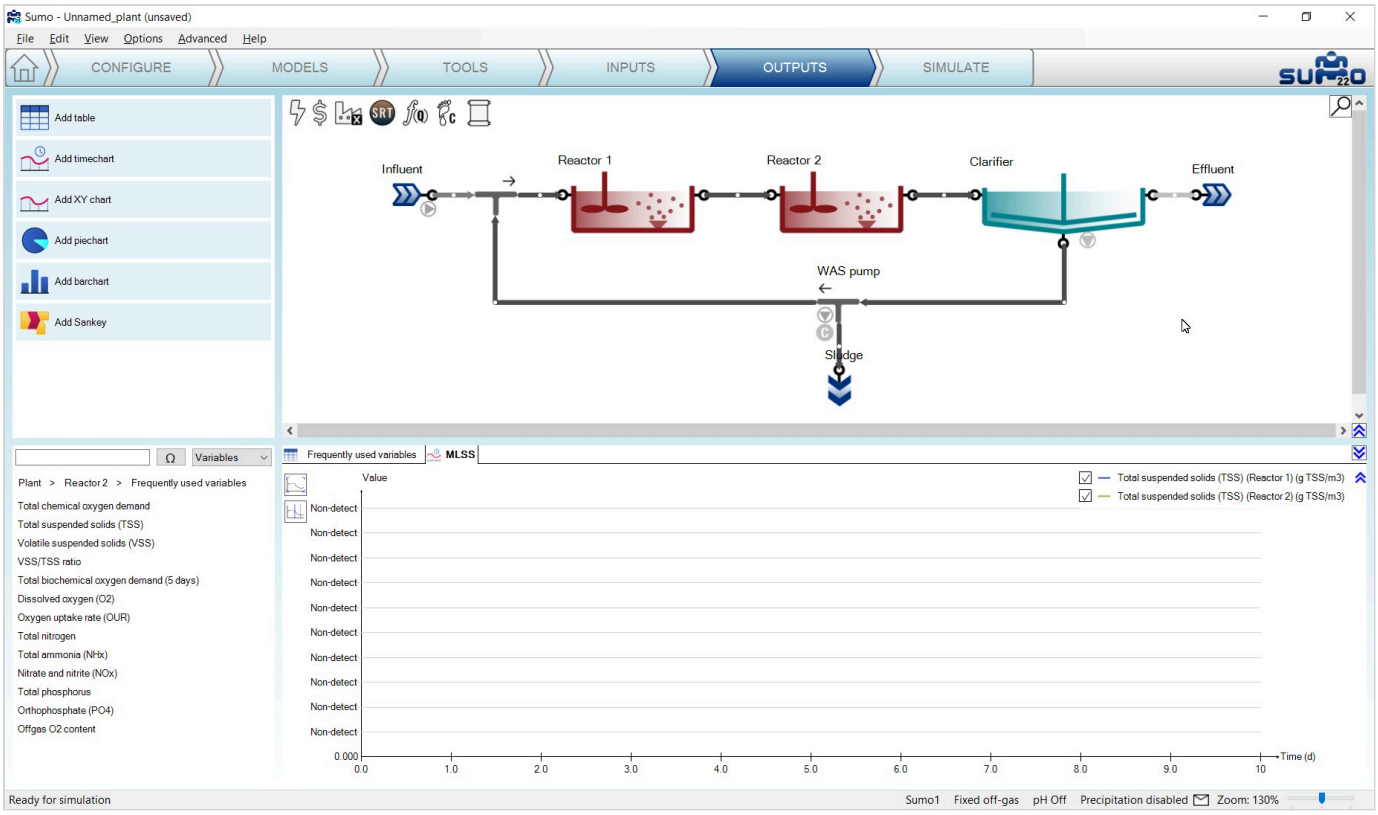


Figure 9 - MLSS timechart setup

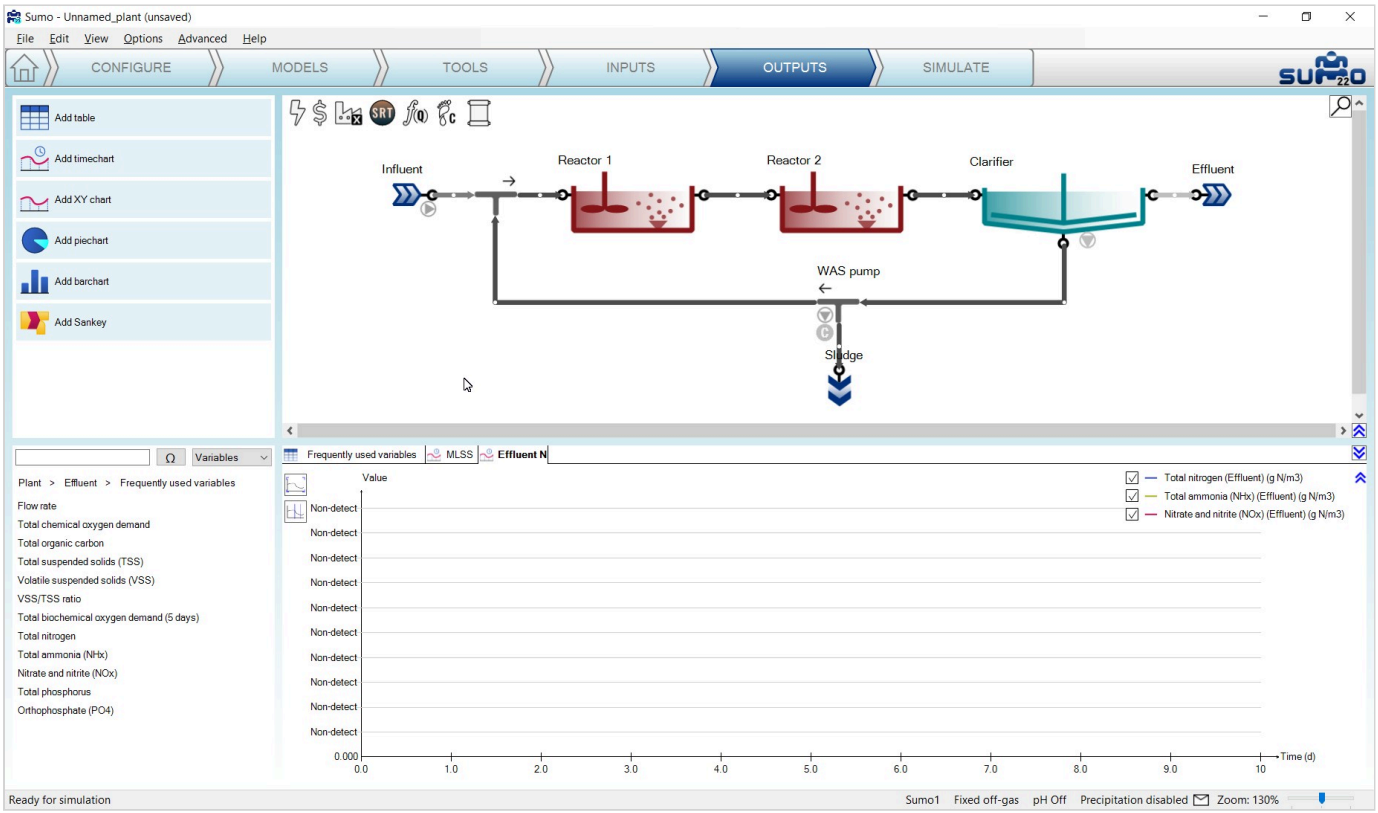


Figure 10 - Effluent N timechart setup

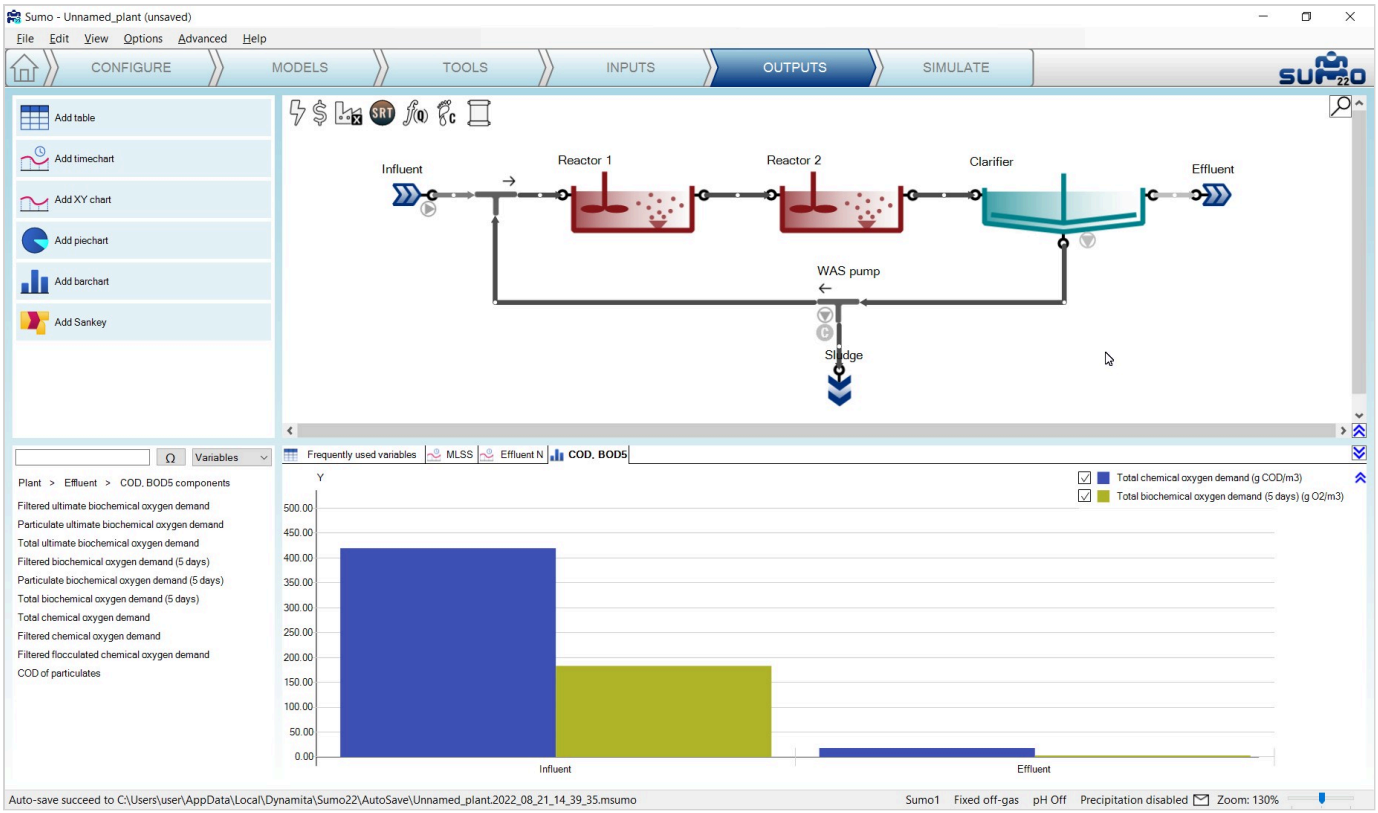
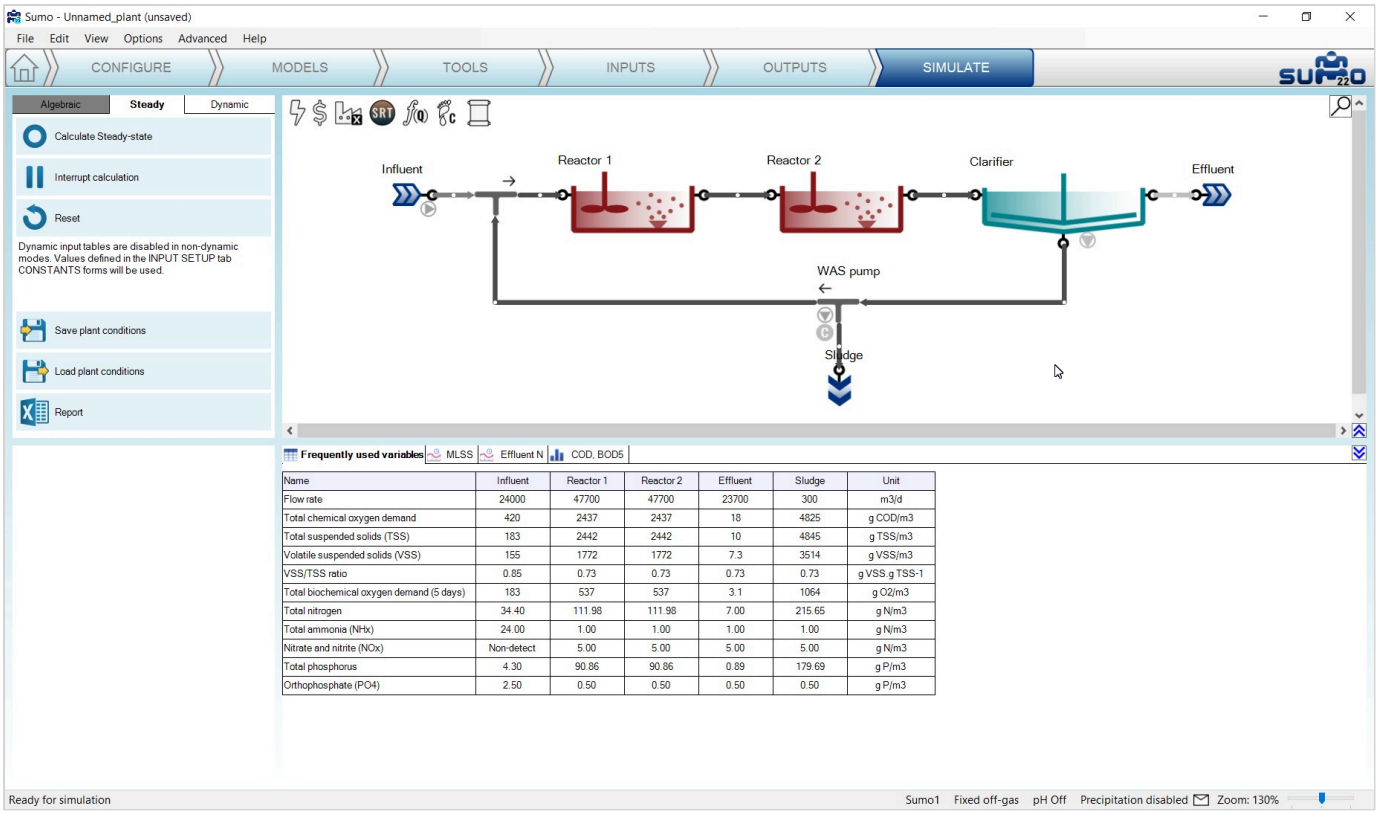


Figure 11 - COD/BOD5 removal setup

Simulate

The last item on the Task Bar can be used to run simulations and observe the results (Figure 12). *Steady* mode can be used to calculate directly the steady-state condition of the variables, whereas using *Dynamic* mode will show the variations with time (switch between the two modes using the tabs on the upper left panel).



Name	Influent	Reactor 1	Reactor 2	Effluent	Sludge	Unit
Flow rate	24000	47700	47700	23700	300	m3/d
Total chemical oxygen demand	420	2437	2437	18	4825	g COD/m3
Total suspended solids (TSS)	183	2442	2442	10	4845	g TSS/m3
Volatile suspended solids (VSS)	155	1772	1772	7.3	3514	g VSS/m3
VSS/TSS ratio	0.85	0.73	0.73	0.73	0.73	g VSS.g TSS-1
Total biochemical oxygen demand (5 days)	183	537	537	3.1	1064	g O2/m3
Total nitrogen	34.40	111.98	111.98	7.00	215.65	g N/m3
Total ammonia (NHx)	24.00	1.00	1.00	1.00	1.00	g N/m3
Nitrate and nitrite (NOx)	Non-detect	5.00	5.00	5.00	5.00	g N/m3
Total phosphorus	4.30	90.86	90.86	0.89	179.69	g P/m3
Orthophosphate (PO4)	2.50	0.50	0.50	0.50	0.50	g P/m3

Figure 12 - Simulation tab, Ready for simulation

Dynamic simulation can be started by pressing the *Start* button. The duration (*Stop time*) and the reporting frequency (*Data interval*) of the simulation can be set before the simulation. Upon first start, the simulation will be run from the initial conditions (defaults specified in the model file and in the process units) and every subsequent run will be initiated with the last system state. A 100-day graph gives a good indication whether the system has settled into stable condition and the results are meaningful for typical dry weather summer operation. (Figure 13 and Figure 14). The COD/BOD_5 removal is shown on the barchart (Figure 15).

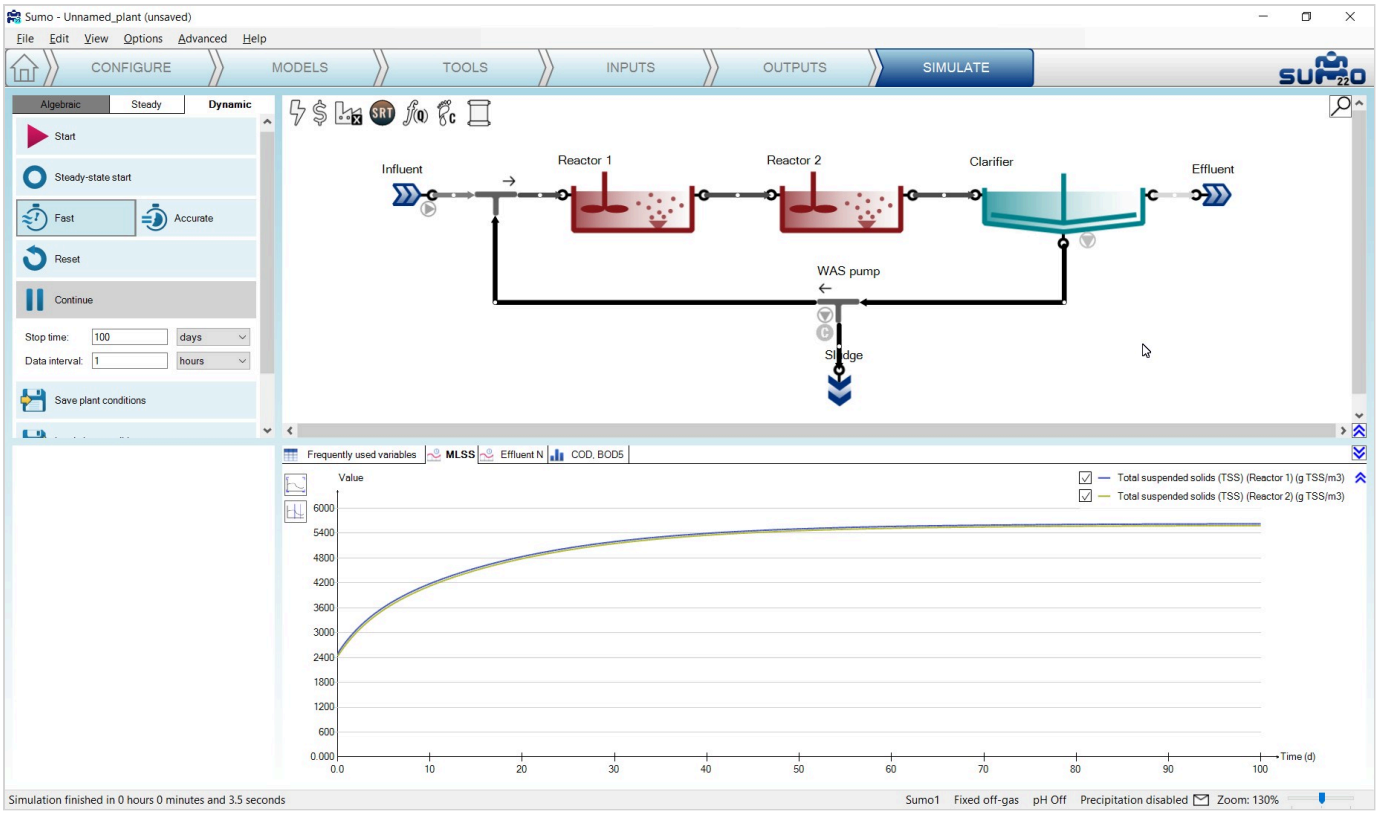


Figure 13 - MLSS timechart results

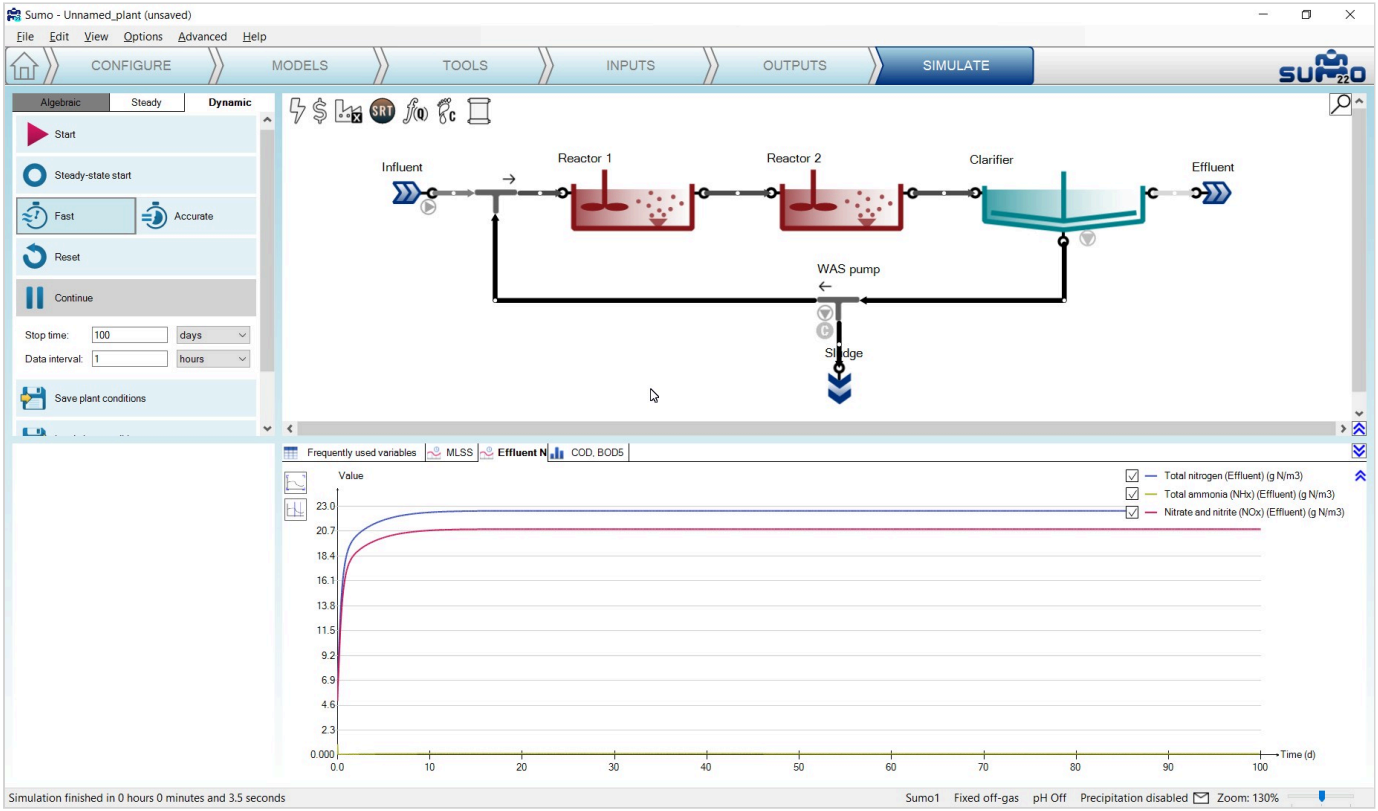


Figure 14 - Effluent N timechart results

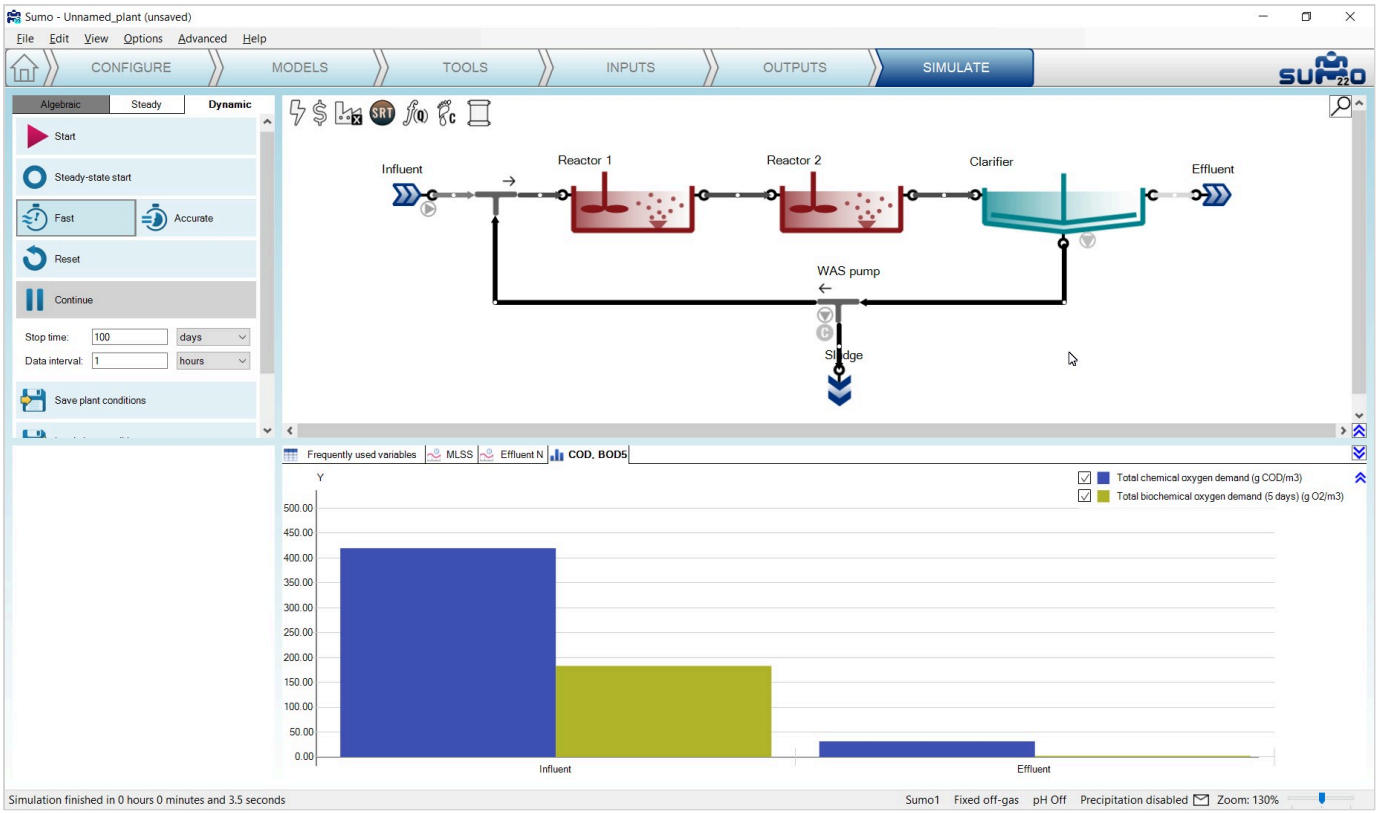
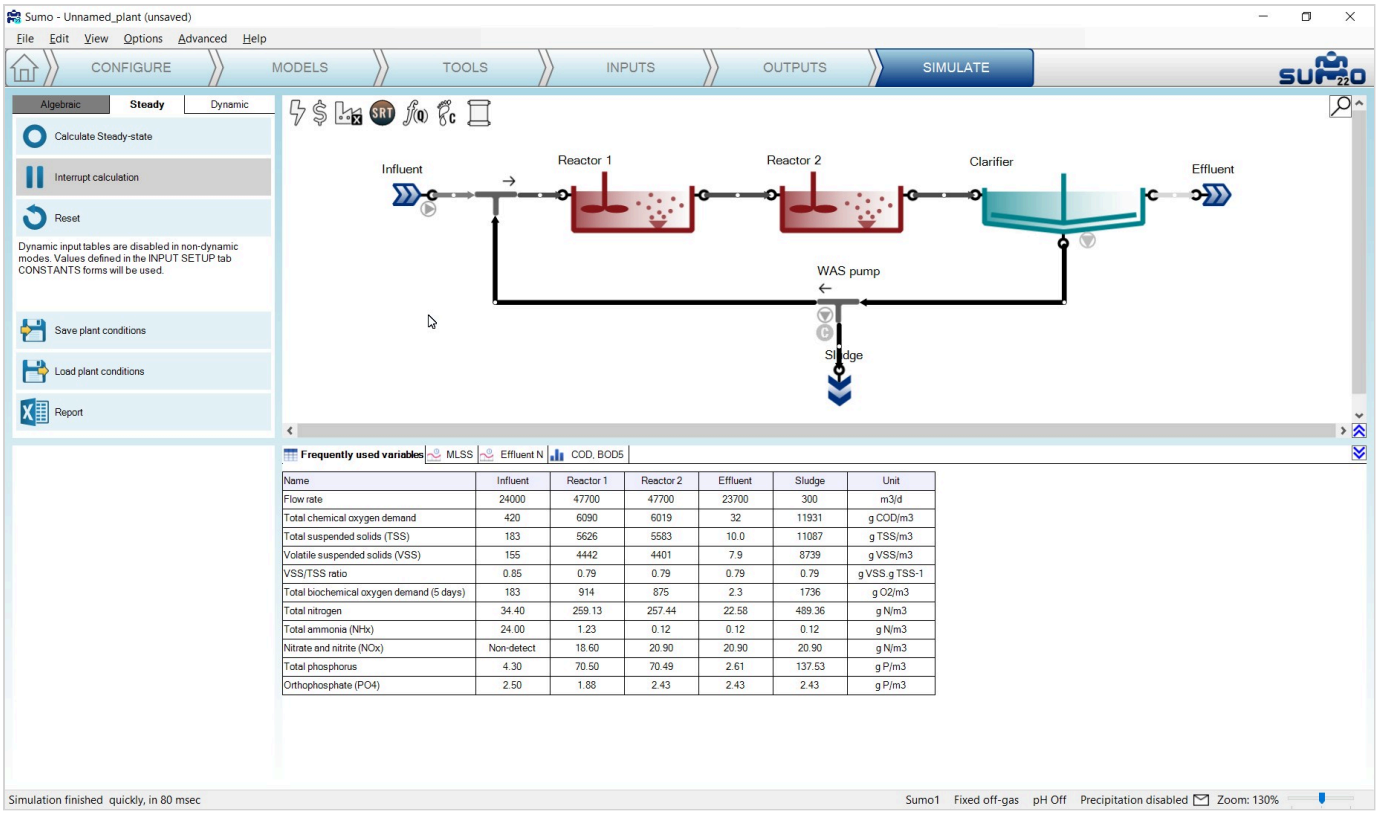


Figure 15 - COD/BOD5 removal results

The steady-state simulation employs different solvers to look for the steady-state condition of the system. In this mode, all dynamic inputs are disabled and the controllers are turned into integrated controllers. The steady-state simulation will find the concentrations in the plant with constant influent and operating conditions, such as monthly average conditions etc. (Figure 16). Please note that steady-state simulation cannot be performed on inherently dynamic processes such as the SBR.



Name	Influent	Reactor 1	Reactor 2	Effluent	Sludge	Unit
Flow rate	24000	47700	47700	23700	300	m3/d
Total chemical oxygen demand	420	6090	6019	32	11931	g COD/m3
Total suspended solids (TSS)	183	5626	5583	10.0	11087	g TSS/m3
Volatile suspended solids (VSS)	155	4442	4401	7.9	8739	g VSS/m3
VSS/TSS ratio	0.85	0.79	0.79	0.79	0.79	g VSS.g TSS-1
Total biochemical oxygen demand (5 days)	183	914	875	2.3	1736	g O2/m3
Total nitrogen	34.40	259.13	257.44	22.58	489.36	g N/m3
Total ammonia (NHx)	24.00	1.23	0.12	0.12	0.12	g N/m3
Nitrate and nitrite (NOx)	Non-detect	18.60	20.90	20.90	20.90	g N/m3
Total phosphorus	4.30	70.50	70.49	2.61	137.53	g P/m3
Orthophosphate (PO4)	2.50	1.88	2.43	2.43	2.43	g P/m3

Figure 16 - Steady-state calculation results

In the *Dynamic* simulation mode, clicking on the *Steady-state start* button will initialize a steady-state run, followed by a dynamic run with the selected *Stop time* and *Data interval* (Figure 17).

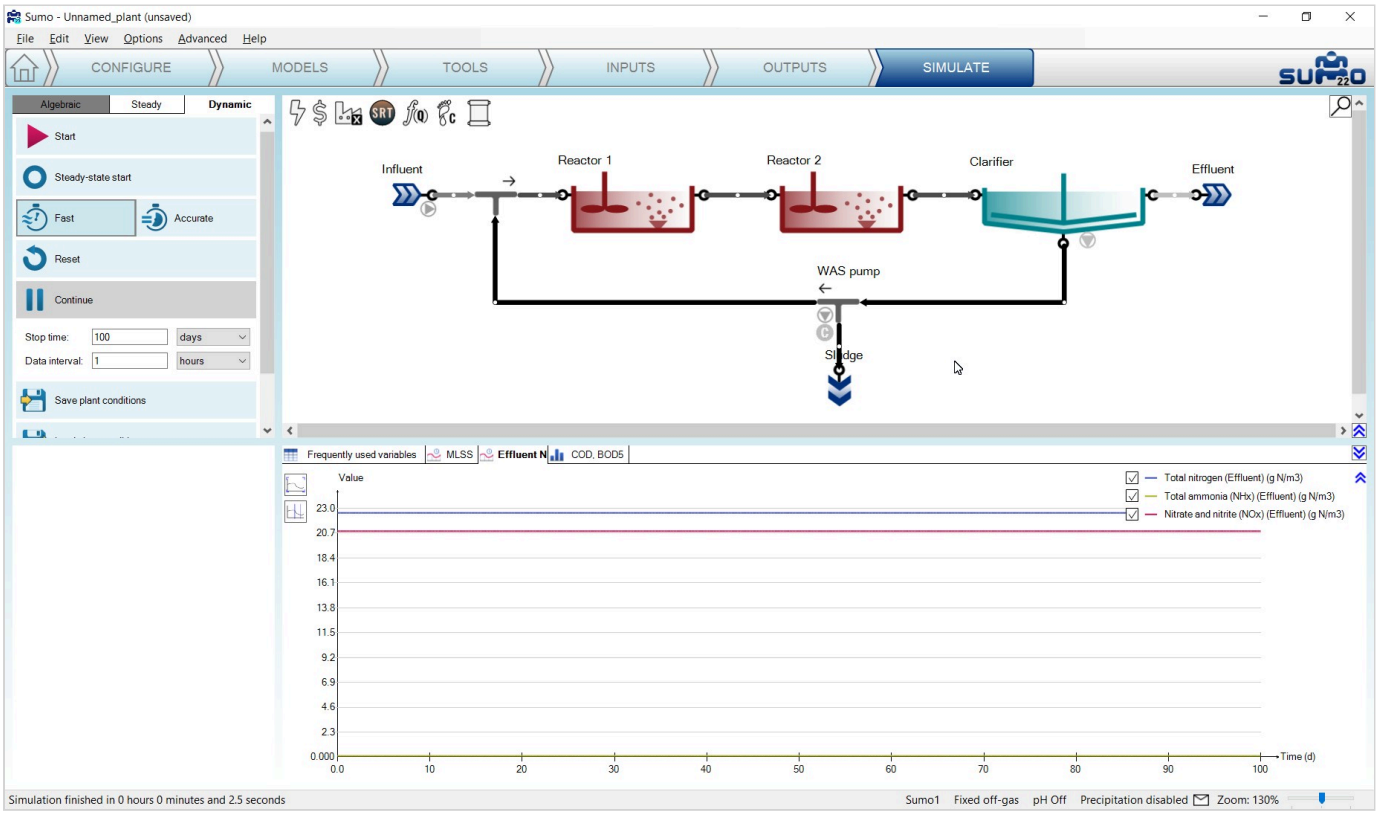


Figure 17 - Steady-state start results

Choosing between *Fast* and *Accurate* modes on the simulation control panel translates to using different pre-configured solver settings. Usually the former is fast and accurate enough for most cases, and therefore its use is generally recommended. However, in certain situations (e.g. with biofilm models), the *Accurate* mode might provide faster simulation. Note that the mode selection will have effect on the steady-state solver as well.

The *Reset* button, which is available in both simulation modes, reinitiates the next simulation with the default concentrations defined in the model and process units. It should be employed thoughtfully, especially when working with complex plants, because reaching steady-state again might be time-consuming in these cases.

Saving plant conditions can be useful to restore system state in case the simulation is driven into an unwanted condition (e.g. accidentally having been reset).

Dynamic Inputs

This ***optional*** task can be used to enter dynamically changing input information, e.g. diurnal flows, DO schedules and more. When choosing the *Inputs* tab, the blue workflow tab automatically splits into *Constants* and *Dynamics*. (Figure 18). According to this, different types of settings become available: we can set either constant inputs (e.g. fixed influent composition, reactor DO setpoints or volumes as we just did) or dynamically changing inputs (e.g. variable influent flow, composition, shifting reactor DO setpoints etc.).

Being on the *Inputs*/*Dynamics* tab, we can copy and paste prepared data tables from an Excel file (i.e. Table 2) into Sumo, simply by clicking on the *Paste table from clipboard* button when the desired process unit is selected. This will apply the selected data ranges to the variables or parameters corresponding to the table headers (Figure 18). The latter have to comply with certain rules (for details, please see the User Manual).

Table 2 – Dynamic input of influent flow pattern

Time	Q
h	m3/d
0	23084.502
1	21581.129
2	20112.819
3	19006.413
4	18538.096
5	18860.780
6	19961.257

Time	Q
7	21658.750
8	23645.574
9	25559.553
10	27069.466
11	27951.420
12	28136.527
13	27717.954
14	26916.230
15	26012.768
16	25269.925
17	24859.318
18	24817.715
19	25042.167
20	25325.377
21	25421.266
22	25122.513
23	24328.482

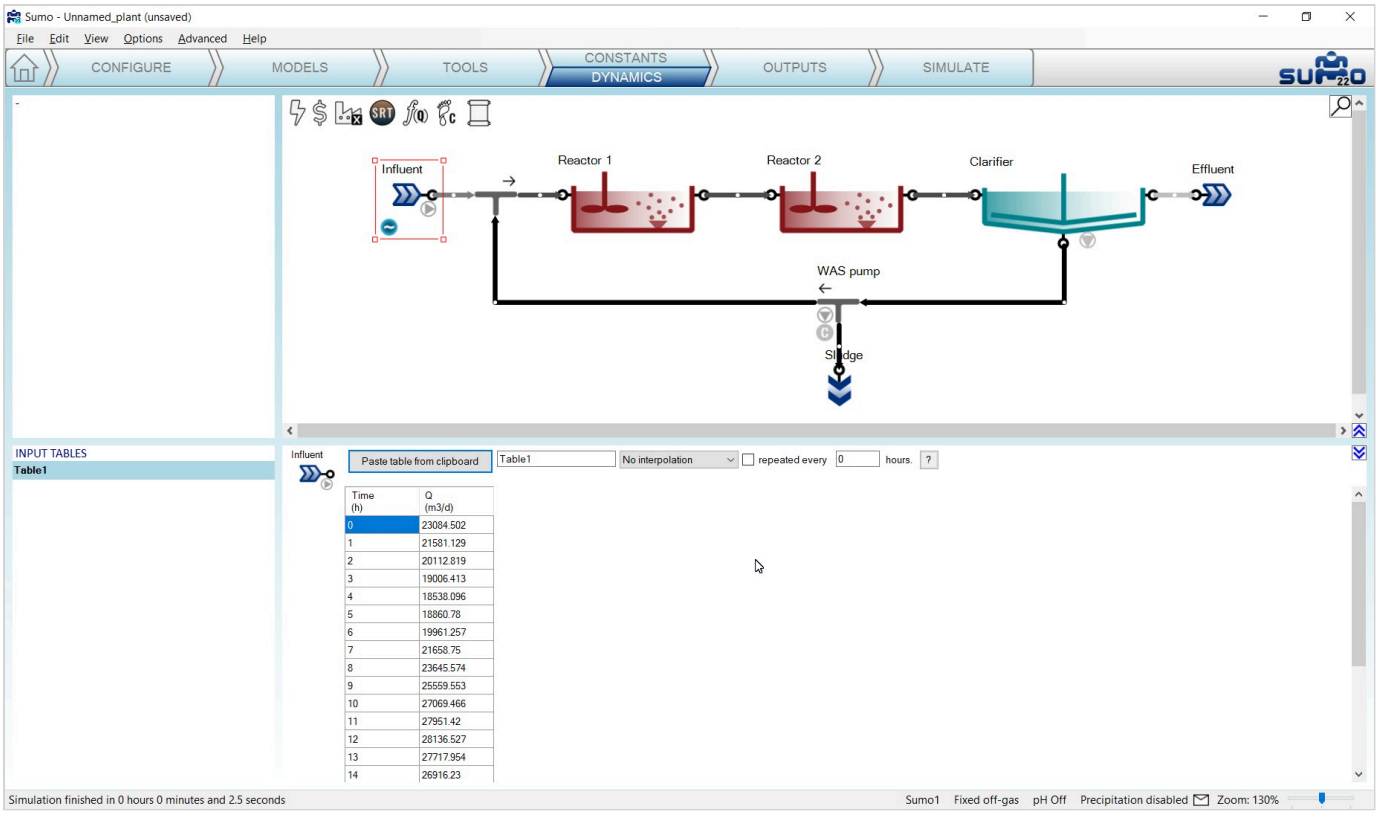


Figure 18 - Dynamic input

Adding measured data to the charts

Plants do collect information and one important task in process simulation is to compare measured data with the simulation results (and potentially using the information to calibrate the model). Let's assume this plant has Wastage flow data logged every 3 hours. The collected data is shown in Table 3.

Table 3 – Measured Wastage flow data for the example plant

Time	Flow (W. pump)
h	m3/d
0	320
3	340
6	360
9	310
12	290
15	300
18	310

Time	Flow (W. pump)
21	310

Copy this table to the clipboard, then in Sumo, switch to the *Outputs* tab, add a timechart (renaming it to “Wastage”) and drop the *Flow rate* for the Wastage pump on the chart (available from *Mass flows in pumped pipe* group). Then right click on the new timechart tab and select *Import data*. The data import is carried out by simply pasting the data from the clipboard (see Figure 19).

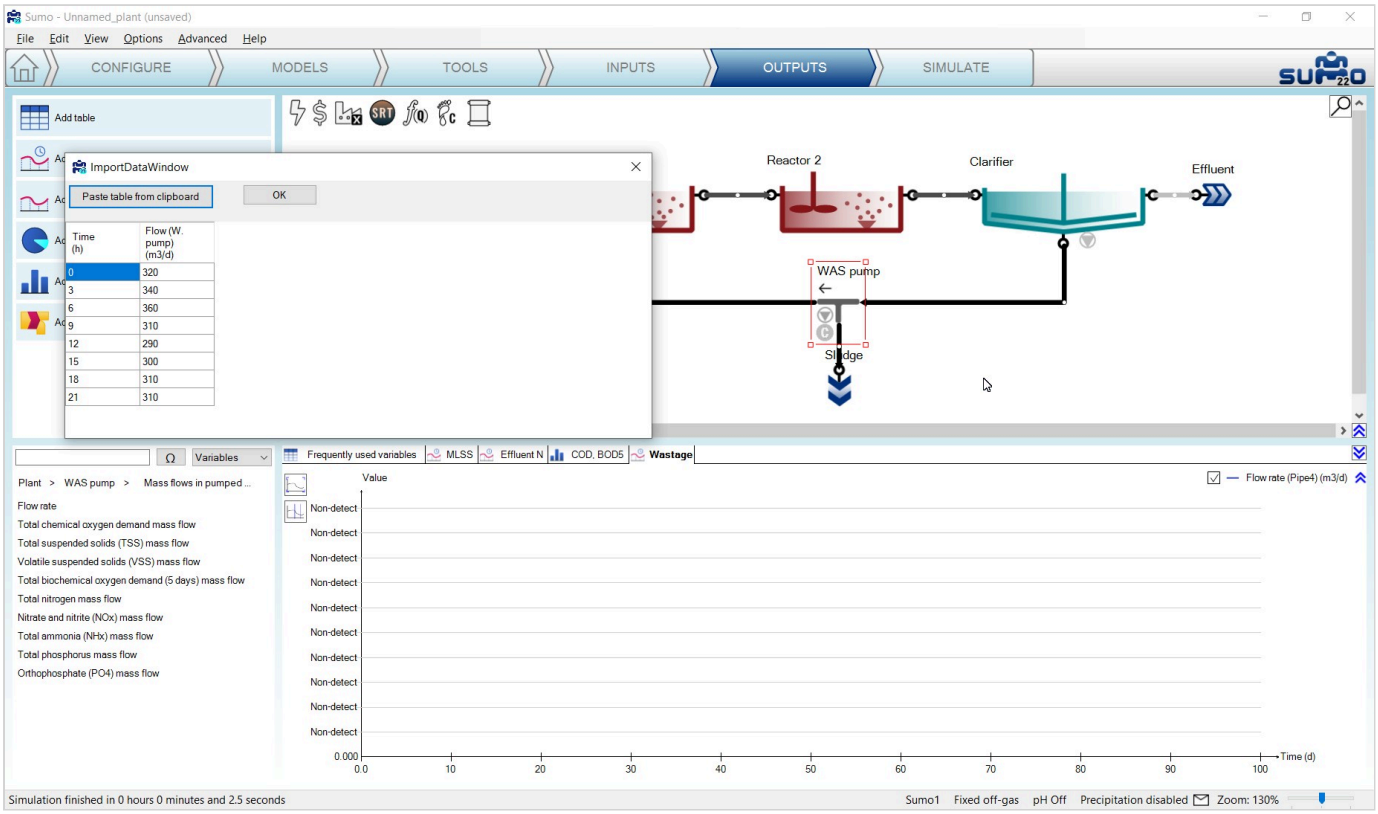


Figure 19 - The data import dialog

In order to have variation in the wastage flow of our plant due to the newly added diurnal flow, let’s activate the SRT control. You can do this by switching to the *Inputs/Constants* tab, selecting the brown SRT icon on top of the drawing board, setting a 15-day SRT and turning on the control, as shown on Figure 20.

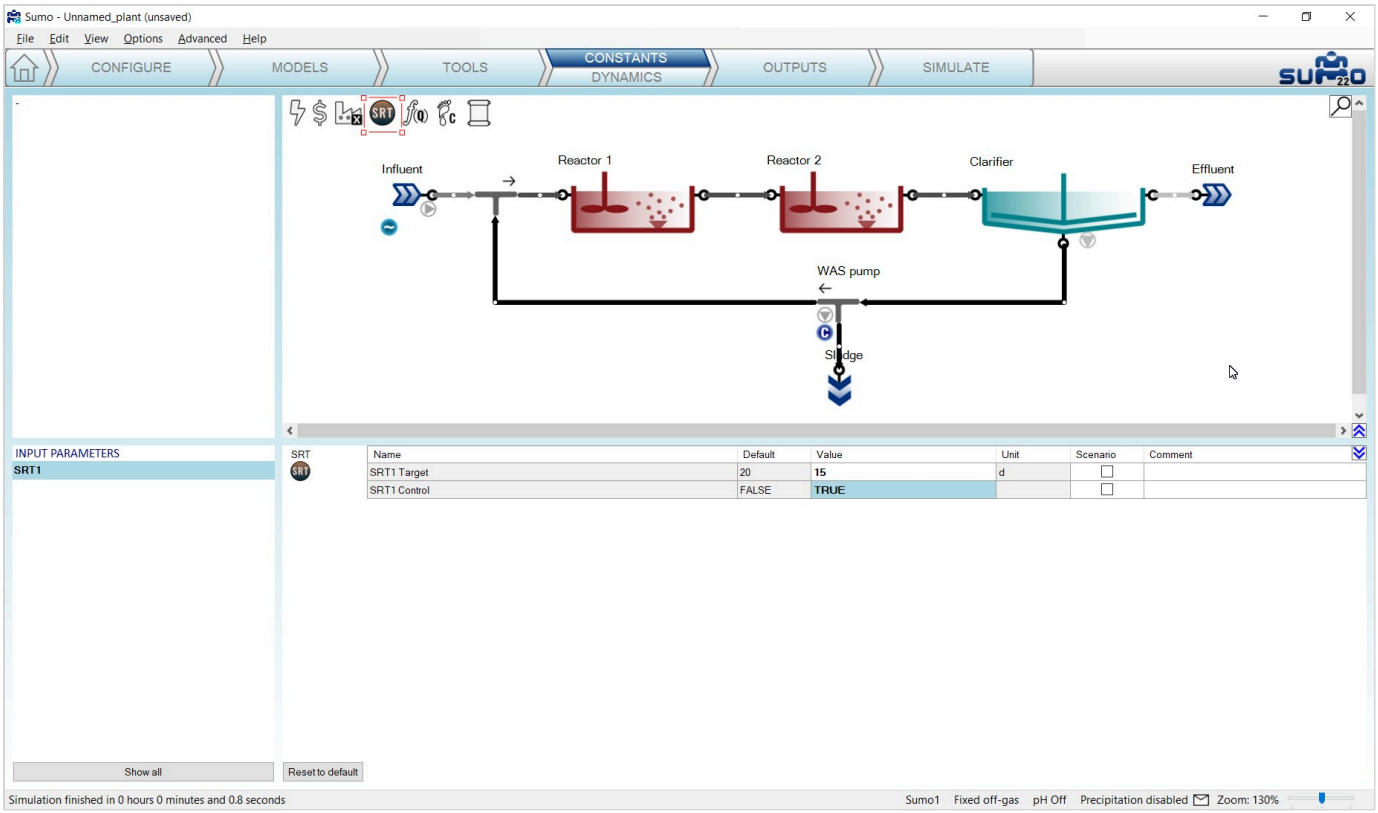


Figure 20 – Activating SRT control

Switch to the *Simulate* tab, set the stop time to 1 day and run a dynamic simulation by clicking on *Start*. Follow the measured and calculated data coherence on Figure 21.

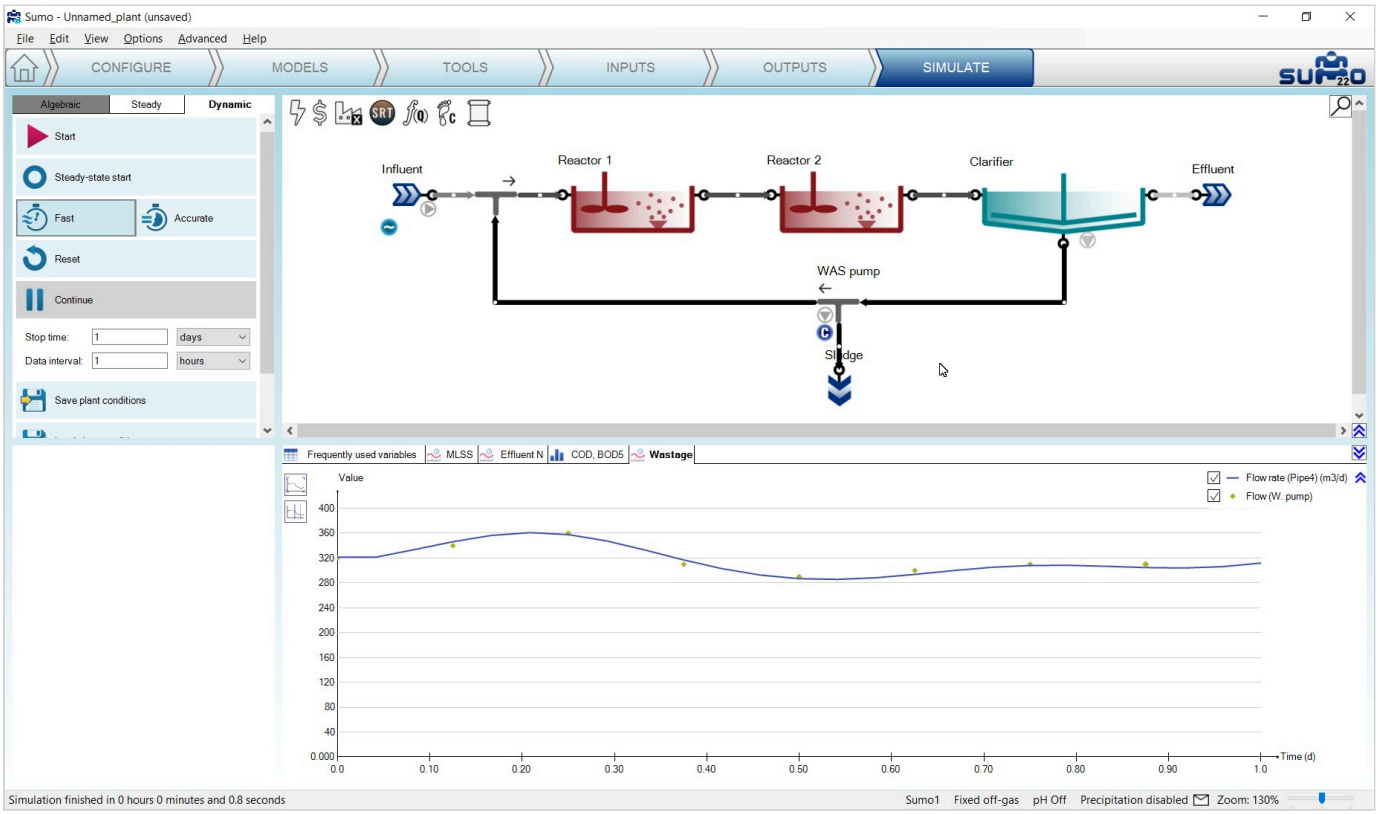


Figure 21 - Wastage timechart with measured data

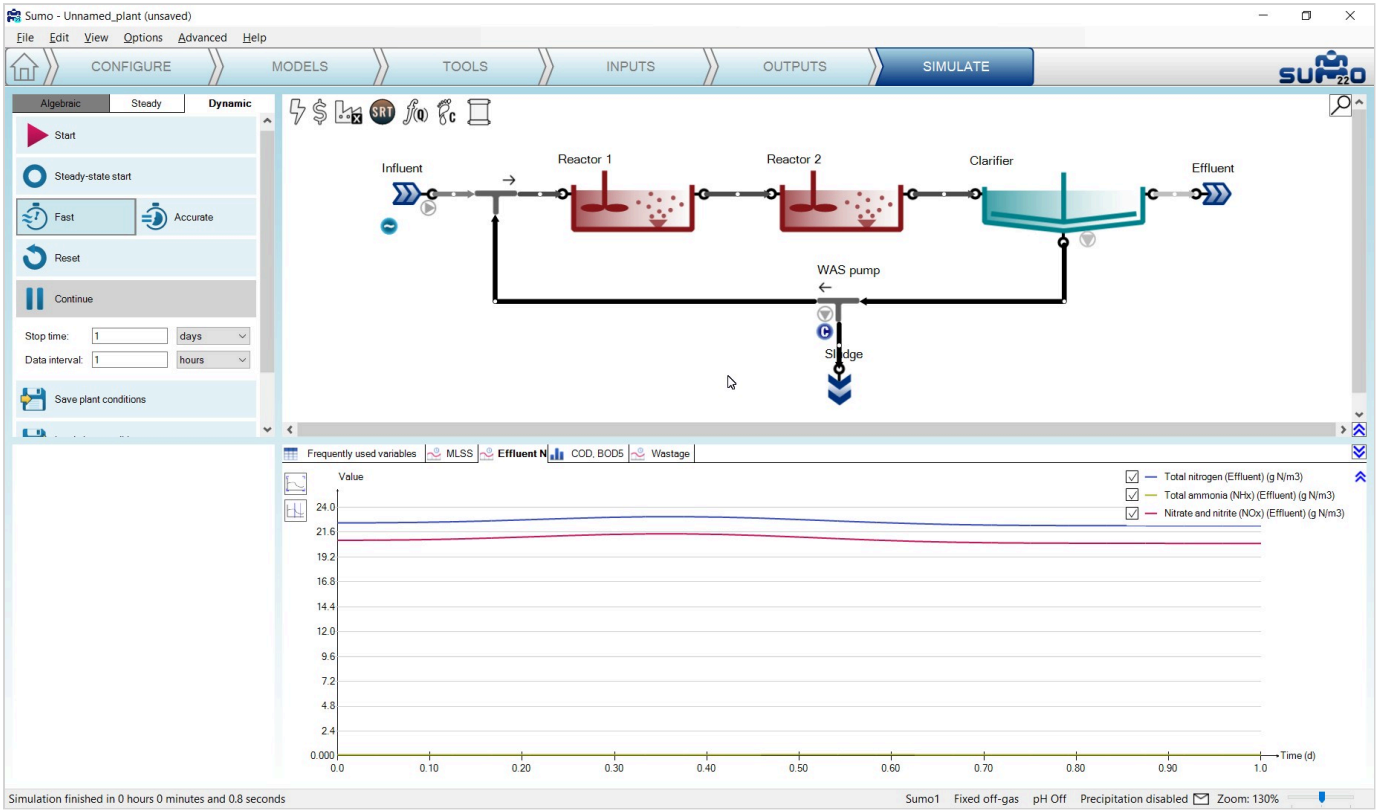


Figure 22 - Effluent N timechart with dynamic input

Writing a report

On the control panel of the *Simulate* tab, a *Report* button is available (you may have to scroll down within the panel in order to reveal it). When clicked, results will be written to an Excel file (saved with the same name as the sumo project file by default). This function creates an Excel file with the following sheets:

- Project overview: contains the configuration layout and basic project information
- Notes: the contents of the *Notes* screen panel from the *Configuration* tab
- Modified parameters: values of all parameters in the project that were changed from default
- Simulation results: all results of the output tabs get saved to separate sheets
- Model: contains all parameter values for the used model (in this example: Sumo1)
- Plantwide calculations: Plantwide, Energy center, Cost center, SRT and Flow dependence settings
- Process Units: all settings and PU parameters are displayed on separate sheets for each unit
- Controllers: all settings and parameters of the controllers employed in the project (if any).

The project can be saved any time during the configuration and project development using the file menu, and reloaded at a later point in time.

Many other operational scenarios can be simulated with Sumo, including more complex reactor configurations and more elaborate operational scenarios. Please see the User Manual and the built-in example layouts.

List of acronyms

Acronym	Definition
A2O	Anaerobic-anoxic-aerobic plant
AB	A-stage (carbon removal) B-stage (nitrogen removal) plant
ACP	Amorphous calcium phosphate
AHO	Carbon adsorption heterotroph organism
ALK	Alkalinity
AMETO	Acidoclastic methanogen
AMX	Anammox organism
AOB	Aerobic ammonia oxidizer
AOP	Advanced oxidation process
AS	Activated sludge
ASM	Activated sludge model
ASRO	Acidoclastic sulfate-reducing organism
AUR	Ammonia uptake rate
BAF	Biological aerated filter
BNR	Biological nutrient removal plant
BOD	Biological oxygen demand
BSH	Brushite
CASTO	Carbon storing organism
CHP	Combined heat and power plant
COD	Chemical oxygen demand

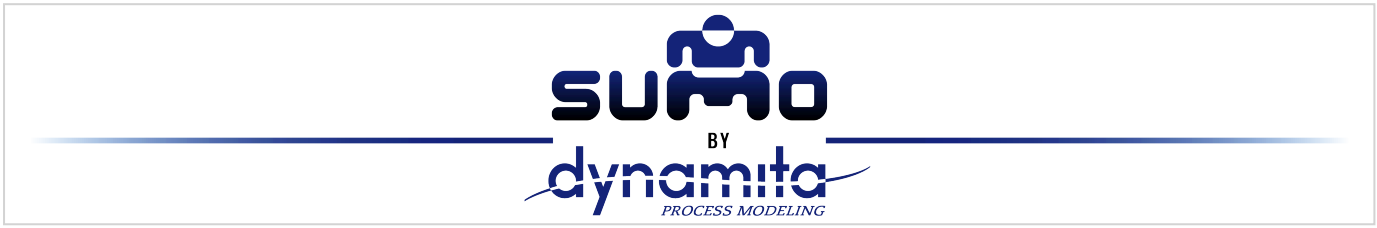
Acronym	Definition
CSTR	Completely stired tank reactor
CVAR	Calculated variable
DAF	Dissolved air flotation
DM	Dry matter
DO	Dissolved oxygen
GAO	Glycogen accumulating organism
GLY	Glycogen
HAO	Hydrous aluminium oxide
HFO	Hydrous ferric oxide
HMETO	Hydrogenotrophic methanogen
HPO	High purity oxygen
HRT	Hydraulic retention time
HSRO	Hydrogenotrophic sulfate-reducing organism
IS	Ionic strength
MABR	Membrane aerated biofilm reactor
MBBR	Moving bed biofilm reactor
MBR	Membrane biofilm reactor
MEOL	Methanol
MEOLO	Anoxic methanol utilizer
MLE	Modified Ludzack-Ettinger plant
MLSS	Mixed liquor suspended solids
N2UR	Nitrite uptake rate
N3UR	Nitrate uptake rate
NITO	Aerobic nitrifying organism
NOB	Nitrite oxidize

Acronym	Definition
NTP	Normal temperature pression conditions (20 °C, 1 atm)
NUR	Nitrate uptake rate
OHO	Ordinary heterotrophic organism
ORP	Oxydo reduction potential
OTE	Oxygen transfer efficiency
OTR	Oxygen transfer rate
OUR	Oxygen uptake rate
PAO	Phosphorus accumulating organism
PFR	Plug-flow reactor
PHA	Polyhydroxyalkanoates
PID	Proportional–integral–derivative controller
PP	Polyphosphate
PRR	Phosphorus release rate
PUR	Phosphorus uptake rate
rbCOD	Readily biodegradable COD
RO	Reverse osmosis
SBR	Sequenced batch reactor
SCCOD	Filtered chemical oxygen demand
SCOD	Filtered flocculated chemical oxygen demand
SOO	Sulfur-oxidizing organism
SOTE	Standard oxygen transfer efficiency
SOTR	Standard oxygen transfer rate
SRT	Sludge retention time
SSOTE	Specific standard oxygen transfer efficiency
STP	Standard temperature pression conditions (0 °C, 1 atm)

Acronym	Definition
STR	Struvite
SV	State variable
THP	Thermal hydrolysis process
TKN	Total Kjeldahl nitrogen
TN	Total nitrogen
TOC	Total organic carbon
TP	Total phosphorus
TSS	Total suspended solids
UASB	Upflow anaerobic sludge blanket
VFA	Volatile fatty acid
Vivi	Vivianite
VS	Volatile solids
VSR	Volatile solids reduction
VSS	Volatile suspended solids
WAS	Waste activated sludge

Sumo User Manual

In-depth introduction to using Sumo



Dynamita, www.dynamita.com , Sigale, France

Sumo *is a third generation wastewater process simulation software. It was put together by a dedicated team with professionalism and thousands of days of tender loving care. Enjoy, and please let us know if you find somewhere it is coming short of your expectations. We will do our best to improve it.*

Imre Takács, on behalf of the whole Dynamita team

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Installing Sumo

The following steps will help to guide you through the installation of Sumo.

Prepare Microsoft Windows for Sumo

Operating system

Make sure your computer is operating Microsoft Windows 7 or later. Sumo supports touch screen computers running Windows 8/8.1 and Windows 10/11.

Sumo can be used on a Mac with Windows installed or through an emulator like “Parallels”.

Microsoft Office

Sumo requires Microsoft Excel 2007 or later installed.

.NET

Please make sure that your computer is running the Microsoft .NET 4.7.2 framework. You can check it in the list of installed applications (Control Panel / Programs / Programs and Features). If the .NET framework’s 4.7.2 version is not installed, please download and install it from the following location:

https://dotnet.microsoft.com/download/dotnet-framework/net472

Windows 10/11 come with the required .NET environment. On other operating systems, if you have .NET already installed on your computer, the downloaded installer will exit or inform you. Proceed to the next step.

Installation of Sumo

You have received a link to the Sumo installer (or in rare cases the install file on a USB key). This is one file and contains everything necessary to install Sumo once Windows is prepared. Download it through the link provided to your computer. From the USB key you can install directly if desired, it is not required to copy the file to the computer.

Install Sumo by starting the install package and follow the instructions. Administrator rights may be required during installation. For workstations, we recommend choosing the “Install for myself only” option.

Obtaining a license

Obtaining a license is a two-step process.

Step 1:

After install, start Sumo from the Windows Start menu. Sumo will display a message providing multiple options. If you don’t have the license file yet, Select “I need a new license” (Figure 1.1). Sumo will display two additional buttons to show information about your hardware (Machine Identifier Code) and to copy this information directly to the Windows clipboard. Please paste this code into an email and send it to support@dynamita.com. Dynamita will provide a license file for you according to our agreement.

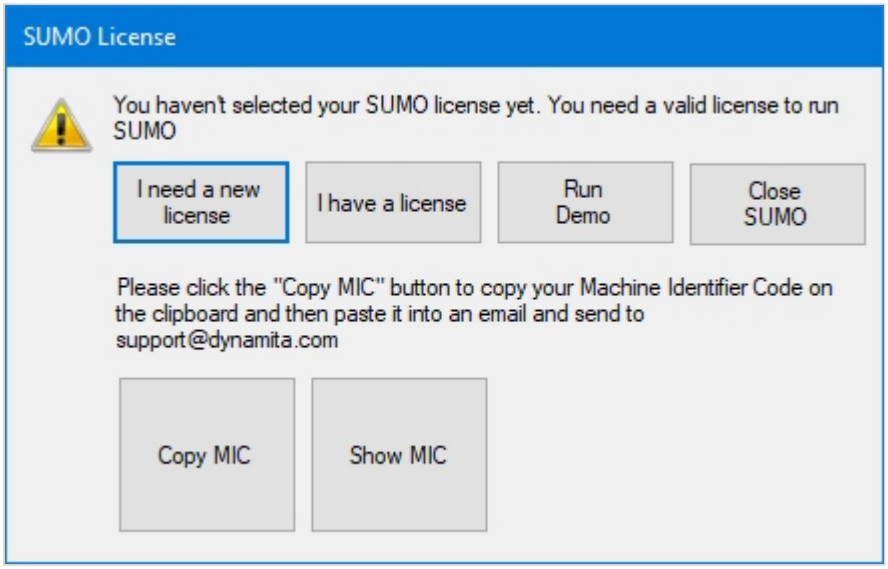


Figure 1.1 - Retrieving Machine Identification Code information

Step 2:

Copy the license file Dynamita provided to a folder on your computer, start Sumo, choose the “I have a license” option, click “Select license file” and navigate to load the license file (Figure 1.2). As long as the license file is not deleted or moved and it is valid, this validation does not have to be repeated. Other options, like using a license server or a hardlock, are also available.

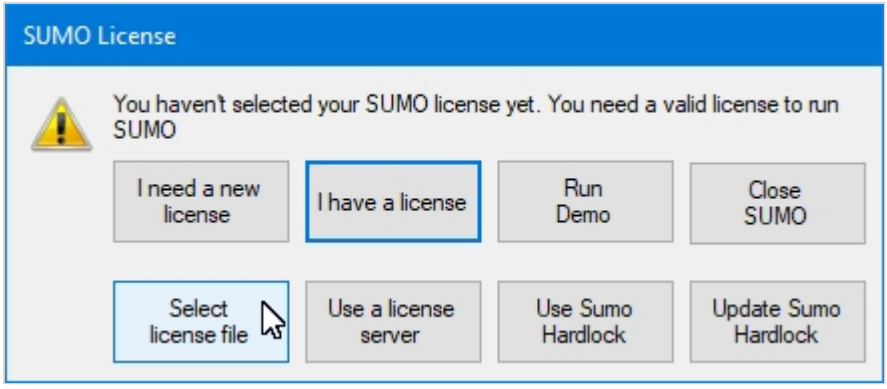


Figure 1.2 - Registering the license file

Note: Demo license

If you already have Sumo installed and running in demo mode, you can go to Step 1 by choosing the “Home” icon and selecting the licensing button in the bottom left window pane.

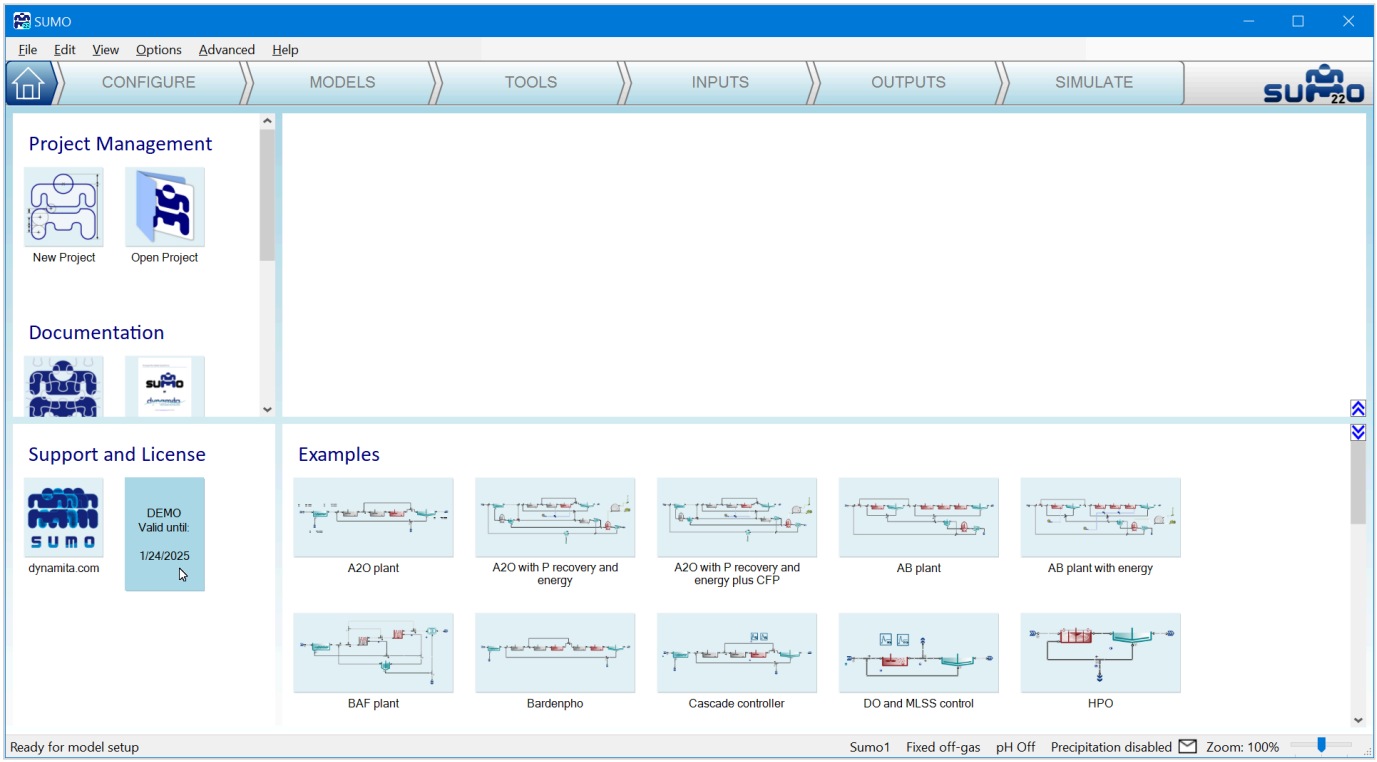


Figure 1.3 - DEMO license: click on it to get to licensing

Introduction

Sumo is a powerful, open process source, multipurpose simulation environment developed for environmental models, particularly municipal and industrial wastewater treatment plant modelling. A wide range of BNR plant configurations can be simulated in Sumo. Sumo models are written in an Excel based open process source code language called SumoSlang (Sumo Simulation Language, copyright Dynamita).

Sumo can simulate traditional biokinetic models dynamically or in steady-state, mixed equilibrium-kinetic models and direct algebraic models, depending on the simulation mode.

Sumo is supplied with internally researched and developed whole plant models as well as focus models (e.g. with focus on sulfur, high rate plants and the fate of nitrogen and GHG). The seven most widely known published models are also included in the Sumo Museum for N and P removal.

Sumo models can be run through several different interfaces. The most widely used is “Sumo”, an intuitive graphical user interface (Figure 2.1).

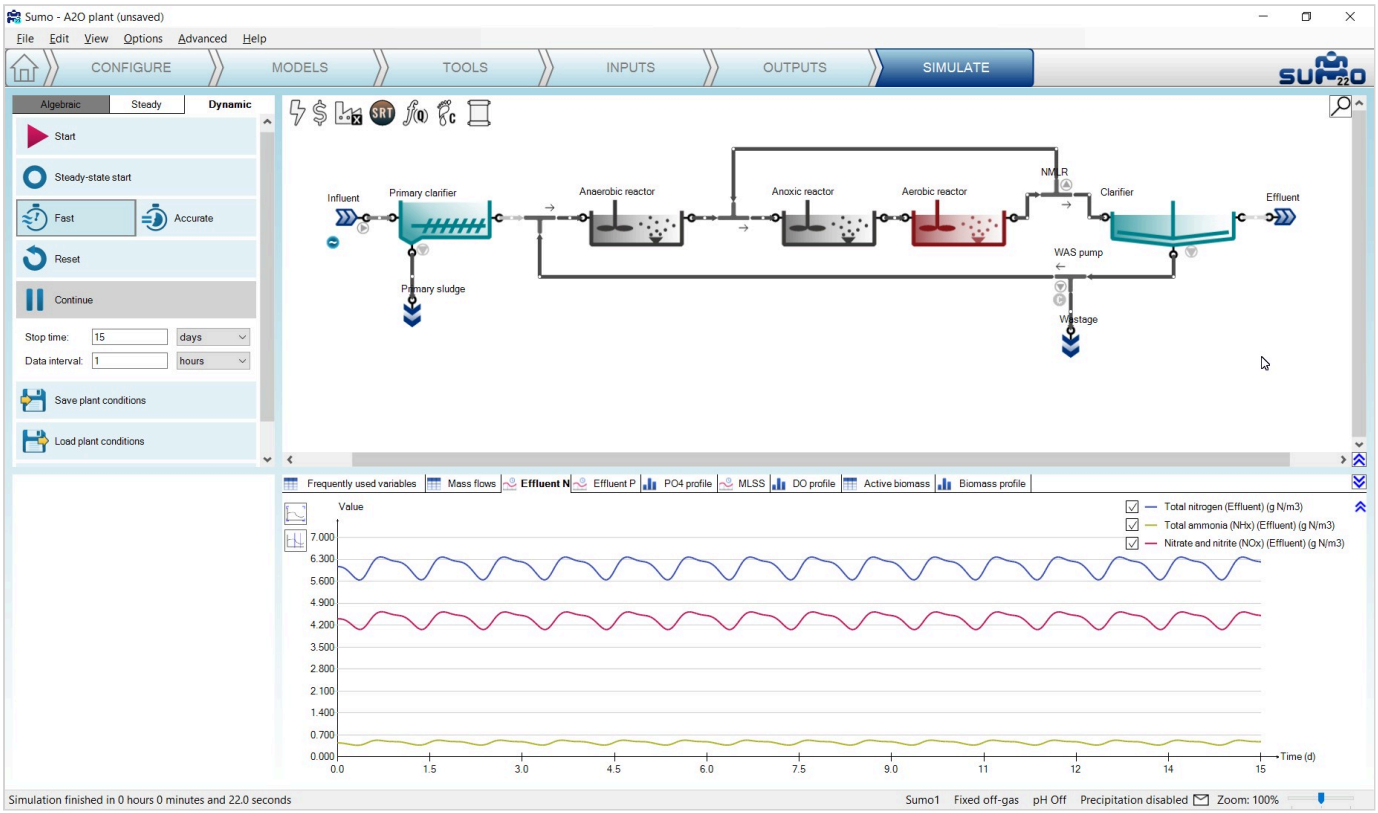


Figure 2.1 - The Sumo graphical user interface

Sumo22 is able to communicate with other programs such as Excel, Python, Matlab, etc., through its Digital Twin Toolkit (DTT). The Sumo22 install comes equipped with a couple of examples:

- Excel based “Operator interface”. This can be customized to a certain plant configuration or SCADA for easy use of plant simulations.
- Sample Python scripts for sensitivity analysis and parameter optimization using Sumo.

Please note that the Digital Twin Toolkit (DTT) will only work with a valid DTT license, which is available separately from the Sumo license.

How to use Sumo for simulations

Start Sumo

On Windows 10 systems, you can use the start menu to launch Sumo. The installer places the software in a folder called “Dynamita”. A quick way of locating the application is to start typing ‘sumo’ once the start screen is on (Windows 10 switches into application search mode in this case, showing the most relevant search results on the left). With drag and drop, you can also pin a Sumo22 quick launch icon to the Start menu tiles or to the Desktop of the computer as well. Note: right clicking on the program launcher icon allows you to open the recent project files.

Sumo will start with showing the Welcome Screen, as illustrated by Figure 3.1. Below the Menu Bar, you will see the Task Bar that guides you through the project workflow, all the way from configuration to simulation.

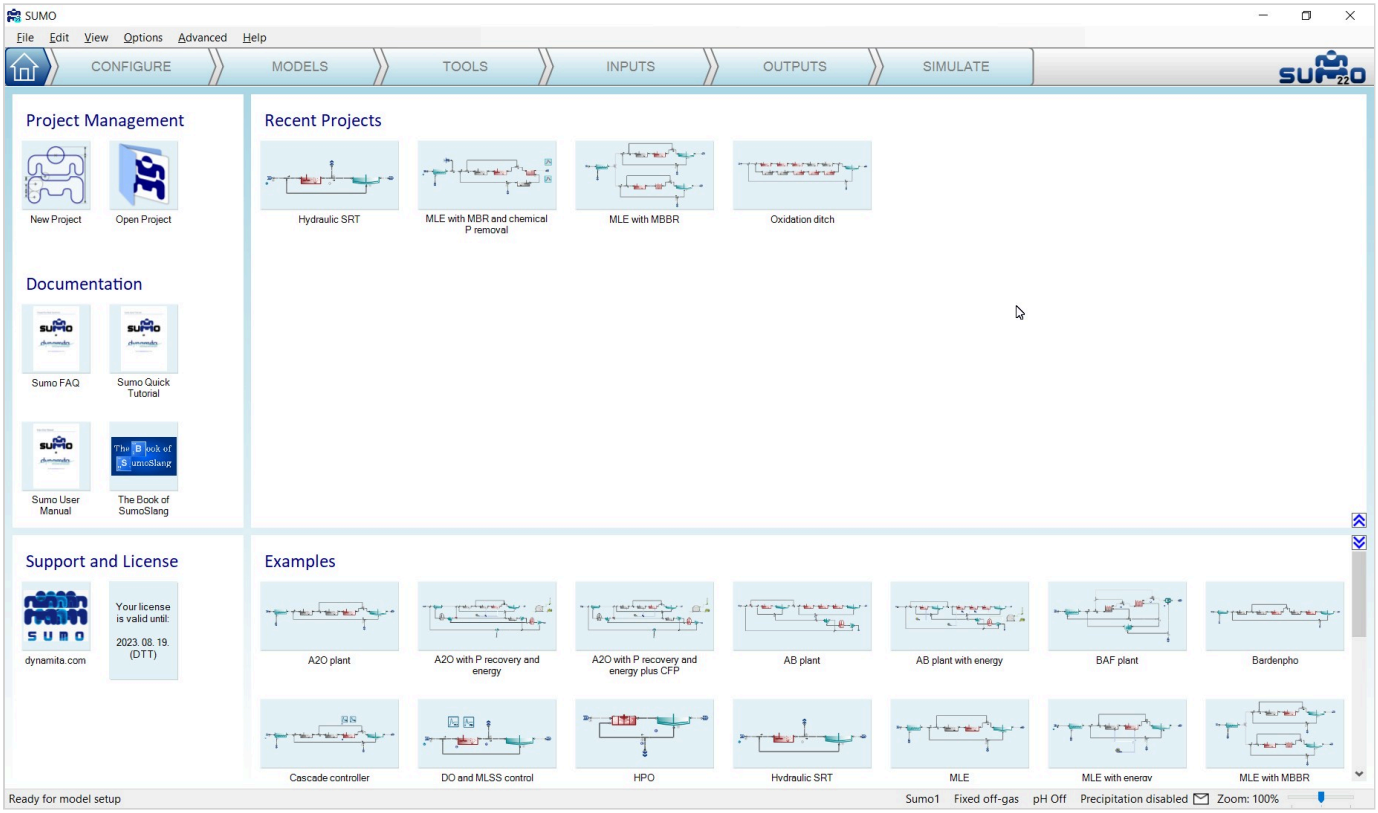


Figure 3.1 – Sumo22 startup screen

The central elements of the Sumo22 Welcome Screen are four screen panels, whose functions and roles are the following:

Top left panel	Project management and documentation

	Starting or opening a new project in a new window (*New Project*), opening a saved project from your own files (*Open Project*) and reaching various documents for how-to-use instructions.
Top right panel	Recent projects Your recently opened projects can be quickly reached from the welcome screen.
Bottom left panel	Support and license information Sumo22 support (link to our website) and the currently used license information can be reached from here.
Bottom right panel	Built-in example project repository All the built-in example configurations can be opened directly from this pane (they are also available from the Help menu).

These functions can be reached later at any point, by clicking either the *Home* icon (the first item of the Task Bar) or the Sumo22 logo (located at the right end of the Task Bar), which will bring you back to the Welcome Screen.

The screen panels can be resized anytime during the workflow to fit the actual needs of the job. In order to do that, just move the mouse to the padding between the panels and drag them to the desired position. The top right panel will always contain the plant configuration, while the content of the other panels depends on the actual task (*Configure*, *Modes*, *Tools*, *Inputs*, *Outputs*, and *Simulate*). Please note that the runtime versions of Sumo are not meant for constructing new models and thus, the *Configure*, *Models* and *Tools* tabs are not available.

The Status Bar in the bottom of the screen provides model/simulation related information. In case of a system notification or model/simulation error, an exclamation mark will appear next to the mailbox icon (Figure 3.2). Red exclamation marks denote errors, while blue and yellow ones inform about warnings and notifications that need attention. Clicking on the mailbox icon will provide the description of the problem and hints about dealing with it.

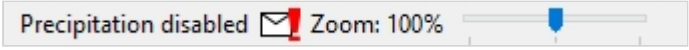


Figure 3.2 - New notification

The following chapters will help you to understand the functions of each main tab of the Task Bar, and teach how to use them for building a project and performing various simulations.

Configure

To start your project, click on the *New Project* icon or the *Configure* tab. This task serves the building of the plant layout.

The roles of screen panels in *Configure* mode are the following:

Top right panel	Plant configuration drawing board
Top left panel	Process unit categories and process units
Bottom right panel	General comment panel – your notes, which will be saved with the project
Bottom left panel	Specific process unit options and information

While the *Configure* tab is selected, we will build a simple AO configuration (also available for reference from the built-in examples as *Tutorial plant*) using the *Flow elements*, *Bioreactors* and *Separators* categories from the top left element list. Select the desired process unit by opening the category and dragging the process unit to the drawing board. To drop the selected unit, just release the mouse button (Figure 3.3).

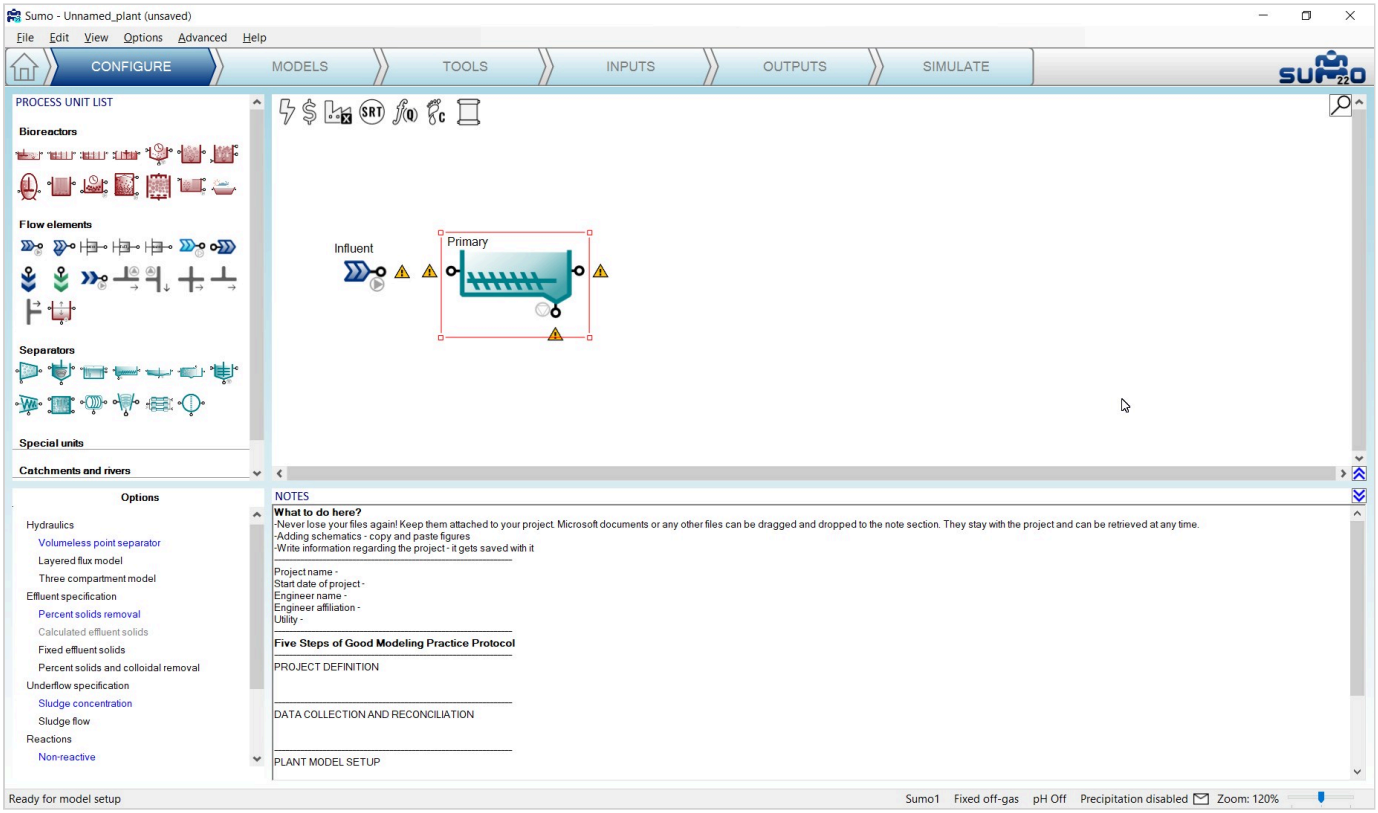


Figure 3.3 - Start building the plant layout

Pipes can be created using two methods. Sumo supports a handy way of establishing connections between process units, which can be triggered by positioning a process unit's output port on top of another process

unit's input port (or vice versa) by moving one of the process units. Once the ports are positioned on top of each other, a pipe connection is automatically created, as it is demonstrated by Figure 3.4 with an Influent and a Primary clarifier. This method is especially useful when Sumo is commanded by fingers on a touch screen. Unconnected ports are indicated by yellow exclamation marks in the *Configure* and *Models* tabs.

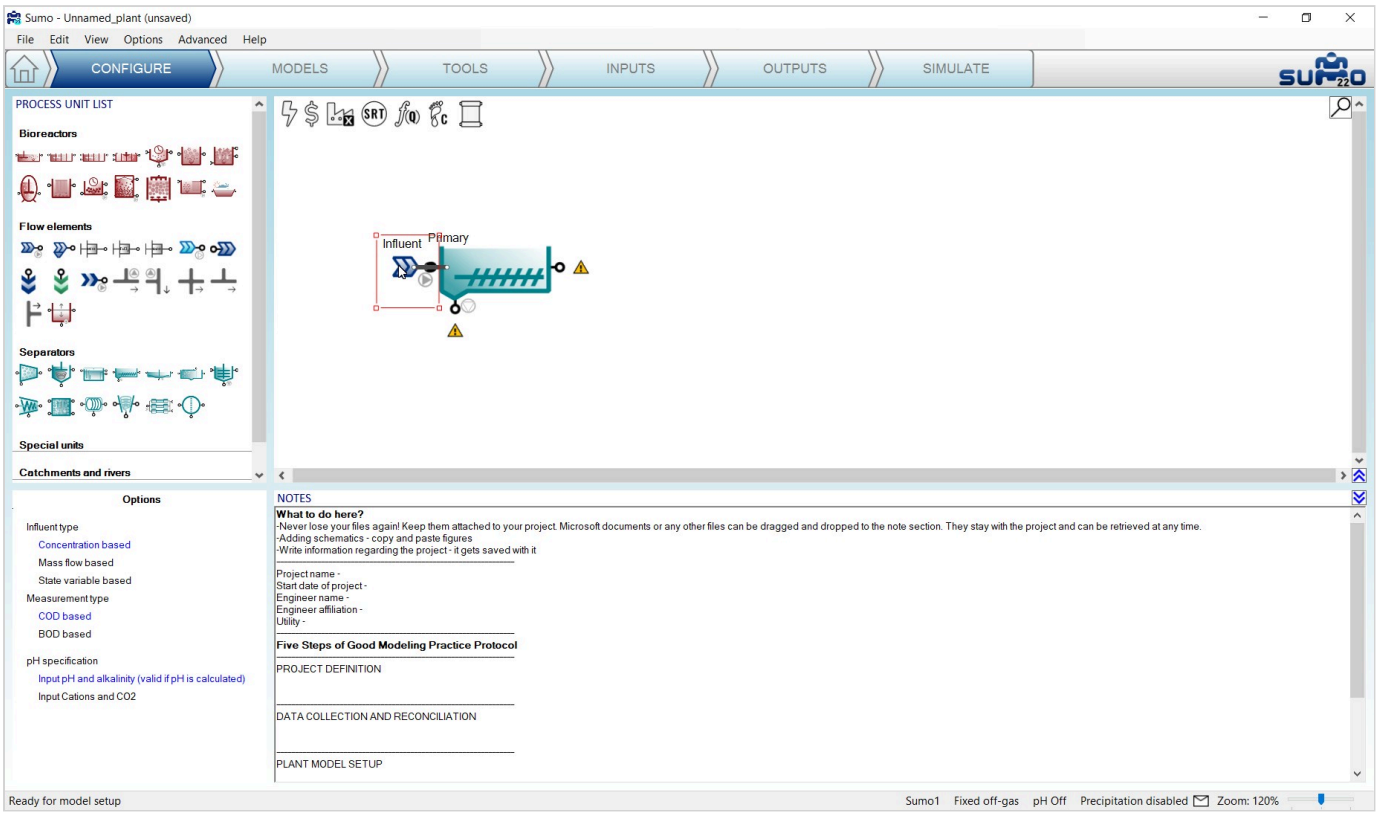


Figure 3.4 - Pipe being created by touching process units

The conventional way also works: position the mouse on an output port of a process unit, press the left mouse button, then move the mouse – and this way drag the pipe, denoted by a red line – to an input port of another process unit (as illustrated in Figure 3.5) and finally release the mouse button to make the connection. Existing pipes can be removed by right clicking on them and selecting *Disconnect pipe* from the pop-up menu.

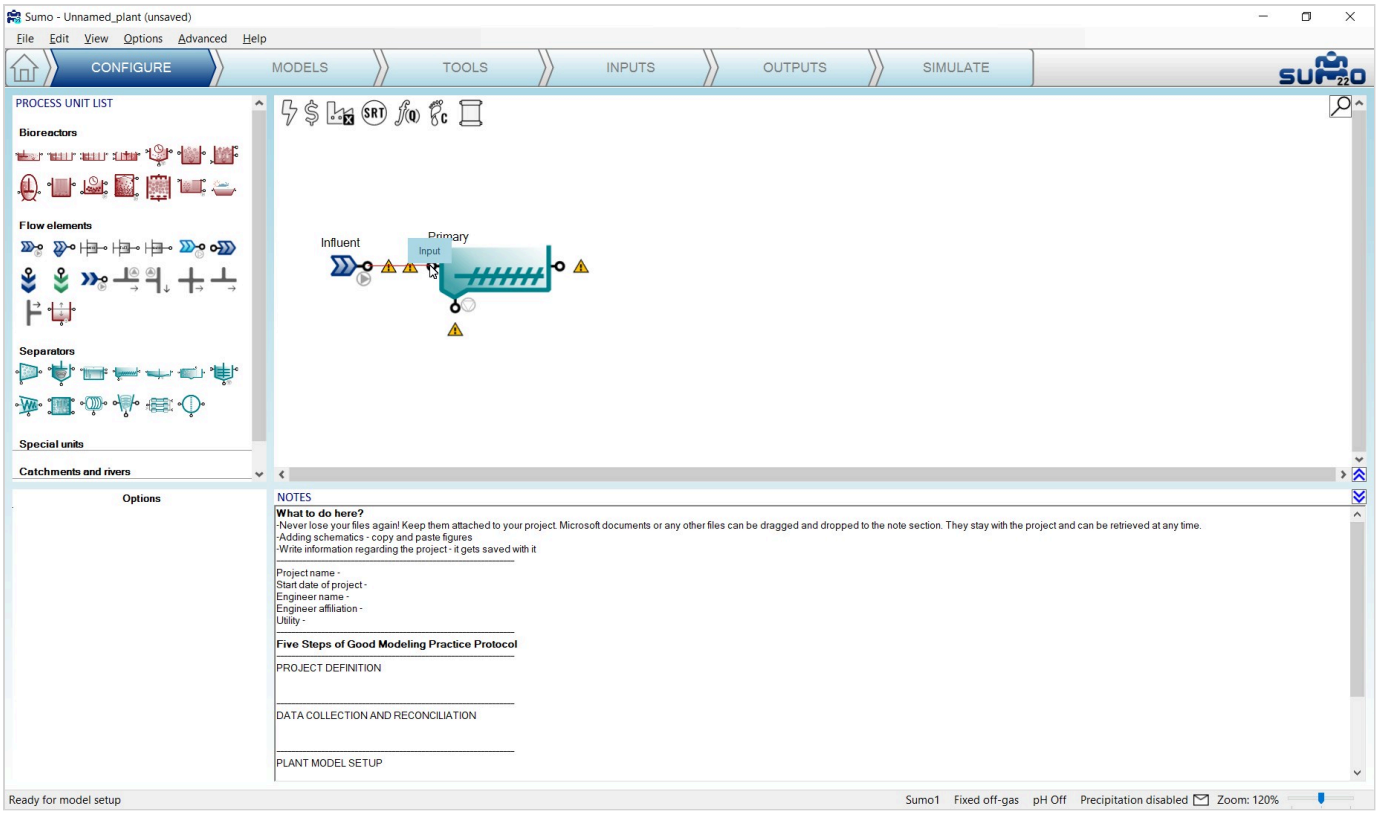


Figure 3.5 - Pipe being created the conventional way

Build the plant configuration and connect the pipes as shown by Figure 3.6. Tooltips provide hints about the purpose of a unit's connection point. This feature comes especially handy for the flow divider and flow combiner (make sure not to mix up these connections – their name is shown on a pop-up tooltip and flow direction is indicated by small arrows). Rotate the flow divider below the clarifier by swiveling the red selection rectangle (or with a right click pop-up menu option) and straighten the lines by grabbing process units or pipe corners. These maneuvers do not change the results of the simulation but will make working with the model a lot clearer.

Upon selecting a process unit on the drawing board, options appear in the bottom left panel, where the most suitable process unit can be chosen, fitted to the model. In this Tutorial we will use:

Influent	
Influent type	Concentration based
Measurement type	COD based
pH specification	Input pH and alkalinity (valid if pH is calculated)
Primary	
Hydraulics	Volumeless point separator
Effluent specification	Percent solids removal

Underflow specification	Sludge concentration
Reactions	Non-reactive
CSTR (both)	
Dissolved oxygen	Input
Aeration	Diffused
Reactions	Reactive
Reactor type	Mainstream
α factor specification	Predicted α
Diffuser system specification	Membrane discs
Clarifier	
Hydraulics	Volumeless point separator
Effluent specification	Fixed effluent solids
Underflow specifications	Sludge flow
Reactions	Non-Reactive
Side flow divider	
Flow divider options	Side flow divider with side pump (with cycling turned off)

Note: The flow divider's connection where the small pump symbol points to needs to be connected to the waste sludge and the other output (where the arrow points to) will be the recycled activated sludge.

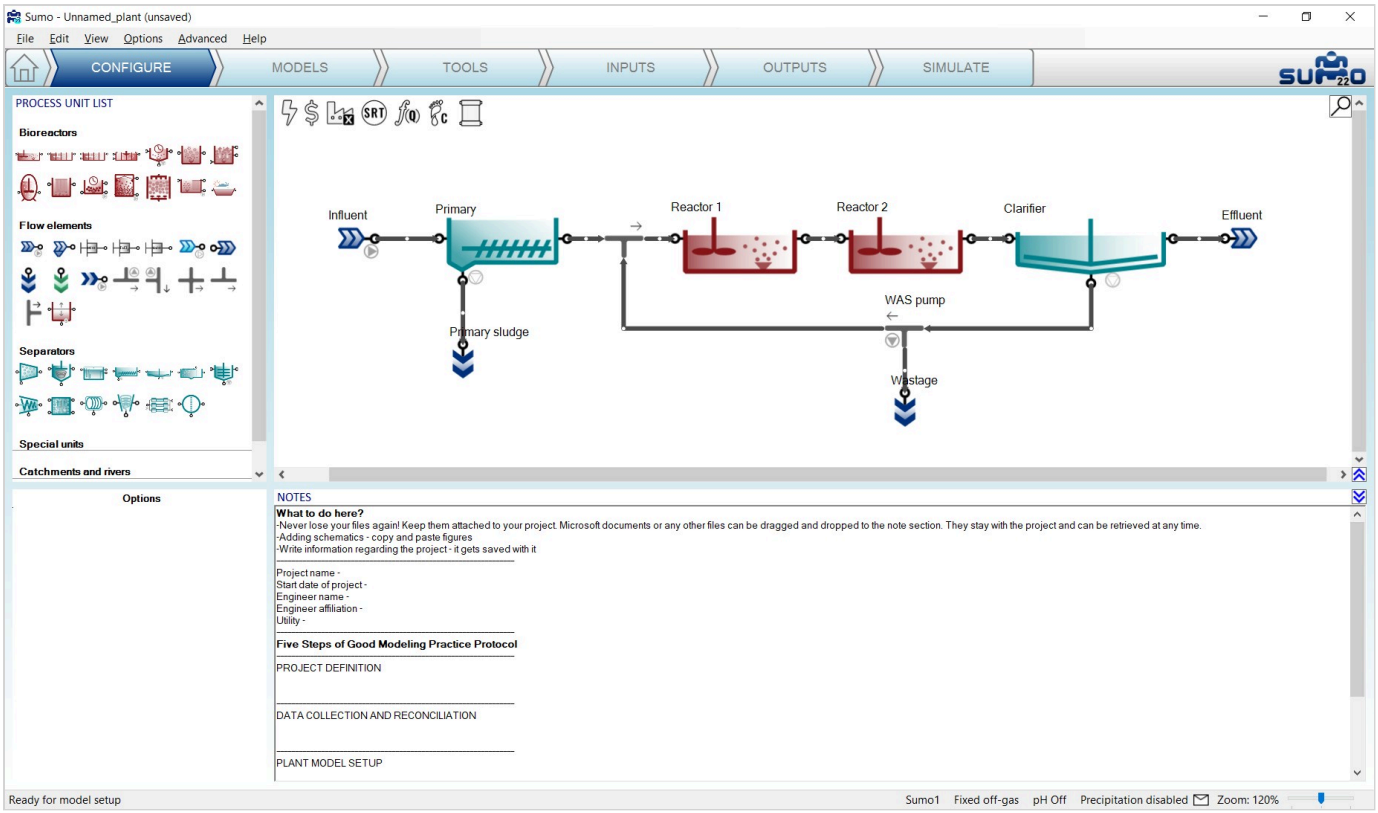


Figure 3.6 - The example layout

The drawing board can be easily zoomed in and out by holding down the CTRL key while scrolling with the mouse wheel, or alternatively by adjusting the zoom slider in the right end of the Status Bar. To move the configuration around the pane, hold down the CTRL key and the middle mouse button simultaneously while moving the mouse. To fit the actual configuration in the center of the viewport with the optimal zoom level, press CTRL+Home.

Rename the process units using the right-click pop-up menu, the F2 function key or double-click on the upper part of the unit. The pipes can be renamed as well, but this is usually not important – the pipe names are hidden by default (this can be changed in the *View* menu on the top). The visibility of process unit names can be controlled on a one-by-one basis. In order to obtain a clear example layout, hide the name of the 'Side flow combiner' process unit (this is the default setting).

Note: the above settings can only be modified in *Configure* mode, but you can return and perform them at any point during your work. Changing the process unit names will not result in recompilation of the project model.

Note: other process units (e.g. Sewer network and Mobile carrier) may be available as add-ons. Please write to support@dynamita.com for information.

Models

In this ***optional*** task, the mathematical model describing the biological, chemical and physical processes can be selected. If no settings are changed, the default settings will be used – the model will be functional.

The role of screen panels in *Models* mode are the following:

Top right panel	Plant configuration
Top left panel	Available model options or models in advanced mode
Bottom right panel	Model parameters
Bottom left panel	Model parameter categories Note: in the case of Sumo models, only selected key parameters are shown by default; click on the *Show all* button to see the entire parameter set.

In this task, we can choose between using the various built-in models for our plant, as well as additional options like turning on or off gas phase, precipitation and different complexity levels of pH calculations.

The current package comes with the Sumo whole plant models listed in Table 3.1.

Table 3.1 – Description of Sumo whole plant models

General full plant models	
Mini_Sumo	Simplified One step whole-plant model Use “Mini_Sumo” for OUR and sludge production prediction.
Sumo1	One step whole-plant model Use "Sumo1" for activated sludge modeling, iron addition for P removal and with plants that have digesters but no iron addition.
Sumo2	Two step whole-plant model Use "Sumo2" for activated sludge modeling and sidestreams, iron addition for P removal and with plants that have digesters but no iron addition.
Focus models	
Sumo2S	Two step whole-plant model

	Use "Sumo2S" for whole plant modeling, (activated sludge, digesters, sidestreams), particularly if iron is dosed and is carried to the digester with the sludge. This is the only model which includes the full interaction of the sulfur and iron cycle.
Sumo2C	Two steps whole-plant model - High rate Use "Sumo2C" for high rate activated sludge modeling and sidestreams, iron addition for P removal and with plants that have digesters but no iron addition.
Sumo4N	Four step whole-plant model Use "Sumo4N" for whole plant modeling, (activated sludge, digesters, sidestreams) when particularly interested in GHG emissions for carbon footprint estimations.

The general full plant models are available directly from the *Model selection* list (top left panel), while the focus models (and other custom models) are accessible either by choosing the *Museum, Focus and custom models* item, or by clicking the *Advanced* button (located in the bottom of the top left panel) – both will open up the complete *Model library* in the top left panel. When the *Model library* is shown, right-clicking on the model name will enable opening the source code in SumoSlang (Excel) format (Figure 3.7). To return to *Model Options* from here, just hit the *Back* button in the bottom part of the screen panel.

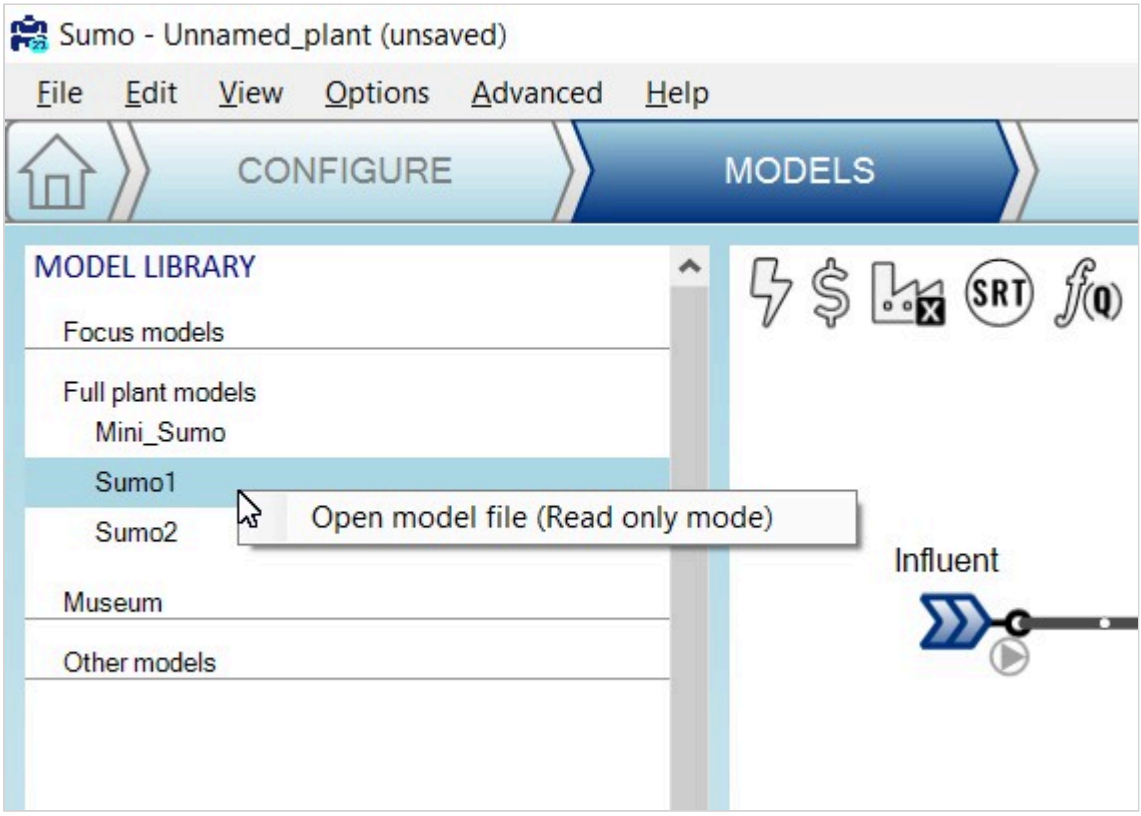


Figure 3.7 – Opening model source files

Table 3.2 lists the main processes included in the Sumo whole plant model family.

Table 3.2 – Main processes included in Sumo whole plant models

	General full plant models			Focus models		
	Mini_Sumo	**Sumo1**	**Sumo2**	**Sumo2S**	**Sumo2C**	**Sumo4N**
COD removal	X	X	X	X	Two populations: OHO and AHO	X
EPS production					X	
Denitrification	1-step	1-step	2-step	2-step	2-step	4-step
Hydrolysis	X	X	X	X	X	X
Fermentation	X	X	X	X	X	X
Anoxic methylotrophs		X	X	X	X	X
Nitrification	1-step	1-step	2-step	2-step	2-step	4-step
EBPR (PAO-GAO model)		X	X	X	X	X
Three-population anaerobic digestion	X	X	X	X	X	X
Temperature sensitivity	X	X	X	X	X	X
Precipitation		X	X	X	X	X
Chemical P removal	based on ASM2d approach	Kinetic approach	Kinetic approach	Kinetic approach	Kinetic approach	Kinetic approach
Sulfur cycle				X		
GHG emissions						X

Important comment on Mini_Sumo: unlike other Sumo whole plant models, Mini_Sumo does not include colloidal components. The user should pay careful attention on the influent fractionation and – if required –

primary clarifier calibration, so that the primary effluent composition in term of BOD and TSS is in agreement with the expectations.

Note: other models may be available as add-ons. Please write to support@dynamita.com for information.

In our example we will use the default model setup with one step nitrification-denitrification model (Sumo1) with specified input gas concentrations (gas transfer is approximated, off-gas concentrations are fixed) and without pH calculation (therefore chemical precipitation is not calculated either), as shown in Figure 3.8.

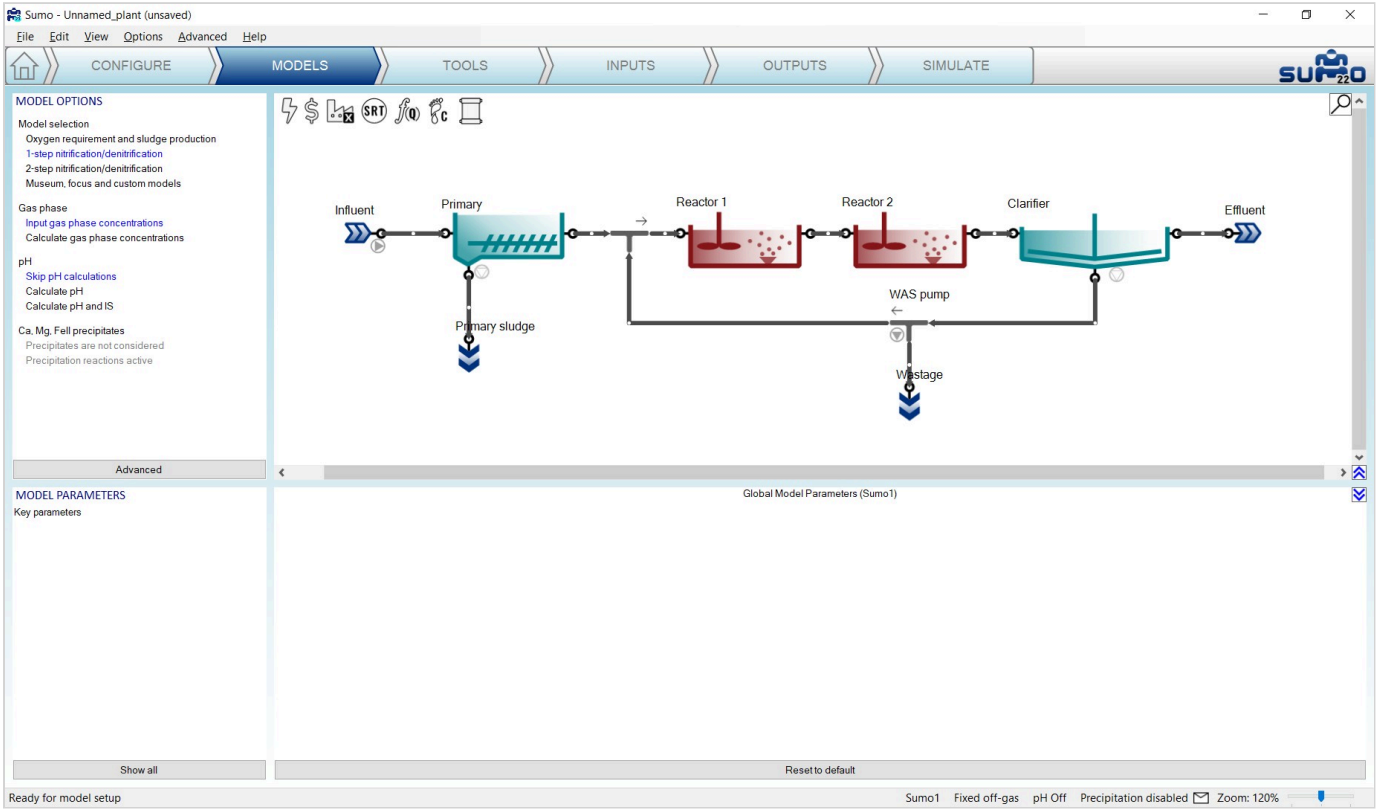


Figure 3.8 – Global model selection in Sumo

Global model parameters

On the *Models* tab, if none of the process units are selected, clicking on the parameter categories listed in the bottom left panel (remember to click the *Show all* button in order to access all parameter tables in Sumo models), global kinetic and stoichiometric model parameters can be reviewed/modified. Each table will open up in the bottom right panel. This way the model parameters can be set globally, for the whole plant (Figure 3.9). These parameters will not be changed in this tutorial.

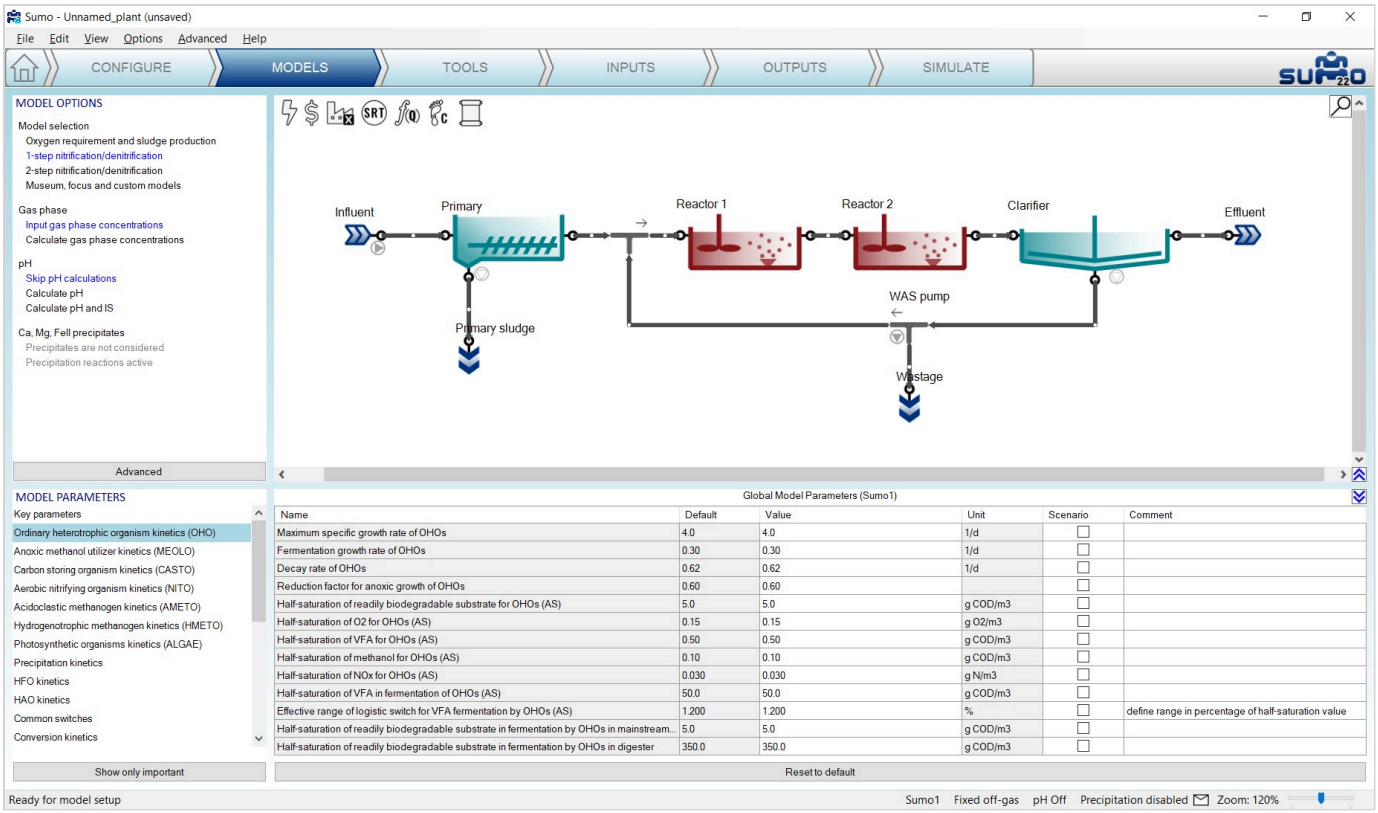


Figure 3.9 - Global model parameter setup in Sumo

Local model parameters

Any model parameter can as well be set as a process unit specific “local parameter”, by selecting the unit and dragging the desired parameter to the right side of the bottom right panel, as shown on Figure 3.10. In this case, the process unit will get a green “L” mark to remind the user for the local changes. Local model parameters will *NOT* be used in the current example, the aim of the above description was to explain this advanced functionality. You can remove local parameter selection by right clicking on the name of the parameter and selecting *Remove*.

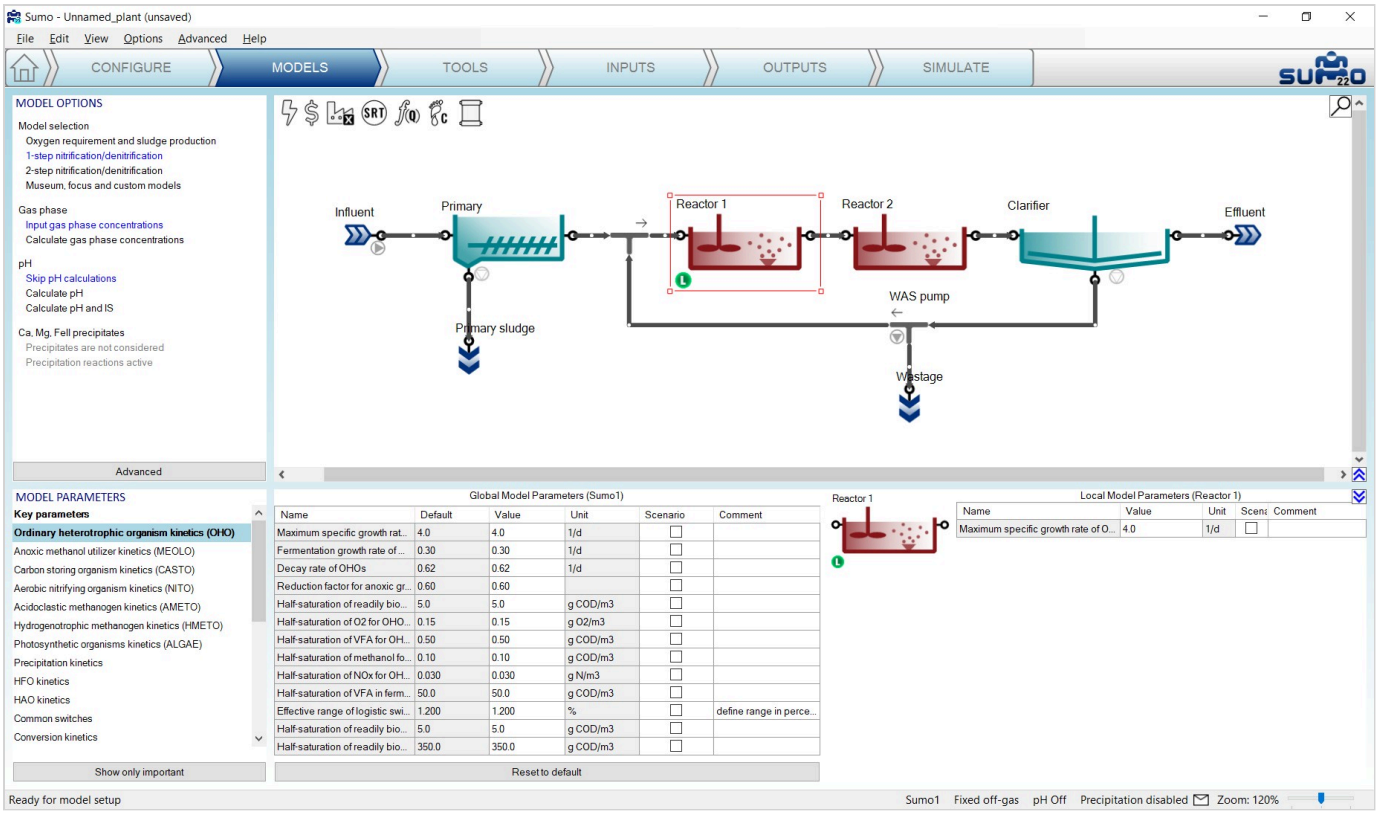


Figure 3.10 – Setting up process unit specific “local” model parameters in Sumo

Tools

Proceeding to the *Tools* tab, complex plantwide calculations can be defined (Figure 3.11).

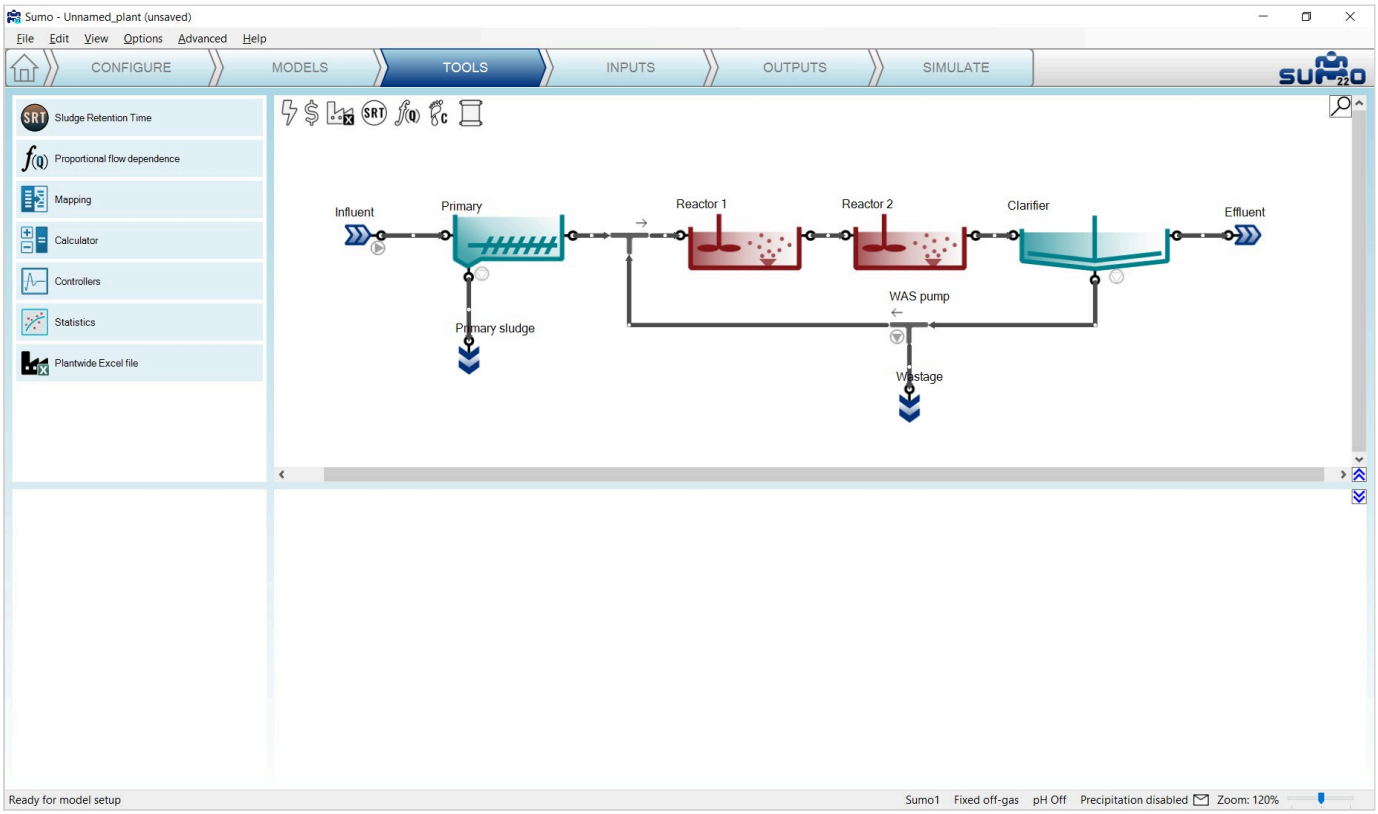


Figure 3.11 - Tools for plantwide calculations

“Plantwide” means that the calculations are based on variables contained in several process units around the plant. The following calculations can be added to the simulation (listed in the top left panel):

- **Sludge Retention Time**

Plant specific SRTs (total, aerobic, etc.) can be calculated.

- **Proportional flow dependence**

Plant specific flow dependence (e.g. RAS flow as percentage of influent flow) can be defined.

- **Mapping**

Parameters can be mapped from one process unit to another one.

- **Calculator**

Variables (e.g. volumes, masses) can be summed up in the plant. Simple and advanced variable ratios can be defined for the plant (e.g. N removal efficiency = effluent TN/influent TKN).

- **Controllers**

Controllers allow the user to configure automatic control (such as time based on/off, PID etc.) of process unit parameters.

- **Statistics**

A few statistical options (Moving average, Noise generator, Totalizer) are available here.

- **Plantwide Excel file**

The plantwide code is not confined to one process unit (PU) but can use variables from all over the plant model. The plantwide code file can be opened from the GUI directly. Further information and an example can be found in the Technical Reference document.

Sludge Retention Time

The SRT calculation is set up the following way: drag reactors that contain sludge mass to the numerator and drag wastage – and if desired, effluent connections (ports) – in the denominator, as illustrated by Figure .

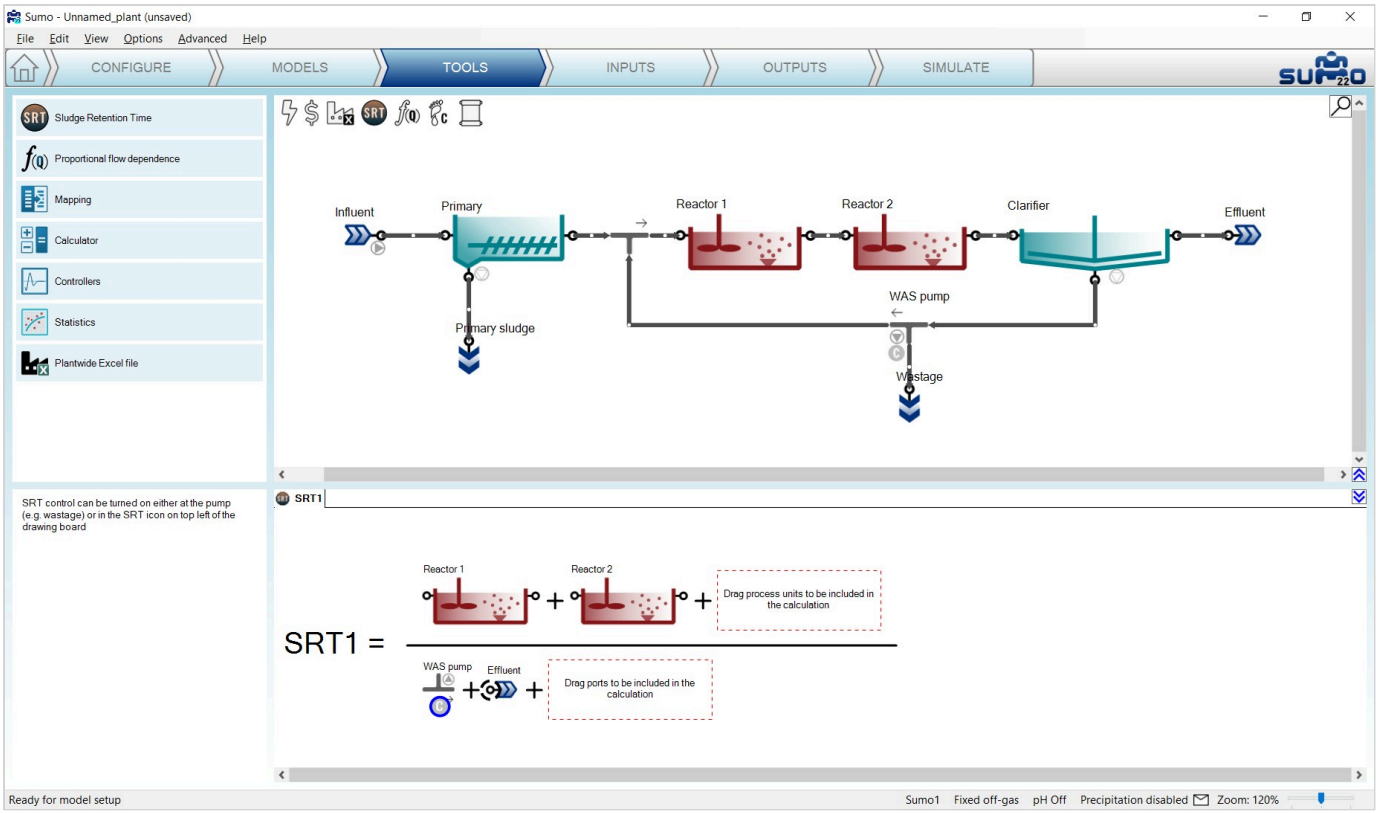


Figure 3.12 – Setting up SRT calculation

Several SRT calculations can be set up, e.g. total and aerobic, or North and South side SRT, etc. In this tutorial the total plant SRT will be calculated (as shown on Figure 3.12).

Note: When the project has an SRT calculation, the SRT icon on top of the drawing board gets a brown color.

Target SRT can be defined as well, by assigning a proper controlled port. These ports, such as the WAS pump in our example, are indicated by a “C” sign within a blue circle. A certain pump can only be used to control one SRT. Pumps can be selected and deselected for SRT control by right clicking their icon in the equation and choosing the desired option. When a pump is selected for control, *Remove Controlled* will deselect it (the “C” sign will disappear from the blue circle), while non-controlling pumps can be set to be controlling ones by choosing *Mark as Controlled* (Figure 3.13).

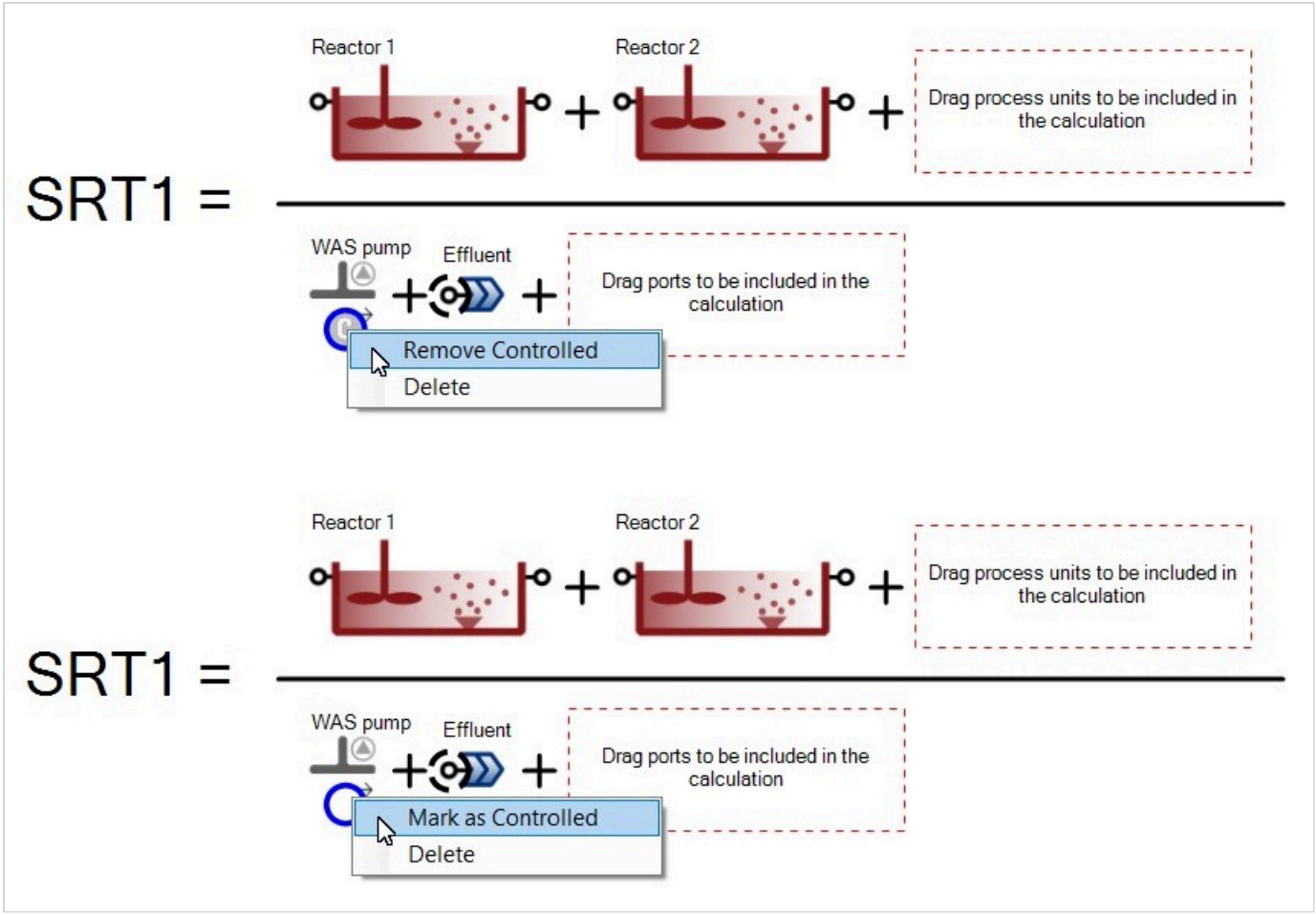


Figure 3.13 – Toggling between pump selection for target SRT control

Note that even though the wastage pump is selected for SRT control, it has not been designated yet for this role at the current stage (this is indicated in the plant layout by a grey “C” sign next to the pumped outflow pipe of the WAS pump). The activation of the SRT control can take place in a subsequent step (see the Plantwide inputs chapter).

Sum of variables

For calculating the Sum of variables, a set of predefined items are available (organized into groups) from dropdown menus in the bottom left panel. If the desired variable cannot be found here, custom variable input can be used well (choosing the last item in the first dropdown menu). In the latter case, make sure that the correct symbol is used, otherwise the built-in GUI check will disallow the calculation. Symbols of variables can be figured out using various methods (hints will be given in a subsequent chapter; details of the naming convention are described in the Technical Reference).

In this example, we will calculate the sum of Suspended solids mass in the reactors by entering “M_XTSS” as custom variable and dragging Reactor 1 and Reactor 2 into the equation from the layout (Figure 3.14).

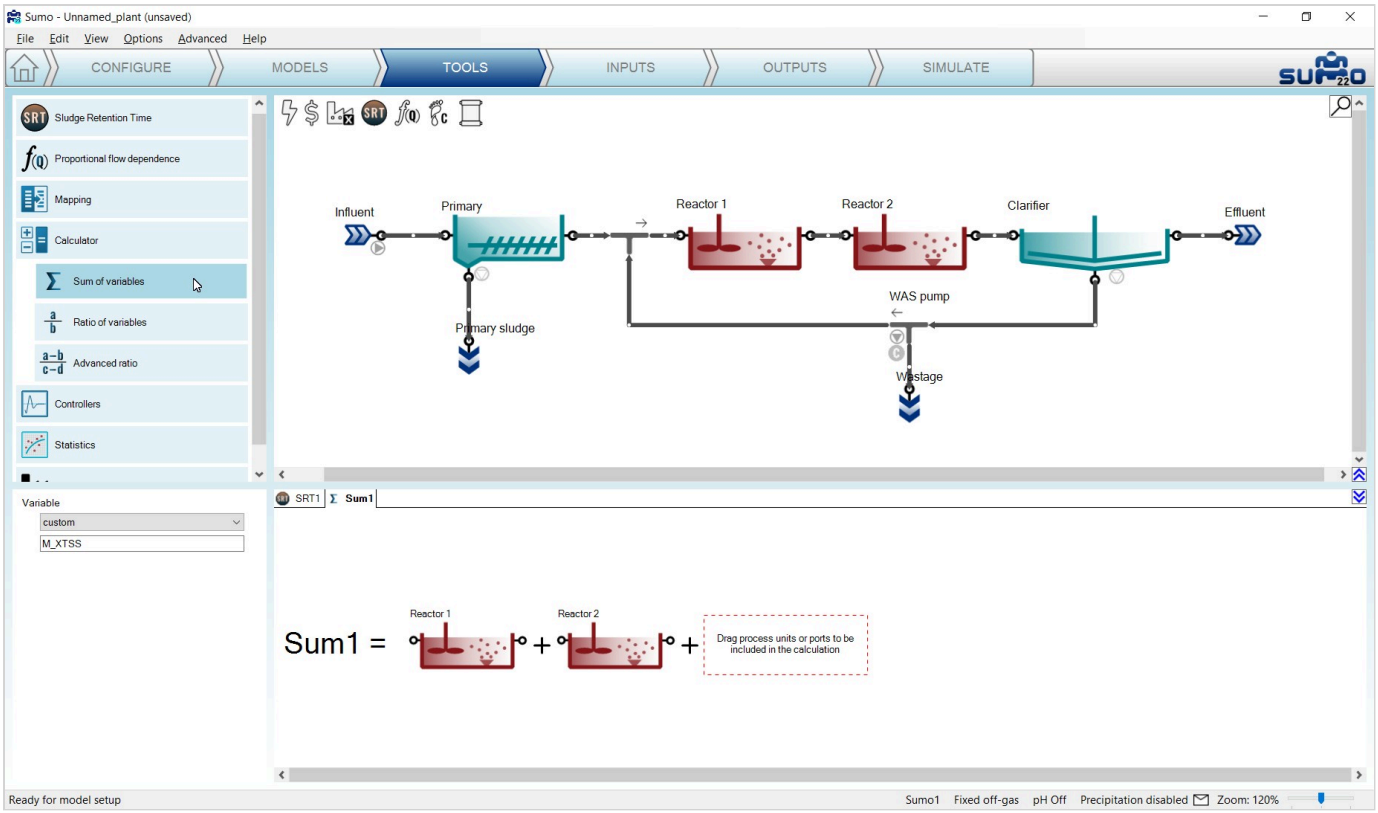


Figure 3.14 - Setting up Sum of variables calculation

Ratio of variables

Adding Ratio of variables can be done in a similar way as the Sum of variables. First select the variables to be used in the numerator and the denominator from the dropdown lists of the bottom left panel, then drag the desired process units to the ratio. In this example, we will calculate the removal ratio of Ammonia, as shown on Figure 3.15.

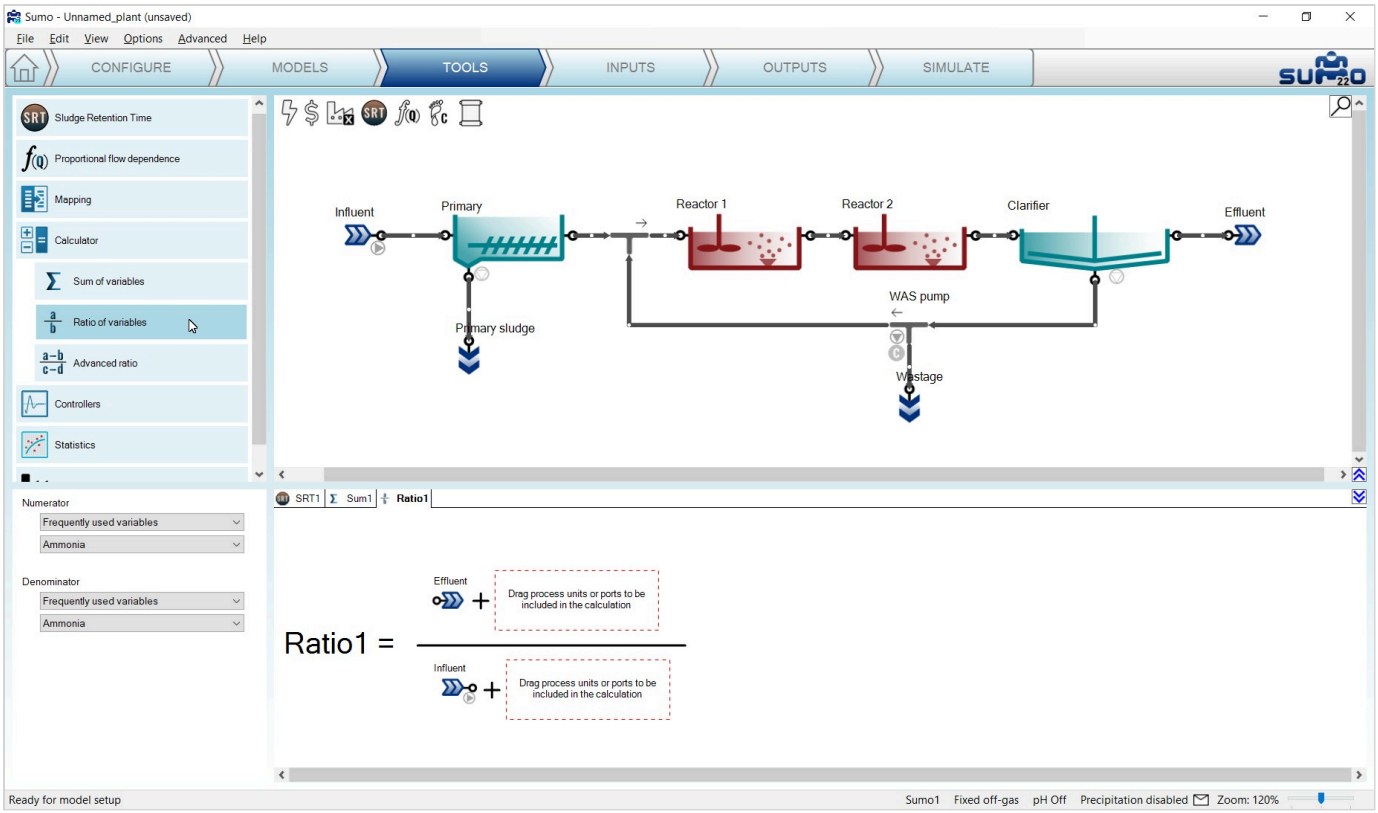


Figure 3.15 - Setting up Ratio of variables calculation

Proportional flow dependence

Adding Proportional flow dependence can be done by dragging the desired process units to the respective slots of the dependence equation. In this example, we are going to set the clarifier sludge recycle flow to be proportional to the influent flow rate, as shown on Figure 3.16. You will see a blue “C” sign showing up beside the clarifier on the drawing board, indicating that its sludge flow became a dependent parameter (controlled by the influent flow). The exact value of the proportional dependency will be set in a subsequent step (see the Plantwide inputs chapter). The controlling flow (e.g. influent) must not be within the loop (i.e. 50% of clarifier input flow to set the RAS flow cannot work as there is no solution to that loop).

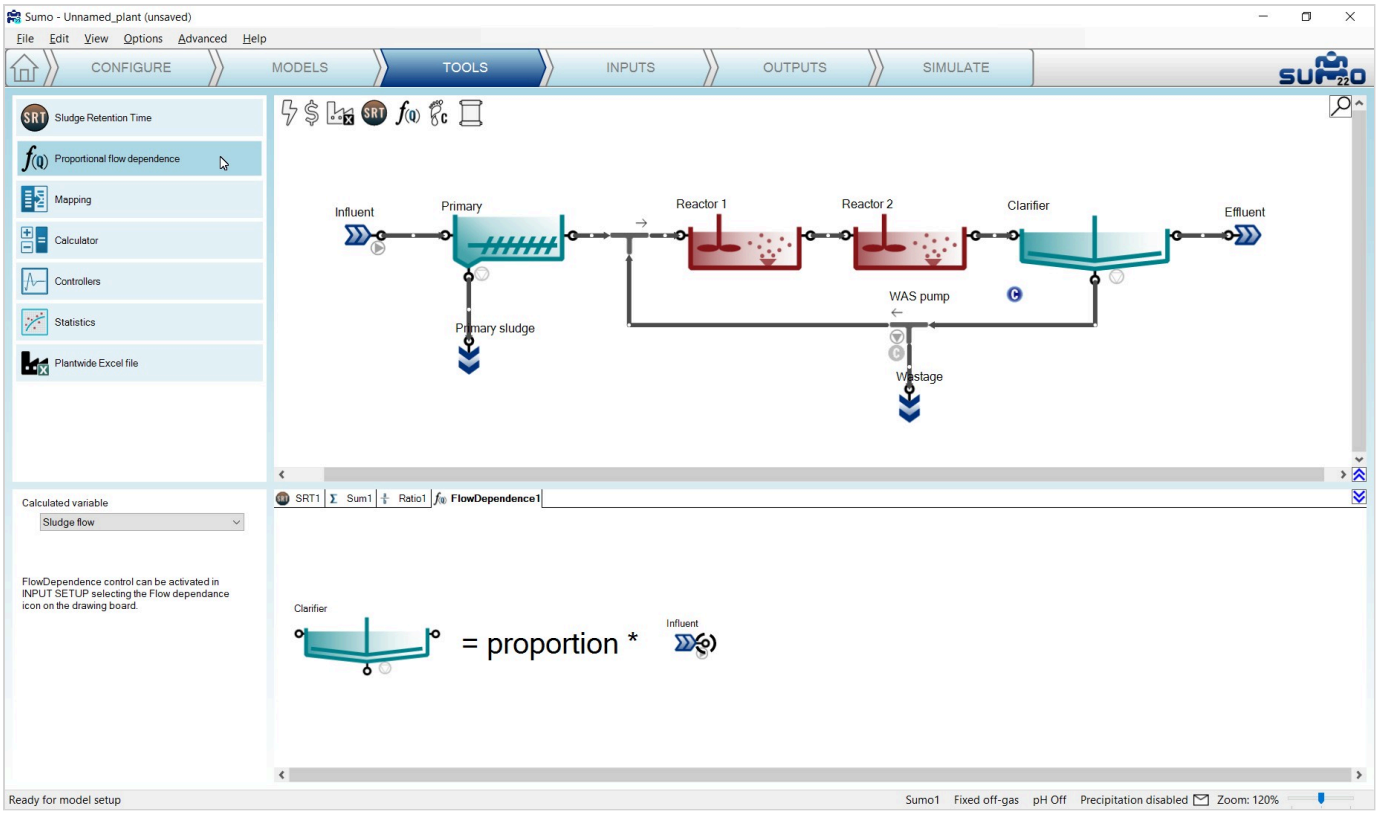


Figure 3.16 – Setting up Proportional flow dependence

Note: When the project has a proportional flow dependency, the “Q” in the f(Q) icon on top of the drawing board gets a blue background.

Controllers

Controllers help to keep certain operational parameters of the selected process unit at a required setpoint or within a band. The following controllers are integrated into Sumo22 (Figure 3.17).

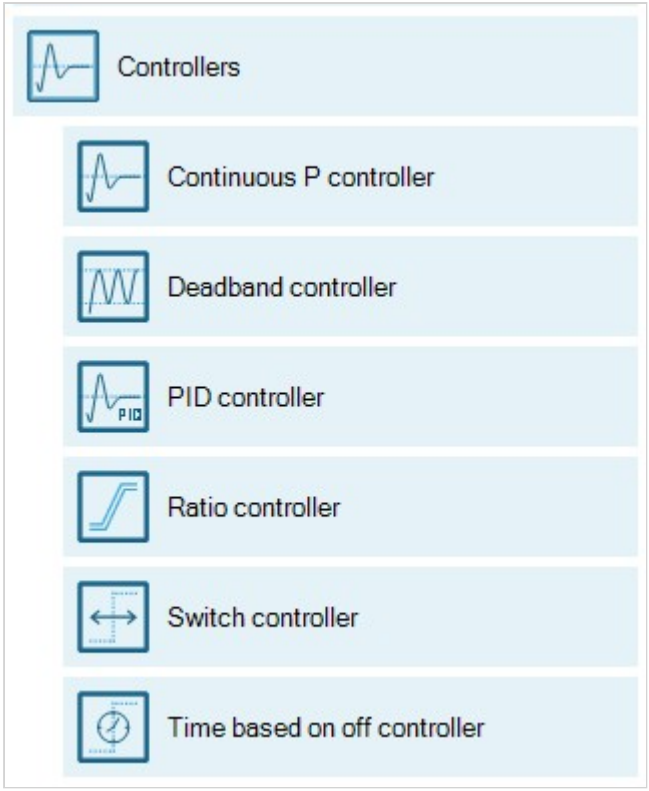


Figure 3.17 – Available controllers

In this example, we will use a *Deadband controller* to control the sludge wastage pump automatically, in order to maintain the MLSS between certain limits. Details about the further controller options can be found in the Controllers chapter.

Deadband controller

Adding a Deadband controller can be done in a similar way as the Sum of variables. First drag and drop the manipulated unit to the left side of the equation in the bottom right screen panel, and then the controlling unit to the right side of the equation. In the bottom left screen panel, you can now select the control variable (CV) and the manipulated variable (MV, a parameter) of the selected units. In this example, we will manipulate the Wastage pump to achieve the desired MLSS range, see Figure 3.18. Note that the “C” sign by the wastage pump will change to blue color, indicating that we have just set up and designated a controller for it that took over the role of the previously defined (but not activated, hence the former grey color) SRT control.

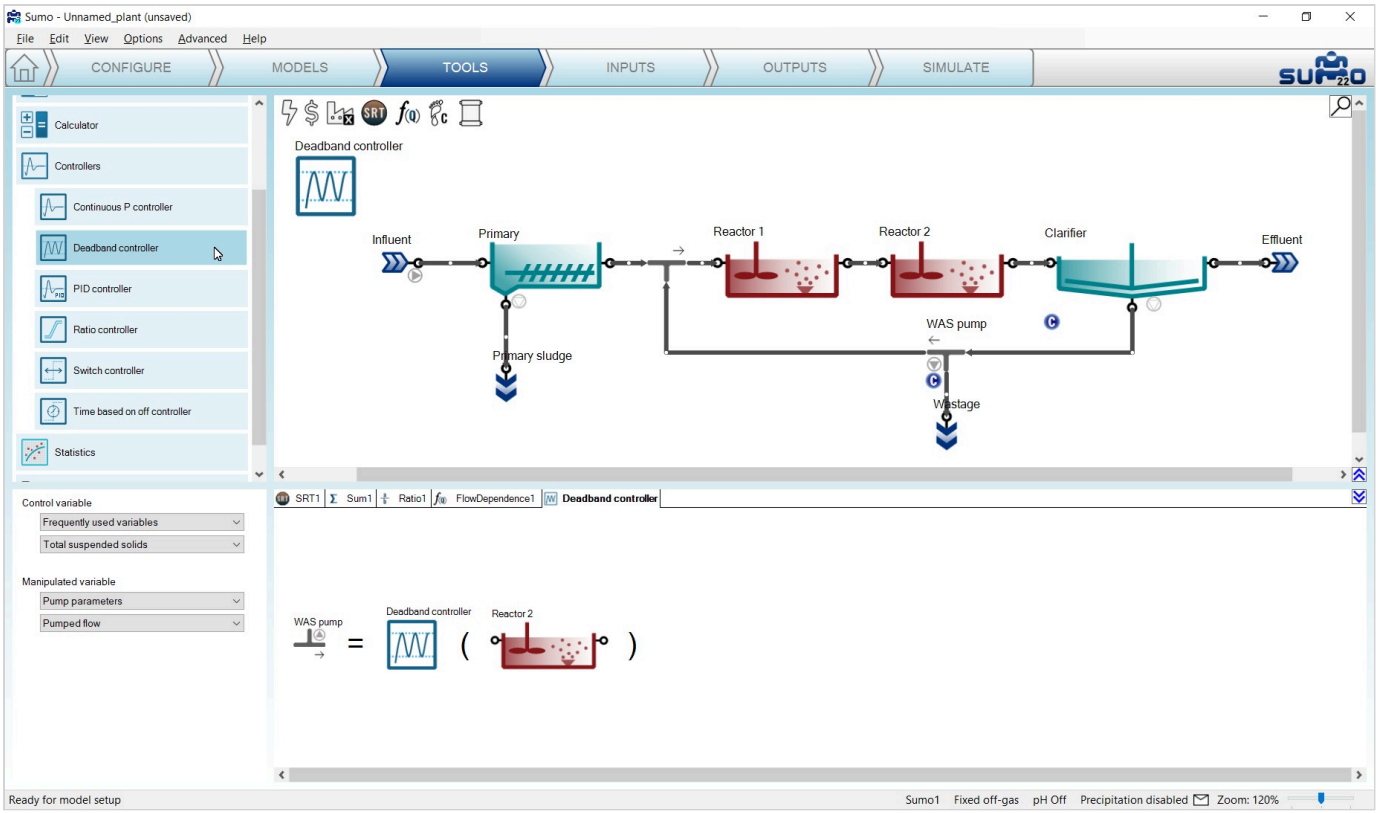


Figure 3.18 – Setting up a Deadband controller

The controller image that appears in the plant layout can be repositioned on the drawing board by holding the CTRL key while the icon is being dragged and moved, so the layout can be better understood. Move the controller icon above Reactor 2, then select it and hit F2 (or alternatively, right click on the tab header in the bottom right panel) to rename it to “MLSS control by WAS”. This will rename the respective tab (or the controller icon) as well.

Statistics

The *Statistics* section contains calculations for easier understanding or presentation of the results, such as average or totalized calculations. The following statistical calculations are integrated into Sumo22 (Figure 3.19).

Figure 3.19 – Available statistical calculations

As an example, we will set up the average effluent concentration of the plant.

Moving average calculation

Moving average can be added in a similar way as Sum of variables. First drag and drop the process unit to which the calculation should apply, to the right side of the equation on the bottom right panel. In the bottom left panel you can now select the desired variable whose average should be calculated. In this example we will calculate the average effluent ammonia concentration, see Figure 3.20.

The statistical unit image can be repositioned on the drawing board and renamed similarly to controllers. Move the icon above the Effluent and rename it to “MA Ammonia”.

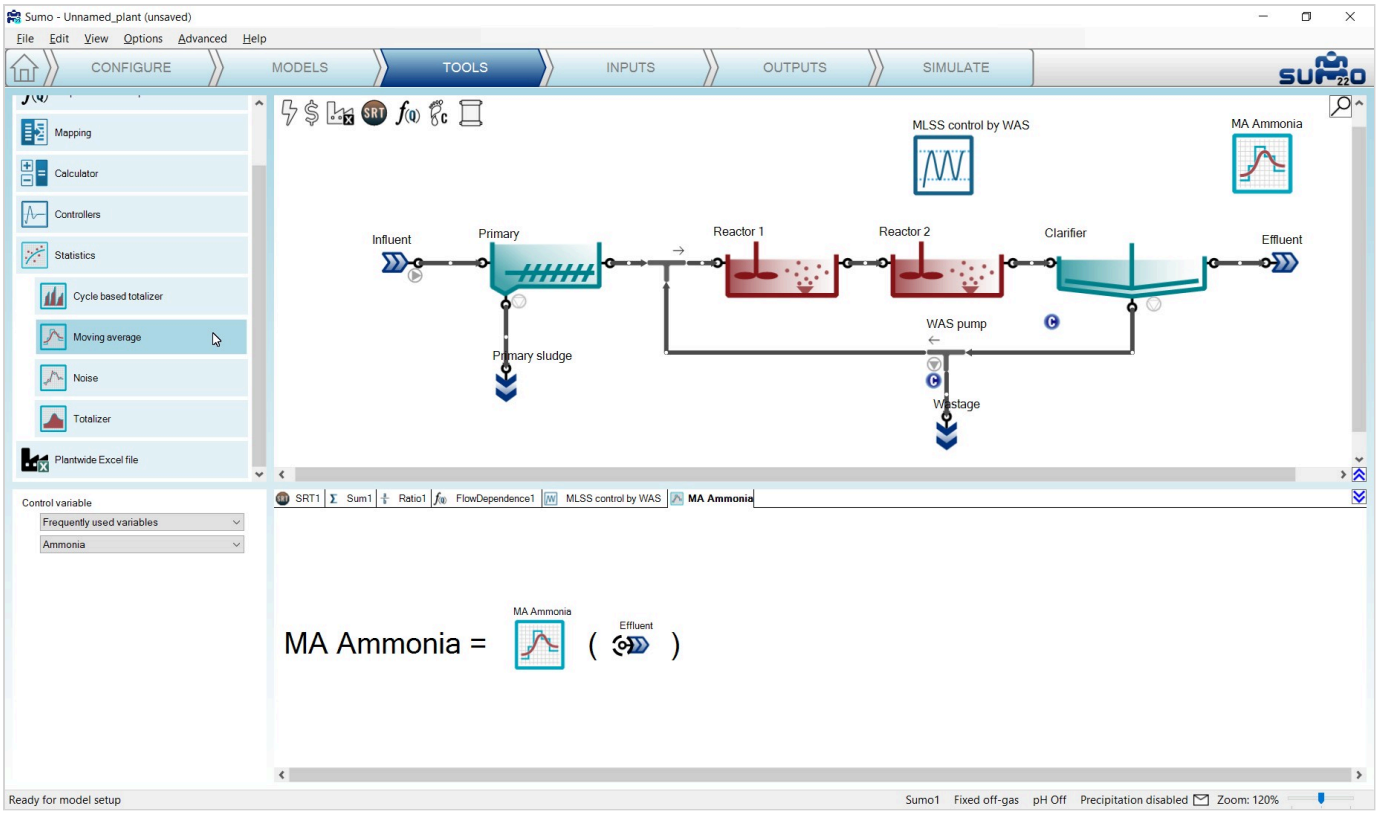


Figure 3.20 – Setting up a Moving average calculation

Inputs

Choosing the *Inputs* task, the blue workflow tab above the drawing board automatically splits into *Constants* and *Dynamics*. According to this, different types of settings become available: we can set either constant inputs (e.g. fixed influent composition, reactor DO setpoints etc.) or dynamically changing inputs (e.g. variable influent flow, composition, shifting reactor DO setpoints etc.). At this point, Sumo will be compiling your model in the background (you can track the progress in the Status Bar). However, in most cases, you can already start providing information to Sumo. When your layout requires using arrays (e.g. layered clarifiers, biofilm), please wait until the model is fully compiled and loaded (status bar message: “Ready for Simulation”). For the initial plant setup, we will only need the *Constants*, as shown on Figure 3.21. Select each object one by one and enter the required values as shown below.

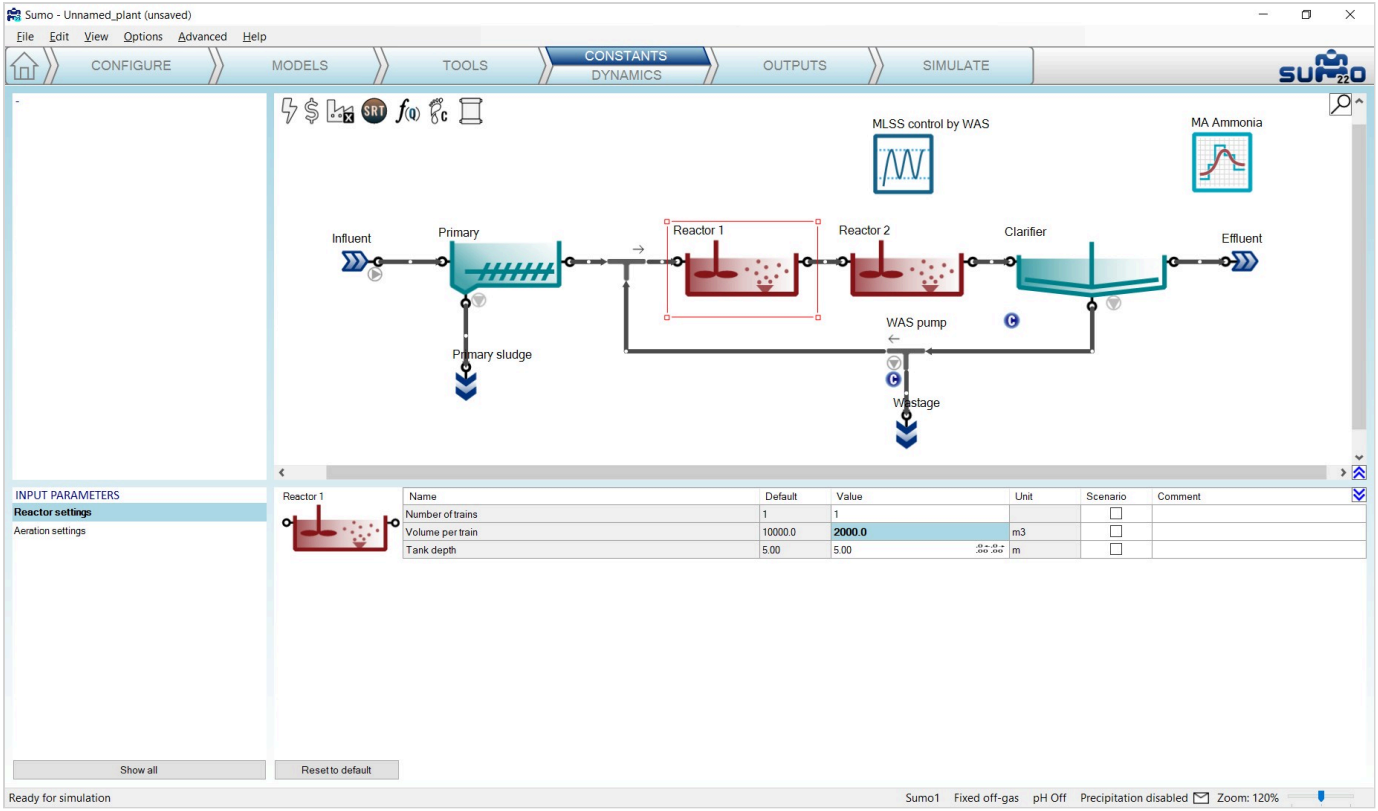


Figure 3.21 – Constant Input setup example

In this simple configuration, we only need to set a few values to build a realistic plant model, first for typical dry weather operation. Use the values from Table 3.3 for this example (leave everything else at default):

Table 3.3 – Input setup for AS plant

Process Unit	Parameter group	Parameter	Value	Unit
Reactor 1	Reactor settings	Volume per train	2000	m^3
Reactor 2	Reactor settings	Volume per train	8000	m^3
Influent	Influent specifications	Flow rate	20000	m^3/d
Influent	Influent specifications	Total COD	500	g COD/m^3
Influent	Influent specifications	Temperature	22	°C

Enter these values by selecting the respective process unit on the drawing board and the parameter group in the *Input parameters* menu (bottom left panel) – the values can be edited in the bottom right panel (Figure 3.22). Each value that is different from the default will be highlighted with bold letter type. There is also a similar indication in the *Input parameters* menu for parameter groups that contain non-default values.

Whenever the entered value is out of the allowed range specified in the model, Sumo will notify you with a prompt window and set the value to the nearest feasible bound, indicating the automatic choice by applying

red color to the text. This value can be overridden manually with a valid number.

If needed, all changes applied to the values of the actual parameter group can be reverted to defaults by clicking the *Reset to default* button located in the bottom right screen panel (Figure 3.22). Also, there is a unit conversion module for US units (MGD, scfm, etc.) in the *Options* menu item if needed.

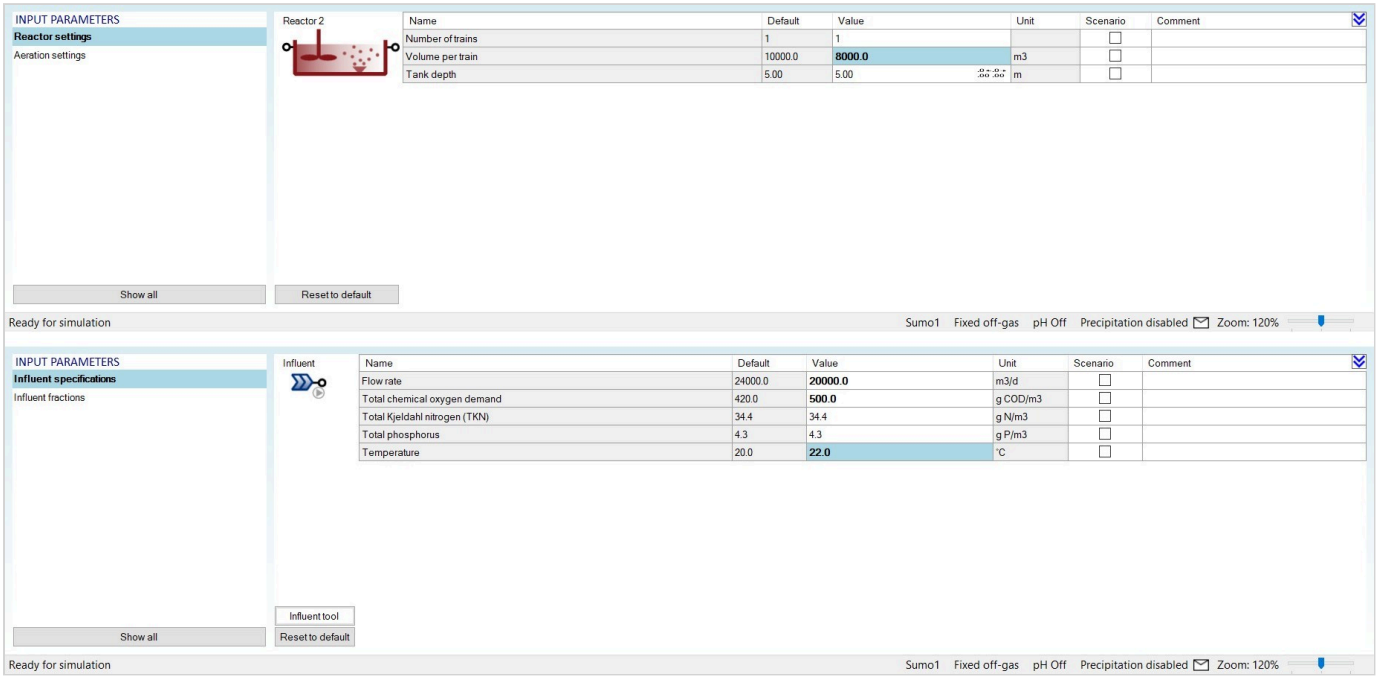


Figure 3.22 - Input parameter table examples

For setting the plant specific influent composition, the use of the *Influent tool* Excel file is recommended. The *Influent tool* can be reached directly from the input setup of the Influent, by clicking the button located in the bottom right screen panel (Figure 3.23).The details of the *Influent tool* are described in the Influent tool chapter. At this point, we will not alter the influent composition, so we will skip using the *Influent tool*.

Parameters for scenario analysis can be selected by using the checkboxes in the *Scenario* column. In this example, we will select the influent flow rate, total COD and the temperature (Figure 3.23). The use of scenarios will be described in the Scenarios chapter.

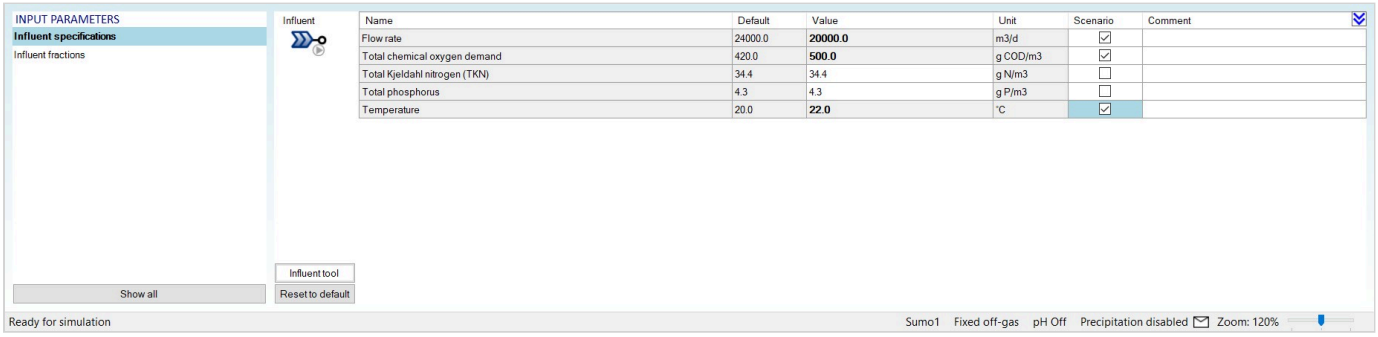


Figure 3.23 – Parameter selection for scenarios

The controller parameters can be setup at this stage as well. In this Deadband controller example, we will set:

- *Controller direction*: inverse (-1), since increasing wastage (MV) will decrease MLSS (CV), i.e. the CV responds inversely to MV change;
- 2600 mg/L as low value and 2800 mg/L as high value for the *Controlled variable* (MLSS in Reactor 2) range;
- 150 m^3/d as low value and 600 m^3/d as high value for the *Manipulated variable* range (the latter represents the physical pump capacity for the Wastage pumped flow);
- *Initial* value of manipulated variable to single pump capacity as 150 m^3/d.

See these settings on Figure 3.24.

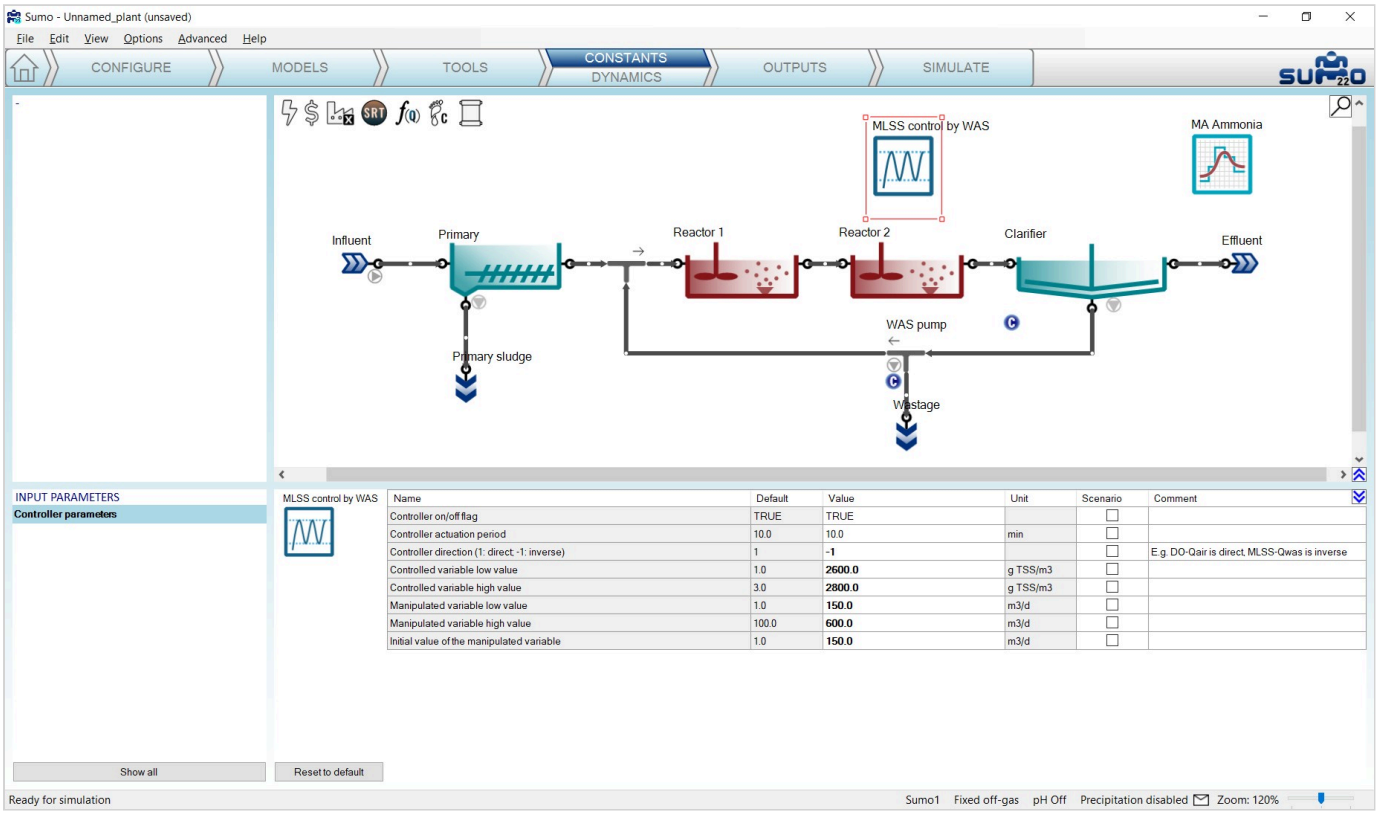


Figure 3.24 – Deadband controller input setup

The input setup of this wastewater treatment plant model is now ready.

Influent tool

The *Influent tool* is a multiple sheet Excel file to help to set up the proper influent composition. The role of each sheet is explained in Table 3.4 below.

Table 3.4 – Description of the Influent tool

Influent tool sheets	
Help	Short description of the file content
Data	Input of the available measurement data of the simulated plant or facility. This sheet provides help to estimate the missing data based on available information for municipal

Influent tool sheets	
	or industrial wastewater composition.
Check fractions	On the left side of the sheet, the estimation of key organic fractions is available, such as COD and N fractions, particulate COD/VSS ratios by component, yield on ultimate BOD and BOD fraction for soluble, colloid and particulate. On the right hand side, the calculated COD, BOD5 and TSS/VSS values can be checked if they match the measured values.
Sumo forms	This sheet gathers all the information that can be used to simply copy into the Sumo *Models* or *Inputs* tab of the Influent process unit.
Fractionation tree	This sheet shows the fractionation graphs of total COD, suspended solids, N and P based on your input data, helping to visualize the organization of the individual fractions used in the model.
Balances	On this sheet, the organic compounds can be checked (how the fractions add up to the total). The sheet will also provide warning when negative component concentrations result from the estimated fractions (such as not enough N for organic TKN if most of TKN is ammonia, and there are solids in the influent)
Diurnal flow	This sheet provides example and usual flow pattern for small, medium and large plants. Based on the influent value, the diurnal flow dynamic input tables are prepared for copy and paste into Sumo.
Birthday cake	On this sheet, you will find a ready-made table for a “birthday cake” type of load analysis, prepared from your input and diurnal flow data.
Calculations	This sheet contains the details of BOD calculation and the error tolerances used on Check fractions sheet.

For a detailed description of the *Influent tool* please refer to the Tools in Sumo chapter of the Technical references, and guidelines for influent fractionation are available in Influent characterisation chapter.

Dynamic Inputs

This ***optional*** task can be used to enter dynamically changing input information, e.g. diurnal flows, DO schedules and more. To activate the dynamic input setup, click on the lower part of the *Inputs* tab on the Task Bar, labeled as *Dynamics*.

The role of screen panels in *Dynamic Inputs* mode are the following:

Top right panel	Plant configuration
Top left panel	Unused in this mode
Bottom right panel	Data entry functionality
Bottom left panel	List of entered dynamic data tables

If we wish, we can copy and paste entire data tables from an Excel file into Sumo. This will be discussed later in the Subjecting the plant to dynamics chapter.

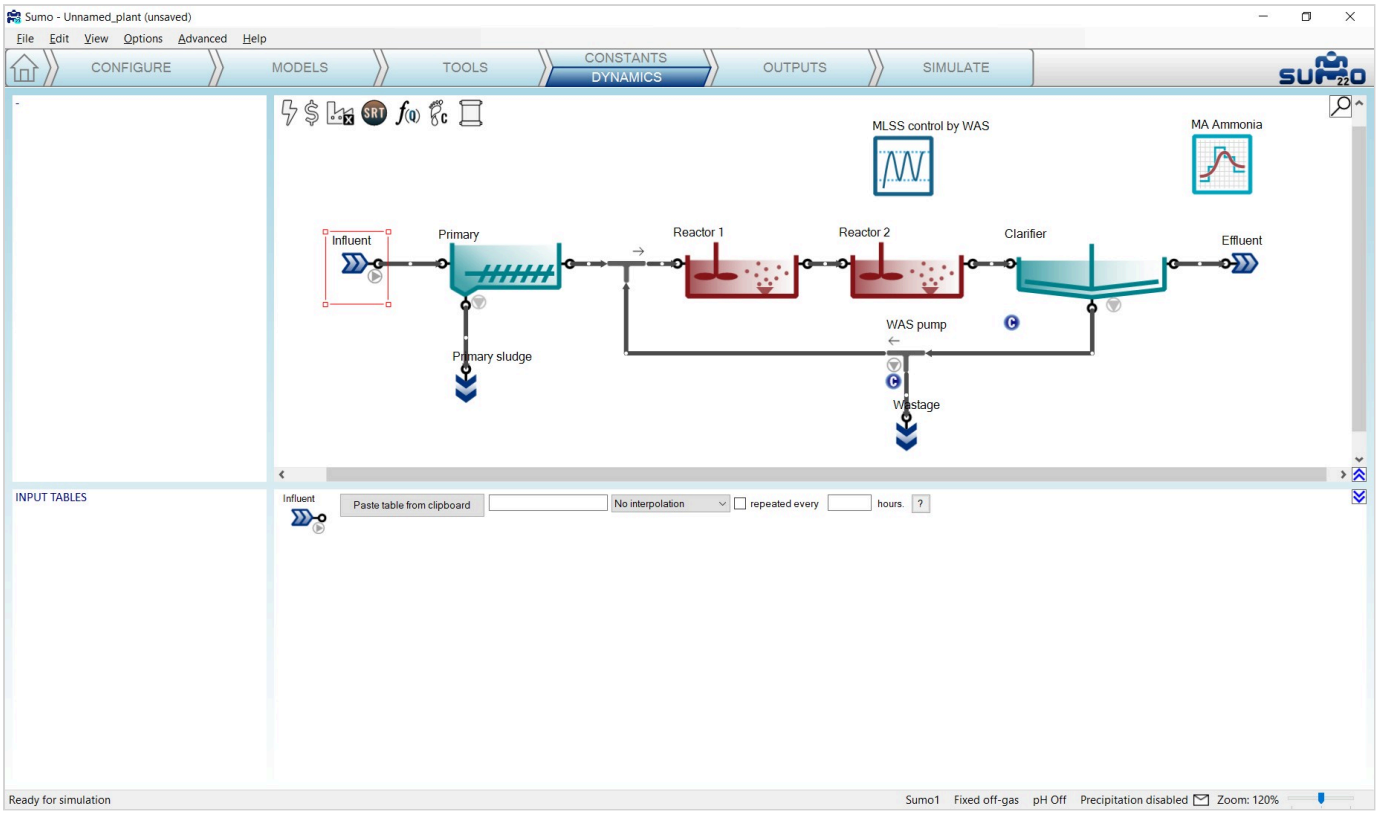


Figure 3.25 - Dynamic input setup

Plantwide inputs

Target SRT and proportional flow dependence input settings can be accessed by clicking on the respective icons listed on the top left part of the layout panel. In this simulation, we will not use the Target SRT controller, but will set up the proportional sludge flow of the clarifier to 100%, as shown on Figure 3.26. This will align the sludge flow rate with the influent flow as 1 to 1.

The plantwide parameters set in the Plantwide Excel file will appear in the *Inputs* tab when the plantwide (factory) icon is selected in the top section of the layout. These can also be changed dynamically, similarly to any other model parameter (for more detailed information on this feature, please consult the Technical Reference). In this simulation, we will not use plantwide parameters.

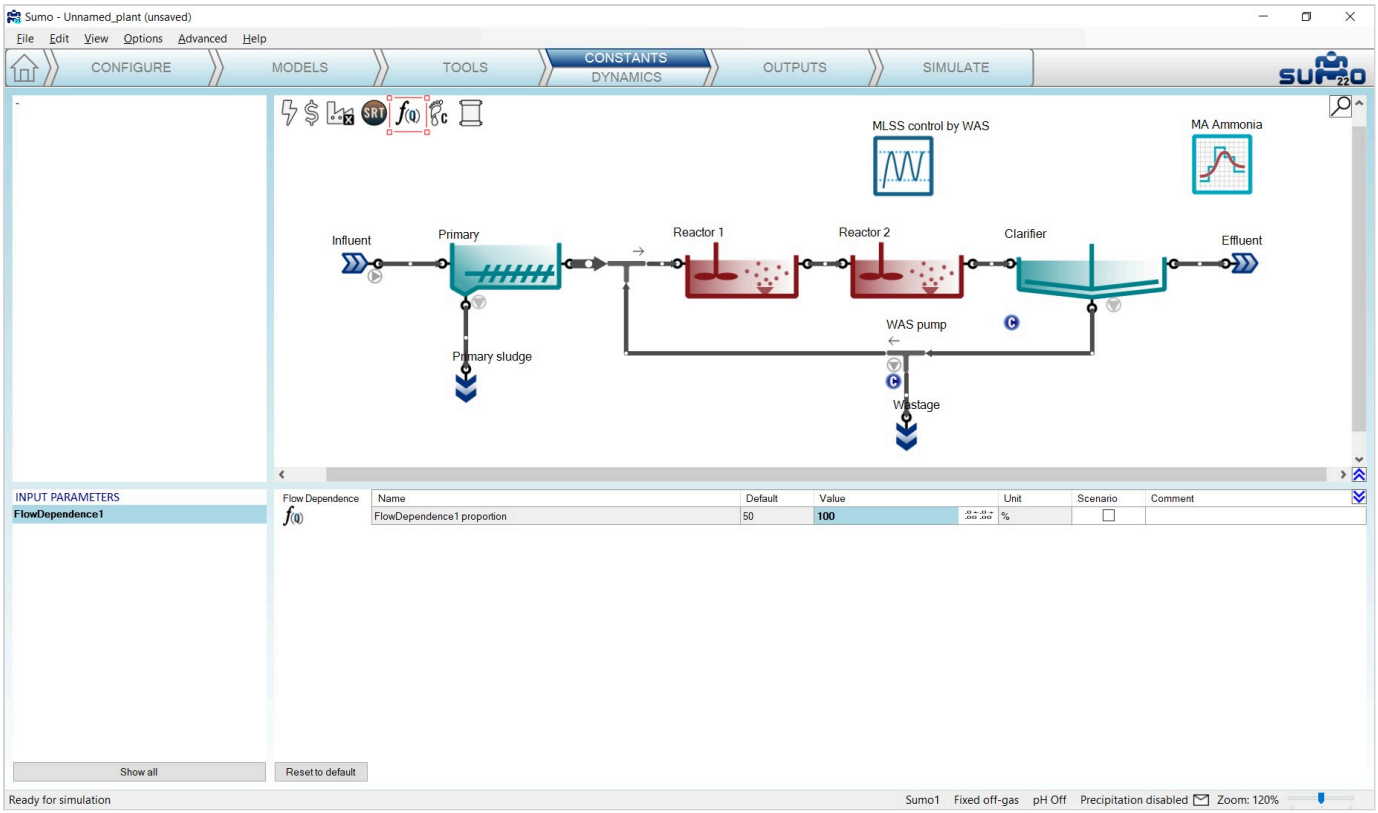


Figure 3.26 – Proportional flow input setup

Outputs

This task can be used to specify which variables and in what format should be displayed and/or saved during the simulation phase (Figure 3.27).

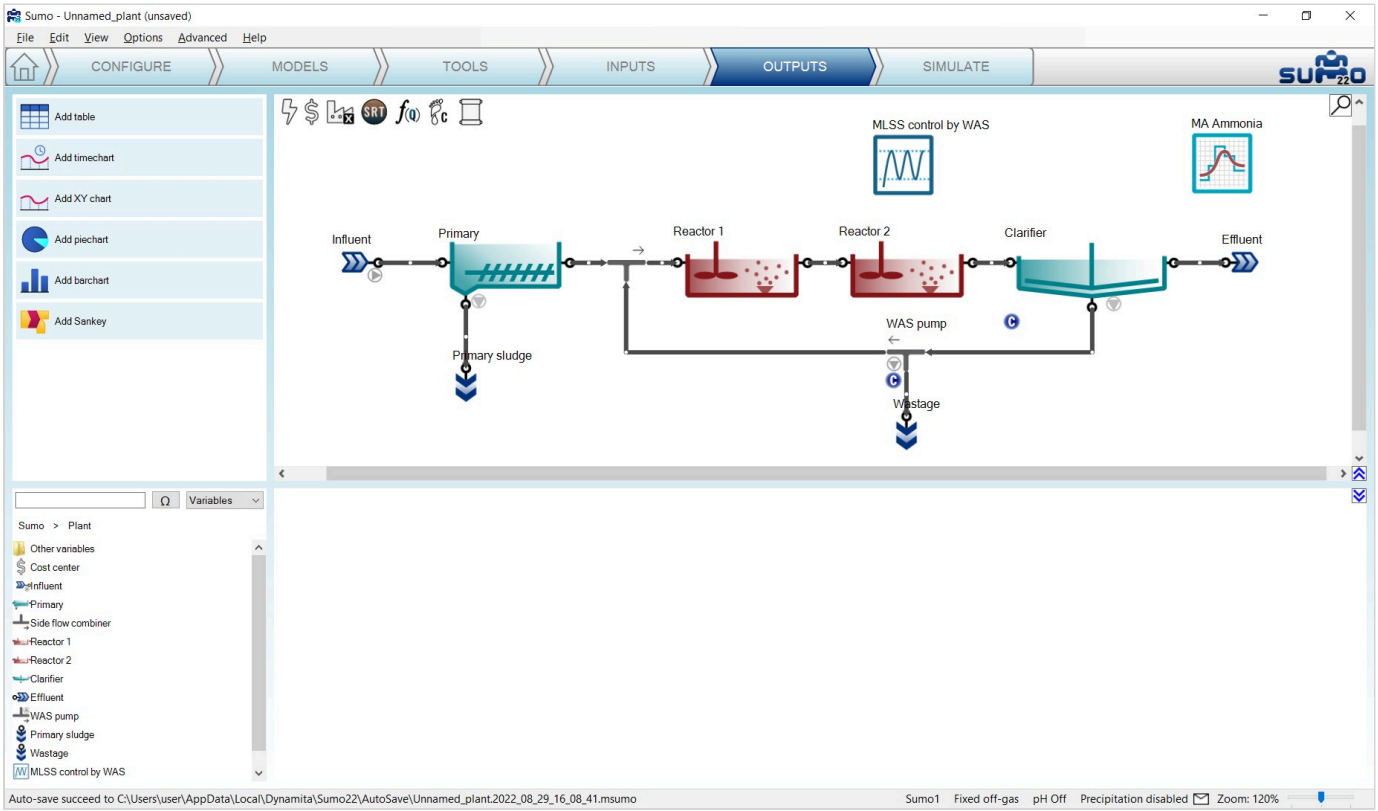


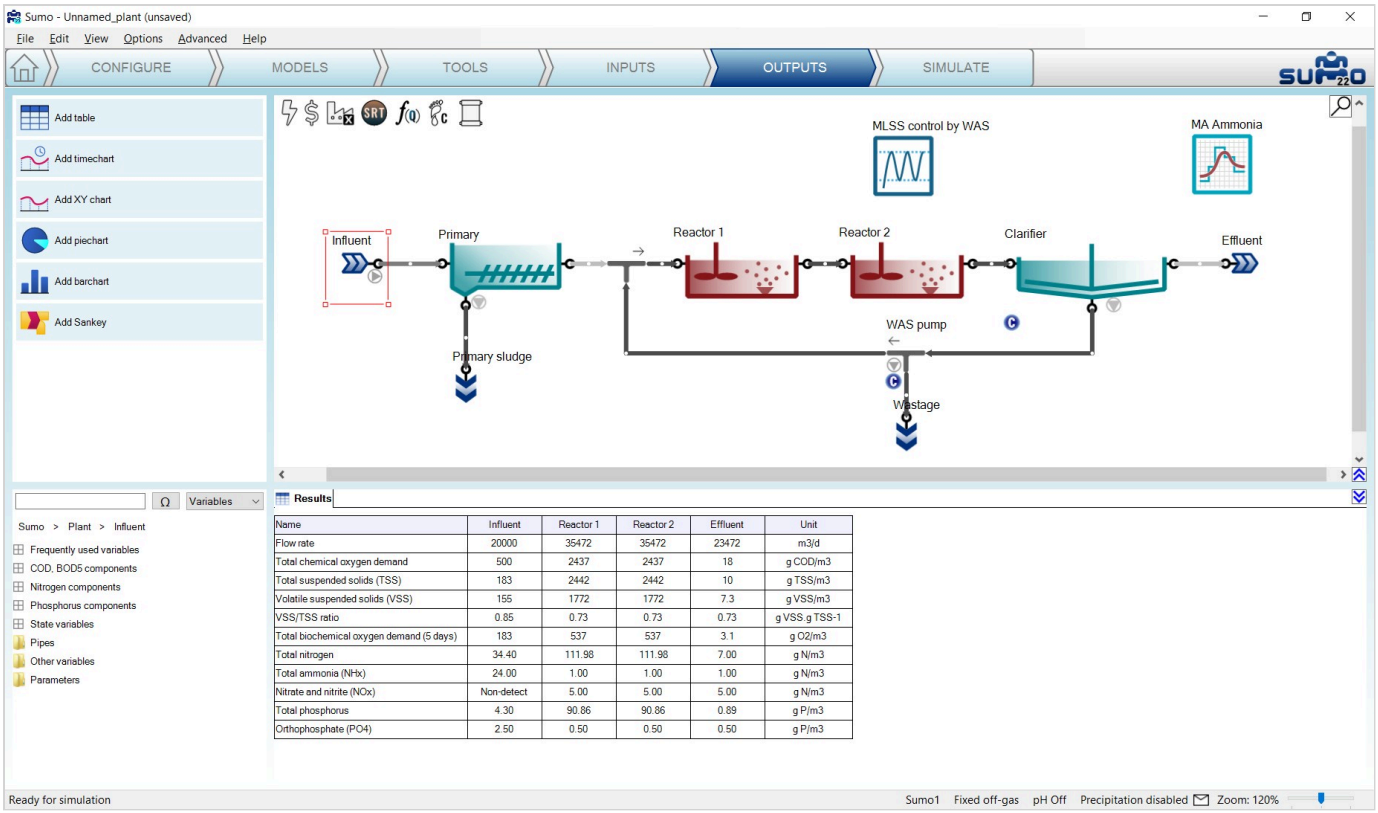
Figure 3.27 – Output setup

The role of screen panels in *Outputs* mode are the following:

Top right panel	Plant configuration
Top left panel	Buttons for different diagram types (Table, Timechart etc.)
Bottom right panel	Added outputs in a series of tabs
Bottom left panel	Output variable list for the selected unit and the connected pipes Available once the model is fully compiled. The user can browse the variables based on their name or symbol. There are also preselected categories (frequently used, operational variables etc.) available to help the work.

Adding a table

Click the *Add table* button in the top left panel: this will add a table to the bottom right panel. The table can be renamed (right click on the tab and choose *Rename* from the pop-out menu or simply just double-click on the tab) and several tables can be added. Name this table “Results”. Add process units to the table by dragging them to the table (by selecting multiple units in the drawing board, they can be added in one go as well). Add variables to the table by selecting and dragging them from the bottom left panel (Figure 3.28). Entire display tables can be added at once by dragging the prepared table e.g. *Frequently used variables* (Note: if the table has not been renamed by the user, it is automatically renamed when a whole display table is added). The exact list of preselected variables varies according to the process units (in this example, the Influent was selected when adding *Frequently used variables* to the table). Initial values will appear in the cells.



Name	Influent	Reactor 1	Reactor 2	Effluent	Unit
Flow rate	20000	35472	35472	23472	m3/d
Total chemical oxygen demand	500	2437	2437	18	g COD/m3
Total suspended solids (TSS)	183	2442	2442	10	g TSS/m3
Volatile suspended solids (VSS)	155	1772	1772	7.3	g VSS/m3
VSS/TSS ratio	0.85	0.73	0.73	0.73	g VSS.g TSS-1
Total biochemical oxygen demand (5 days)	183	537	537	3.1	g O2/m3
Total nitrogen	34.40	111.98	111.98	7.00	g N/m3
Total ammonia (NHx)	24.00	1.00	1.00	1.00	g N/m3
Nitrate and nitrite (NOx)	Non-detect	5.00	5.00	5.00	g N/m3
Total phosphorus	4.30	90.86	90.86	0.89	g P/m3
Orthophosphate (PO4)	2.50	0.50	0.50	0.50	g P/m3

Figure 3.28 - Adding a table

You can add also the DO and Offgas O_2 content from the *Frequently used variables* of Reactor 1 (or 2).

Add another table and drag the *Active biomass* and *Uptake rates* for both reactors.

Note that the table columns (except for *Name* and *Unit*) can be reorganized by dragging the column header and dropping to the desired slot. Table rows can be rearranged likewise: first highlight the rows to be moved with the mouse, then drag and move the pointer out to the bottom left screen panel for a moment, and finally drop the rows to the desired new place. Units can be changed by clicking and selecting from the dropdown list. The number of decimal digits displayed can be customized to show meaningful detail by hovering the mouse over the numbers and clicking the respective icons – the action will apply to all numbers in the active table row.

Adding a timechart

Click the *Add timechart* button in the top left panel: this will add a timechart to the bottom right panel as a new tab. Select a process unit on the layout and drag a variable from the bottom left panel on the timechart to be plotted (a legend will appear in the top right corner of the timechart). Several variables can be added to each timechart (new items will be appended to the legend), and several timecharts can be added as well (increasing the number of tabs). In this example we will plot MLSS in the reactors and wastage flow on one timechart (select the reactors one by one and add TSS from *Frequently used variables*); and effluent total nitrogen, ammonia, as well as nitrate and nitrite (available from *Nitrogen components*) on the second one (see Figure 3.29). Graphs will be plotted during the simulation phase.

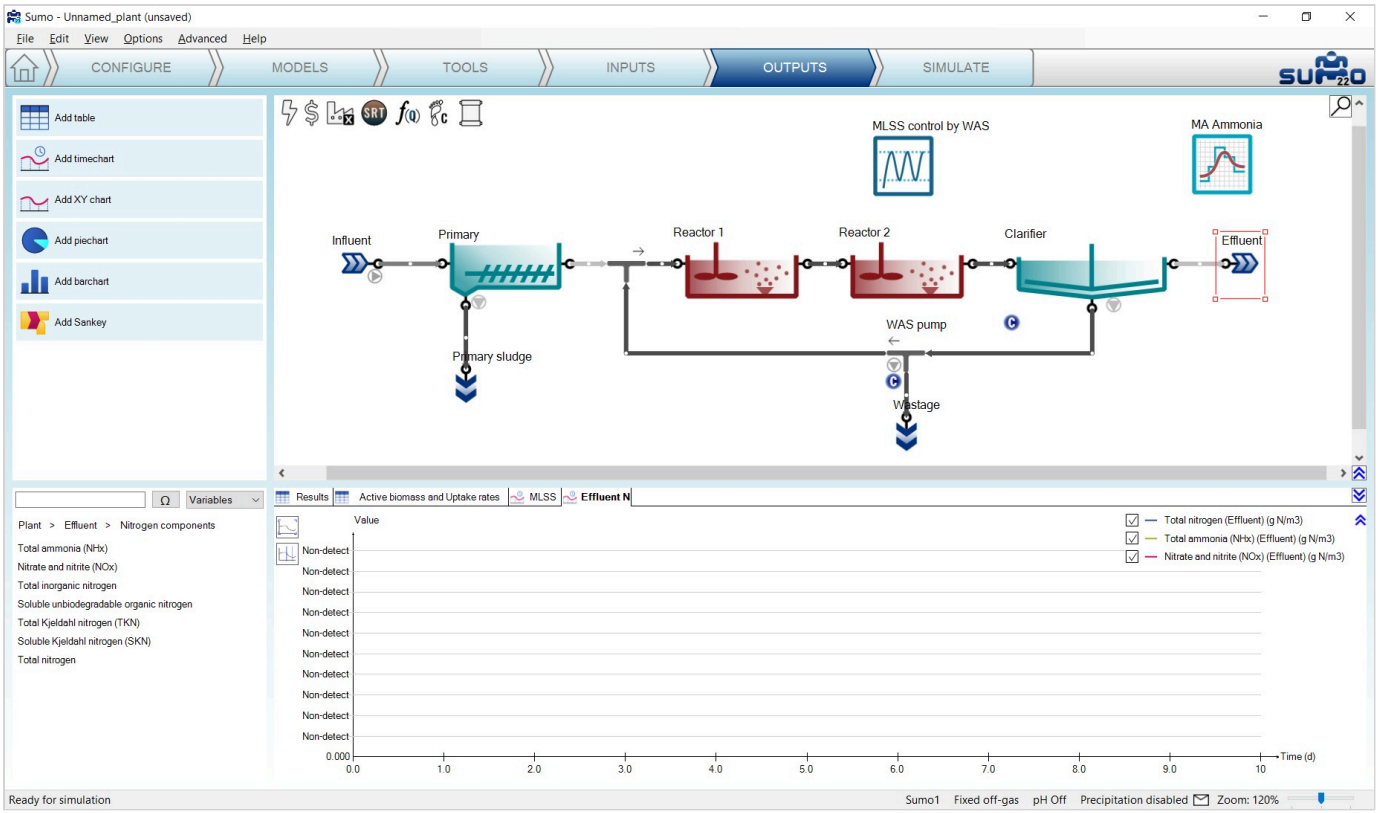


Figure 3.29 - Adding a timechart

Adding an X-Y chart

This type of diagram can be used to demonstrate the relation between selected variables (e.g. equilibrium species) depending on another variable (e.g. pH). A practical application is shown in the example called Titration of ammonia solution.

Adding a piechart

Click the *Add piechart* button in the top left panel: a new tab for labeled piechart will appear in the bottom right panel. Select the desired process unit on the layout and drag the variables to be depicted from the bottom left panel to the – yet empty – bottom right panel (a legend will appear in the top right corner). For this example, we will use Total Kjeldahl Nitrogen along with Nitrate and nitrite (available from *Nitrogen components*) in the effluent. Rename the tab to “N fractions” (Figure 3.30). The piechart will be rendered during the simulation phase.

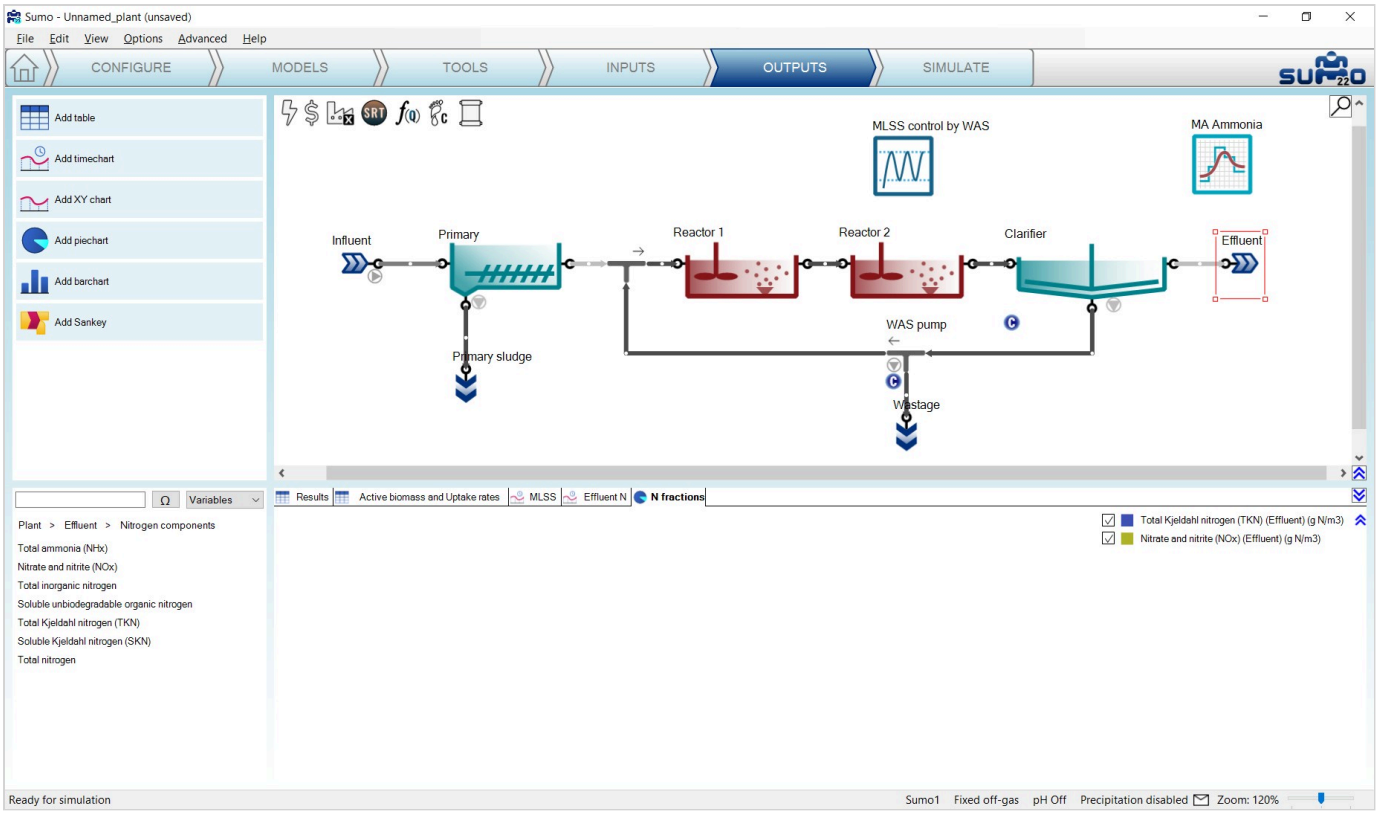


Figure 3.30 - Adding a piechart

Adding a barchart

Click the *Add barchart* button in the top left panel: this will add a barchart to the bottom right panel as a new tab. Choose a process unit and drag variables from the bottom left panel to be shown on the barchart, just like in the previous chart types. Multiple variables can be added to each barchart, and several barcharts can be added as well. Dragging additional process units to the chart will add them with the actual set of variables and initial values will be shown. For this example, choose Total chemical oxygen demand and Total 5-day biochemical oxygen demand from the *Frequently used variables* in the influent and in the effluent (Figure 3.31). Rename the tab as “COD & BOD5”. The barchart will be continuously updated with the changes during the simulation phase.

Note that the order of process units in the barchart can easily be reorganized by dragging the name of the process unit and dropping it to the desired slot.

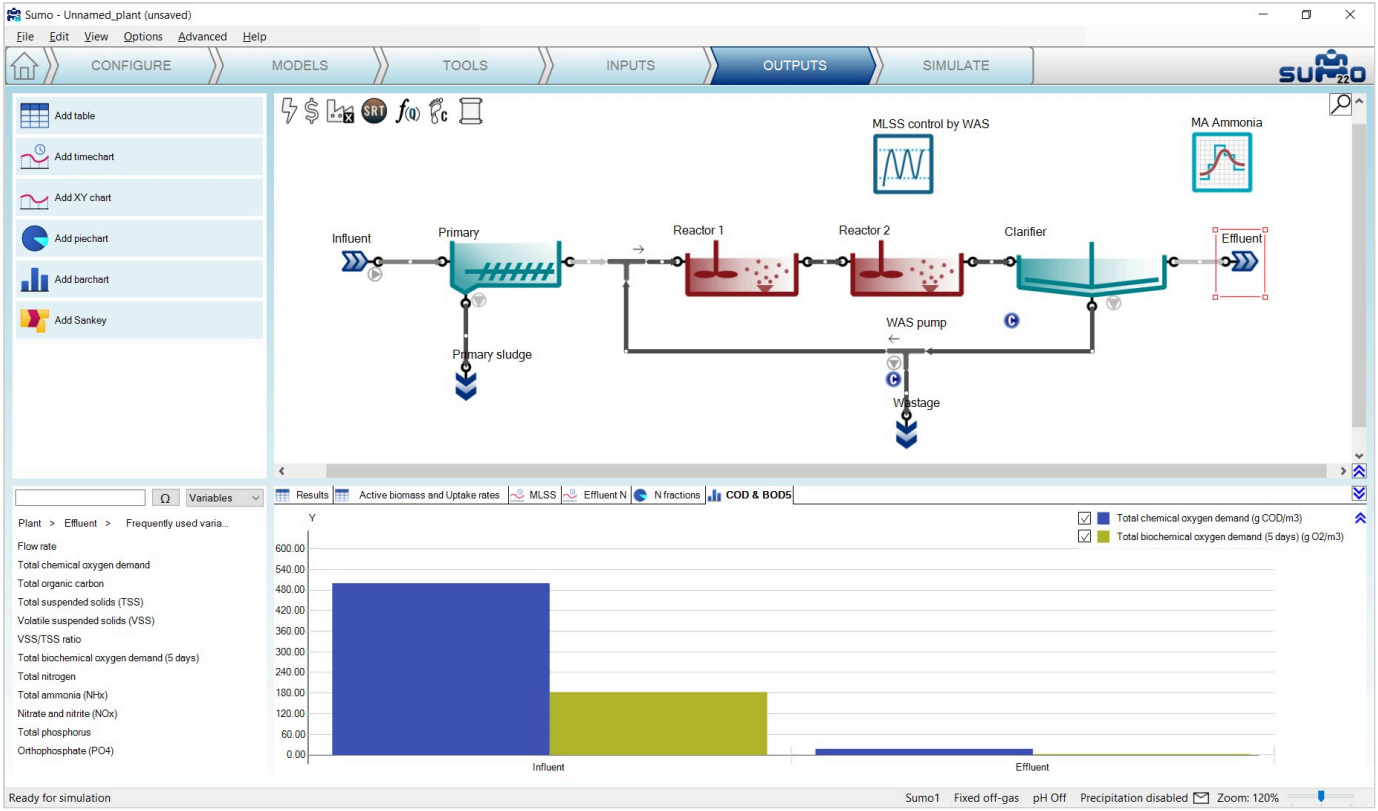


Figure 3.31 - Adding a barchart

Adding Sankey

Click the *Add Sankey* button in the top left panel: this will add the Sankey diagram of flow by default. The variable can be changed by dragging any other item from the bottom left panel over to the bottom right panel. Several Sankey diagrams can be added, with one variable plotted on each Sankey. This example will use one Sankey with the default setting (renamed to “Flow”) and another one showing the mass flows of ammonia (renamed as “Ammonia mass flow”) as shown on Figure 3.32. Use the search field in the bottom left panel to find the latter: type in “Total ammonia” and locate “Total Ammonia (NHx) mass flow” under the “Mass flows of frequently used variables” list item in the search results. The search field works with all of the other output options as well.

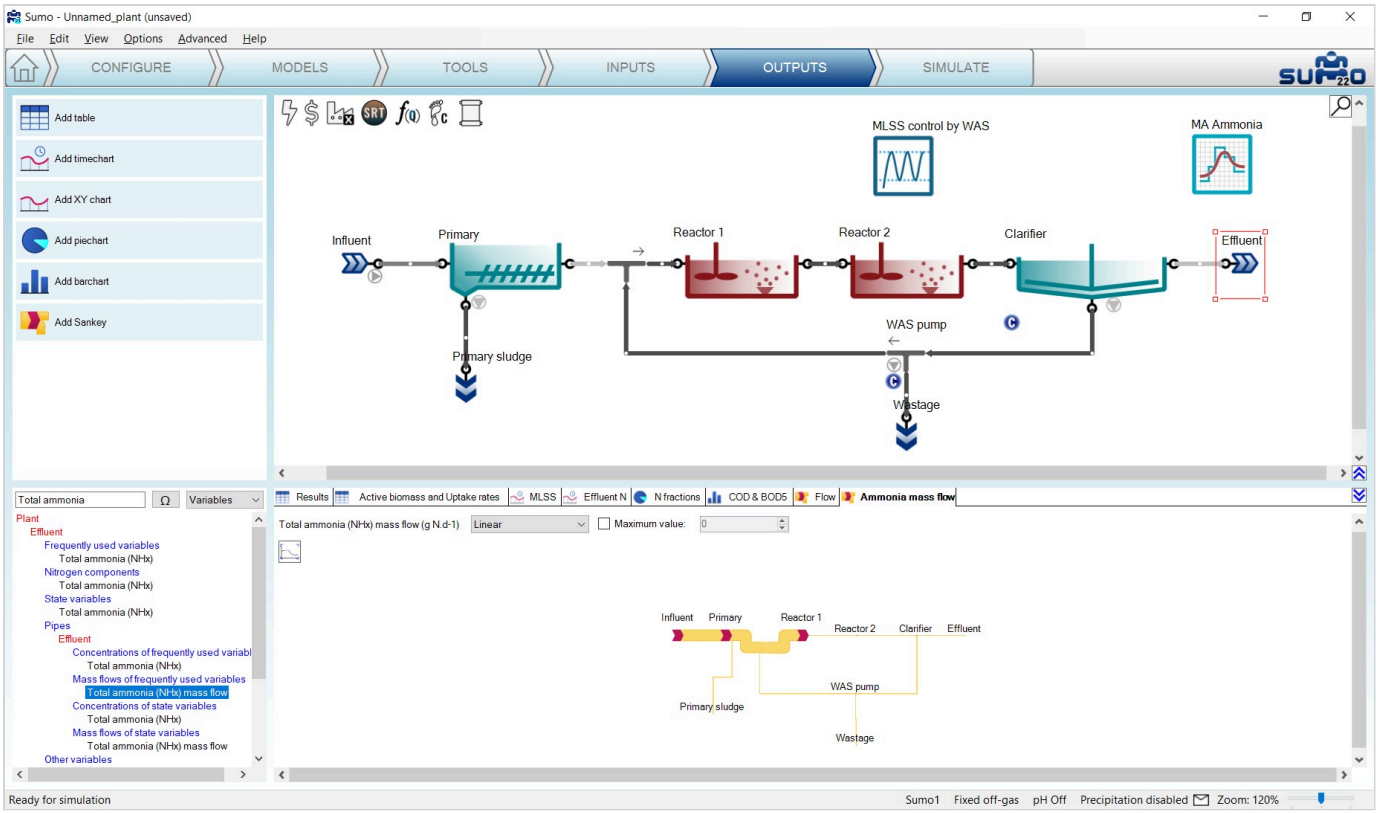


Figure 3.32 - Adding a Sankey diagram

At this point, the example is prepared for simulation with all the inputs and outputs provided. If desired, the output tabs can be reordered by dragging them to the aimed sequence. The file can be saved using the *File* menu (this function is not available in the demo version).

Simulate

The last item on the Task Bar can be used to run simulations and observe the results.

The role of screen panels in *Simulate* mode are the following:

Top right panel	Plant configuration
Top left panel	Simulation control panel Different function buttons for the simulation, including report preparation in Excel format.
Bottom right panel	Tabs for the previously defined outputs Display of results.

Bottom left panel	Tabs for scenario definition

Simulation Control Panel

The top left screen panel enables operating the model, to run dynamic or steady-state simulations (as well as algebraic calculations, when being in design mode). *Steady* mode can be used to calculate directly the steady-state condition of the variables, whereas *Dynamic* mode will show the variations with time.

Steady mode

In systems theory, a system or a process is in a steady state if the variables which describe the behavior of the system or the process do not change with time. If a system is in steady state, then the recently observed behavior of the system will continue into the future.

After setting up the plant, all process units get a predefined initial value for each state variable (taken from the model defaults). However, most often this will not equal the values that can be observed in steady-state condition. The steady-state calculation will find the proper state variable values when the system is in steady state.

The steady-state simulation employs different solvers to look for the steady-state condition of the system. In this mode, all dynamic inputs are disabled and the controllers are turned into integrated controllers. Please note that steady-state simulation cannot be performed on inherently dynamic processes such as the SBR.

The roles of the control panel buttons on the *Steady* tab (Figure 3.33) are the following:

Calculate Steady-state	Start steady-state simulation from current system state
Interrupt calculation	Interrupt simulation (or resume a previously interrupted one)
Reset	Reset the system to default initial conditions
Save plant conditions	Save actual conditions to a Sumo System State file
Load plant conditions	Load previously saved conditions from a Sumo System State file
Report	Generate a report in Excel format

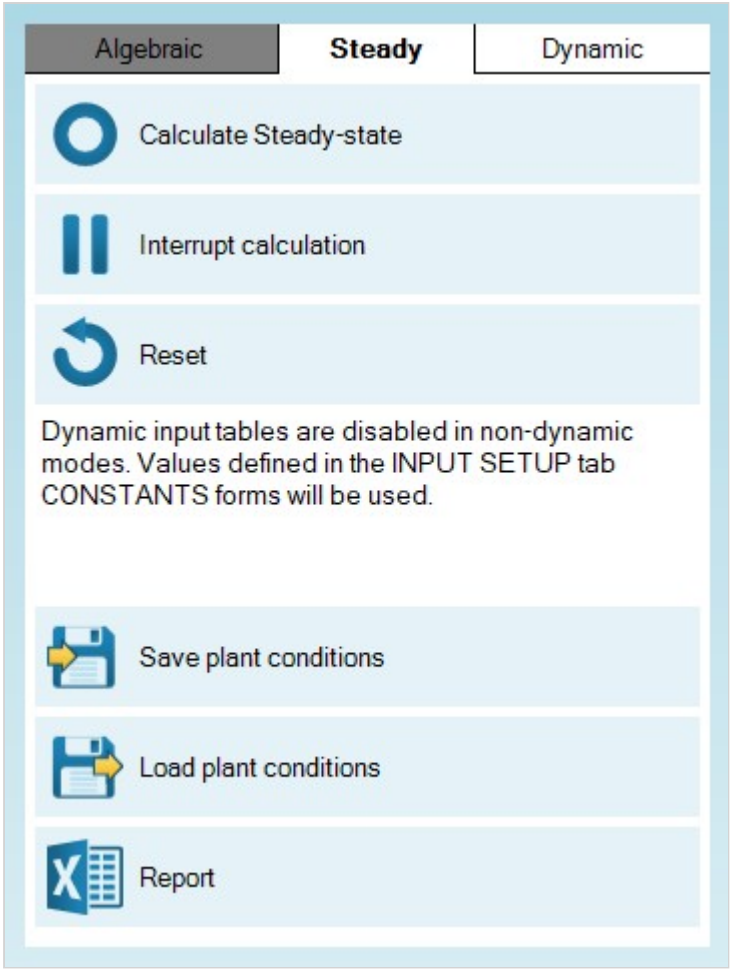


Figure 3.33 - The “Steady” control panel

One should use the *Reset* button thoughtfully, especially when working with complex plants, for it will reinitiate the simulation with the default concentrations defined in the model and process units, and reaching steady-state again might be time-consuming in these cases. Saving plant conditions (especially if steady-state has been found) can be useful to restore system state in case the simulation is driven into an unwanted condition (e.g. accidentally having been reset).

Dynamic mode

Dynamic simulation will follow changes within the system as time passes, starting from the actual state of the system, and applying all dynamic inputs and behaviors that were defined during the setup process.

The roles of the control panel buttons on the *Dynamic* tab (Figure 3.34) are the following:

Start	Start a simulation from actual conditions
Steady-state start	Start a simulation from steady-state
Fast / Accurate	Choose between Fast and Accurate modes

Reset	Reset default conditions
Continue	Continue/Pause simulation
Stop time	Length of dynamic run
Data interval	Data plotting/updating interval
Save plant conditions	Save actual conditions to a Sumo System State file
Load plant conditions	Load previously saved conditions from a Sumo System State file
Report	Generate a report in Excel format

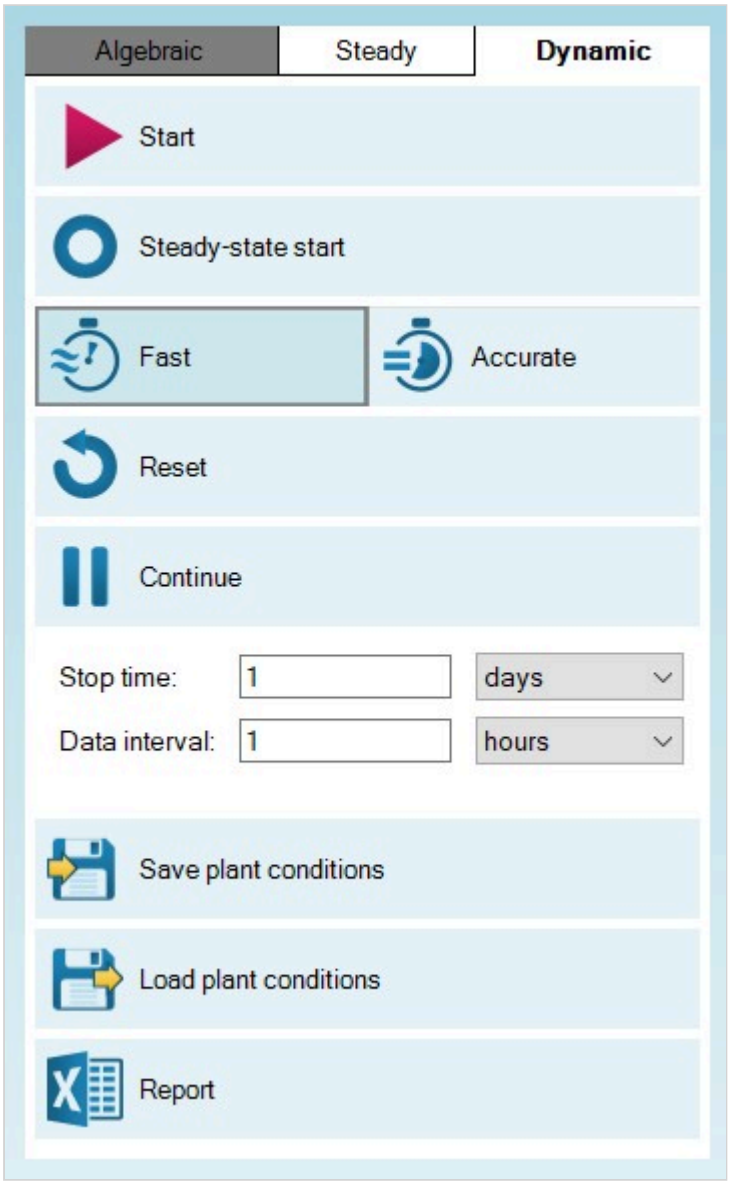


Figure 3.34 - The “Dynamic” control panel

Dynamic simulation can be started by pressing the *Start* button. Upon first start, the simulation will be run from the initial conditions (defaults specified in the model file and in the process units). Every subsequent run will

be initiated with the last system state. Pressing the *Steady-state start* button will run a steady-state simulation prior to starting the dynamic one (so that steady-state will be used as the initial condition). The role of the *Reset* button is the same as it is in the *Steady* mode – use it only if the goal is to restart the simulation process entirely from scratch.

The dynamic simulation will run until the end of the period defined by *Stop time* is reached (default setting: 1 day) and will plot/update results in the bottom right screen panel with the frequency described by the *Data interval* (default setting: 1 hour). The *Stop time* and *Data interval* can be modified before the simulation is started, or also when it is paused.

Choosing between *Fast* and *Accurate* modes translates to using different pre-configured solver settings. The differences between the two are described in Table 3.5. Usually the *Fast* mode is fast and accurate enough for most cases, and therefore its use is generally recommended. However, in certain situations (e.g. with biofilm models), the *Accurate* mode might provide faster simulation. If the plant seems to be complex and takes a long time to find a solution in *Fast* mode, then try switching over to *Accurate*. In such rare cases, it is the trial-and-error of coming to solver settings that lead to a speedy solution.

Table 3.5 – Explanation of Fast and Accurate solver settings

	Fast	**Accurate**
Type of configuration	Simple plant layouts will provide a speedy simulation	Best for complex plant layouts, specifically which have biofilm processes (MBBRs, and trickling filters) and several return or recycle streams.
Solver types	GISA → Relaxation solver → Newton-Raphson	Relaxation solver → Newton-Raphson

Note that the mode selection will also have effect on the steady-state solver: GISA introduces a strong perturbance to the system state, therefore it is quite suitable for finding steady-state from a distant initial system state, while not so necessary when the system is already close to steady-state. There is no difference however in the stop criteria for the solvers.

A process simulation example – aerobic plant

The plant configuration we have just built is an aerobic plant, with 12-hour hydraulic residence time:

$$HRT = \frac{10000\ m^3\ volume}{20000\ m^3/d\ influent} \times 24 \frac{h}{d}$$

A 10-day MLSS graph gives a good indication whether the system has settled into stable condition and the results are meaningful for typical dry weather summer operation, so let us start by setting the stop time to 10 days with 1-hour data interval and running a dynamic simulation. MLSS and effluent N plots are presented by Figure 3.35 and Figure 3.36, respectively. The effect of the MLSS control strategy can be observed as well.

In the bottom left screen panel rename the *Default scenario* to *Summer* (in order to differentiate from an another scenario that will be added later on).

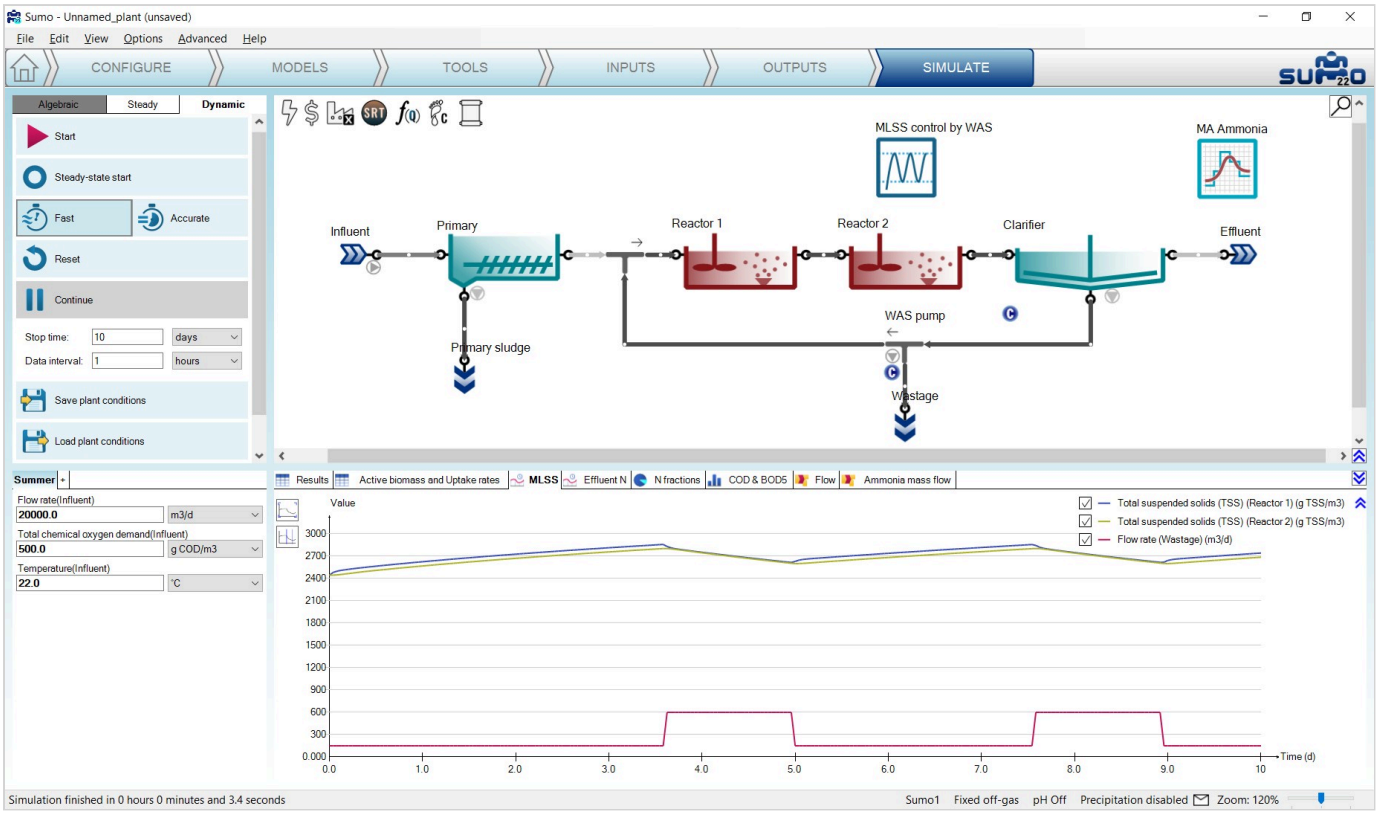


Figure 3.35 - Simulation results of the example plant with MLSS control

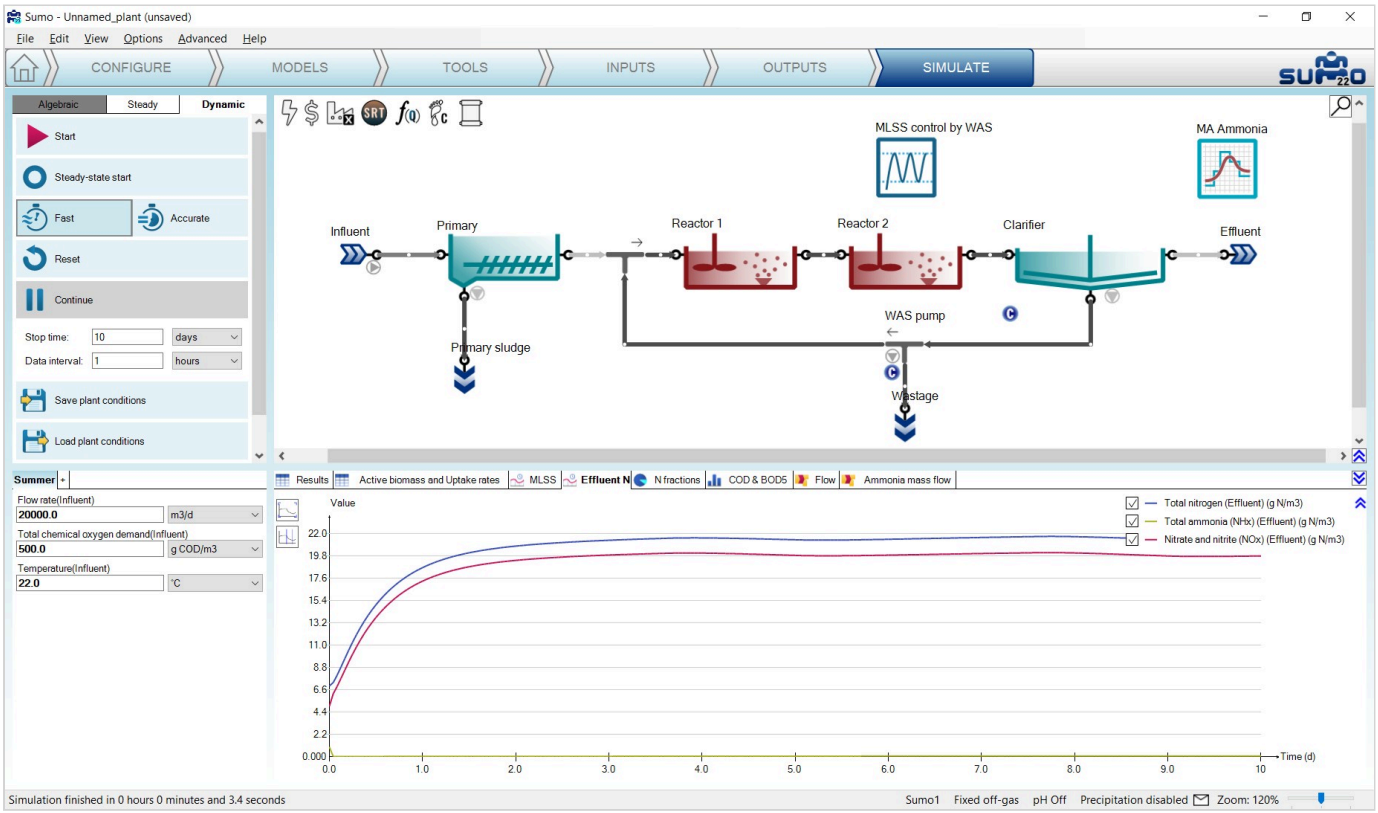


Figure 3.36 - Effluent total nitrogen, ammonia and nitrate at nitrification plant

The tabular results are shown in Figure 3.37 and Figure 3.38.

Results | Active biomass and Uptake rates | MLSS | Effluent N | N fractions | COD & BOD5 | Flow | Ammonia mass flow

Name	Influent	Reactor 1	Reactor 2	Effluent	Unit
Flow rate	20000	39327	39327	19327	m3/d
Total chemical oxygen demand	500	3084	3000	36	g COD/m3
Total suspended solids (TSS)	218	2740	2684	10	g TSS/m3
Volatile suspended solids (VSS)	185	2224	2172	8.1	g VSS/m3
VSS/TSS ratio	0.85	0.81	0.81	0.81	g VSS.g TSS-1
Total biochemical oxygen demand (5 days)	218	604	567	2.8	g O2/m3
Total nitrogen	34.40	150.48	148.13	21.44	g N/m3
Total ammonia (NHx)	24.00	2.14	0.11	0.11	g N/m3
Nitrate and nitrite (NOx)	Non-detect	16.96	19.80	19.80	g N/m3
Total phosphorus	4.30	54.49	54.60	3.24	g P/m3
Orthophosphate (PO4)	2.50	2.24	2.97	2.97	g P/m3
Dissolved oxygen (O2)	Non-detect	2.00	2.00	2.00	g O2/m3
Oxygen gas (O2) off-gas concentration in v/v%		18.8	18.8		%

Figure 3.37 - Tabular presentation of simulation results

Results | Active biomass and Uptake rates | MLSS | Effluent N | N fractions | COD & BOD5 | Flow | Ammonia mass flow

Name	Reactor 1	Reactor 2	Unit
Ordinary heterotrophic organisms (OHO)	1037.4	1008.1	g COD/m3
Carbon storing organisms (CASTO)	97.4	98.0	g COD/m3
PAO (Phosphorus accumulating organisms) fraction of CASTO	17.7	17.6	g COD/m3
GAO (Glycogen accumulating organisms) fraction of CASTO	79.7	80.4	g COD/m3
Anoxic methanol utilizers (MEOLO)	0.71	0.70	g COD/m3
Aerobic nitrifying organisms (NITO)	54.0	53.0	g COD/m3
Acidoclastic methanogens (AMETO)	0.22	0.21	g COD/m3
Hydrogenotrophic methanogens (HMETO)	0.071	0.055	g COD/m3
Oxygen uptake rate (OUR)	55.5	15.8	mg O2/L/h
Carbonaceous oxygen uptake rate (COUR)	27.5	10.9	mg O2/L/h
Nitrification oxygen uptake rate (NOUR)	28.0	4.9	mg O2/L/h
Nitrate uptake rate (N3UR)	0.77	0.53	mg N/L/h
Ammonia uptake rate (AUR)	10.5	2.8	mg N/L/h
Phosphorus uptake rate (PUR)	1.2	0.47	mg P/L/h

Figure 3.38 - Tabular presentation of simulation results

These tables show:

- TSS and VSS profile from the influent through the reactors to the effluent;

- High effluent nitrate and low effluent ammonia (full nitrification);
- DO of 2 mg/L in both reactors (due to input settings);
- Oxygen Uptake Rate (OUR) in the two reactors: higher in the first one, lower in the second, as expected.

This fully aerobic plant does nitrify completely, producing low ammonia and high nitrate concentrations in the effluent. Both reactors are aerated to 2 mg/L DO, which requires energy and comes with costs.

Implementing denitrification

In the system above, the main electron acceptor for biochemical reactions is dissolved oxygen. We can use the abundant nitrate as electron acceptor, and with this process reduce our energy requirement and improve the effluent quality at the same time. For this, we need to reconfigure the plant – in this case simply creating an anoxic zone by switching off the aeration in Reactor 1. (In the actual plant, mixers would need to be installed in the anoxic zone to keep the MLSS in suspension, but in the model, the reactors are always ideally mixed.)

To implement this change, select *Inputs* on the Task Bar, switch to *Constants* mode, select Reactor 1 and select the *Aeration settings* item from the *Input parameters* (bottom left panel), then change the DO setpoint to zero in the bottom right panel (Figure 3.39).

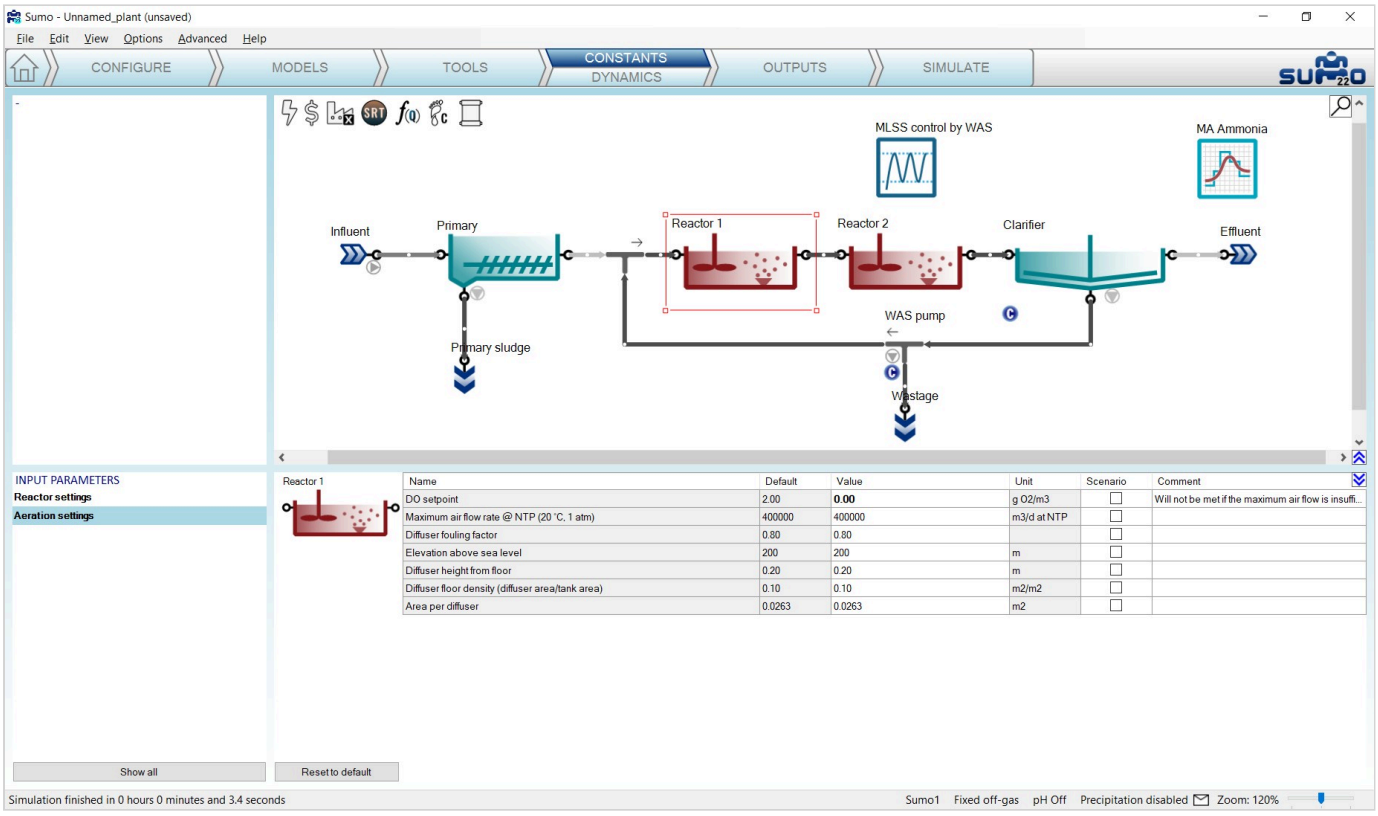


Figure 3.39 - Modifying DO setpoint in 'Reactor1'

Go back to the *Simulate* tab, set the *Stop time* to 20 day and click *Continue* to go on with the simulation while keeping the results of the previous 10 days in the graphs. Note that the color of the first tank will change to grey: this feature serves for easier visual identification of anoxic/anaerobic reactors. The effluent nitrate will be reduced because it is used up to oxidize organic material in Reactor 1 (the anoxic zone). On the contrary,

effluent ammonia increases slightly as nitrification requires aerobic conditions and the aerobic reactor volume was reduced from 10000 m^3 to 8000 m^3. The effect of the DO setpoint change in the Reactor 1 can be followed in Figure 3.40. The drop in effluent nitrate concentration after 10 days is a due to the Reactor 1 having been turned anoxic. The time frame of the change can be followed as well: within 24 hours the nitrate concentration drops to the lower value.

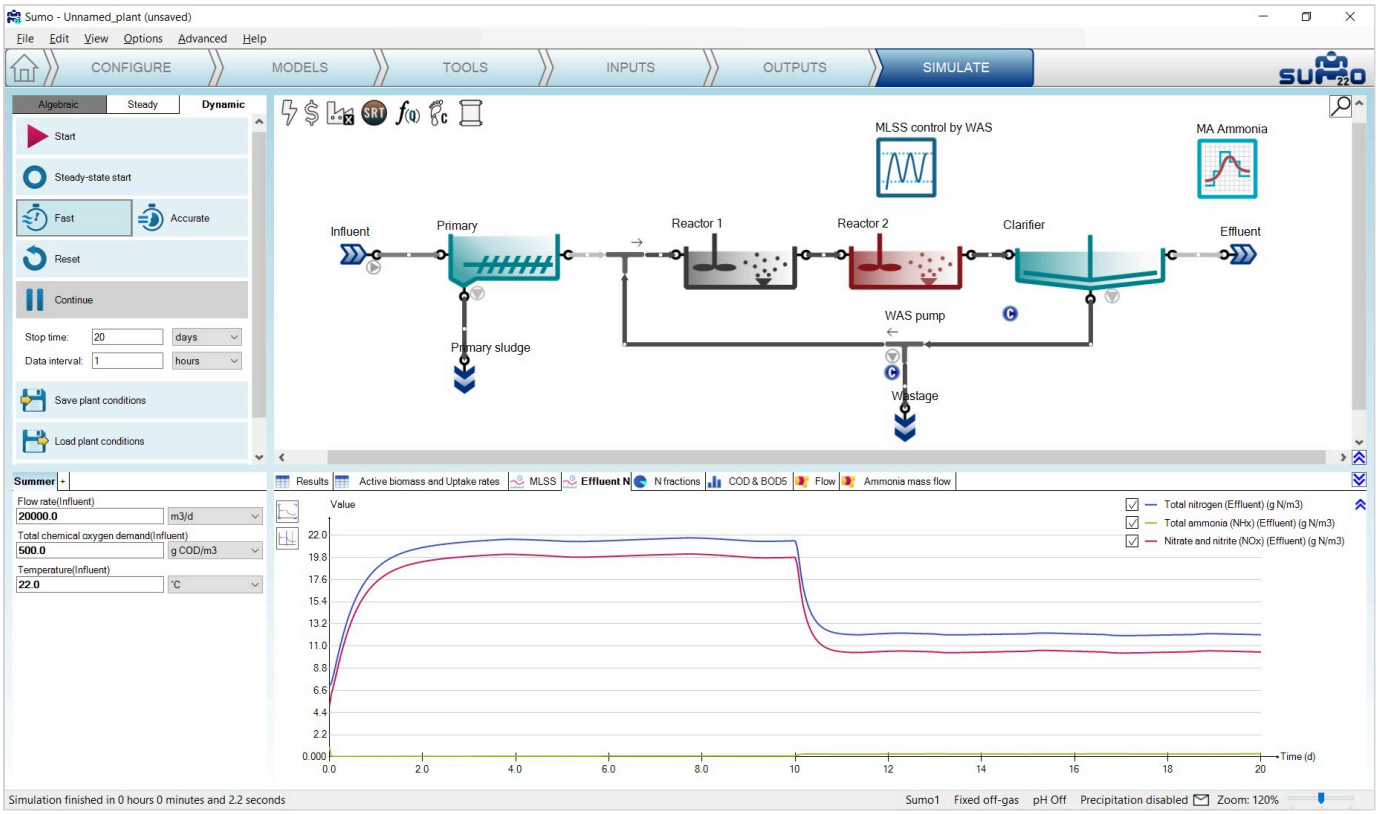
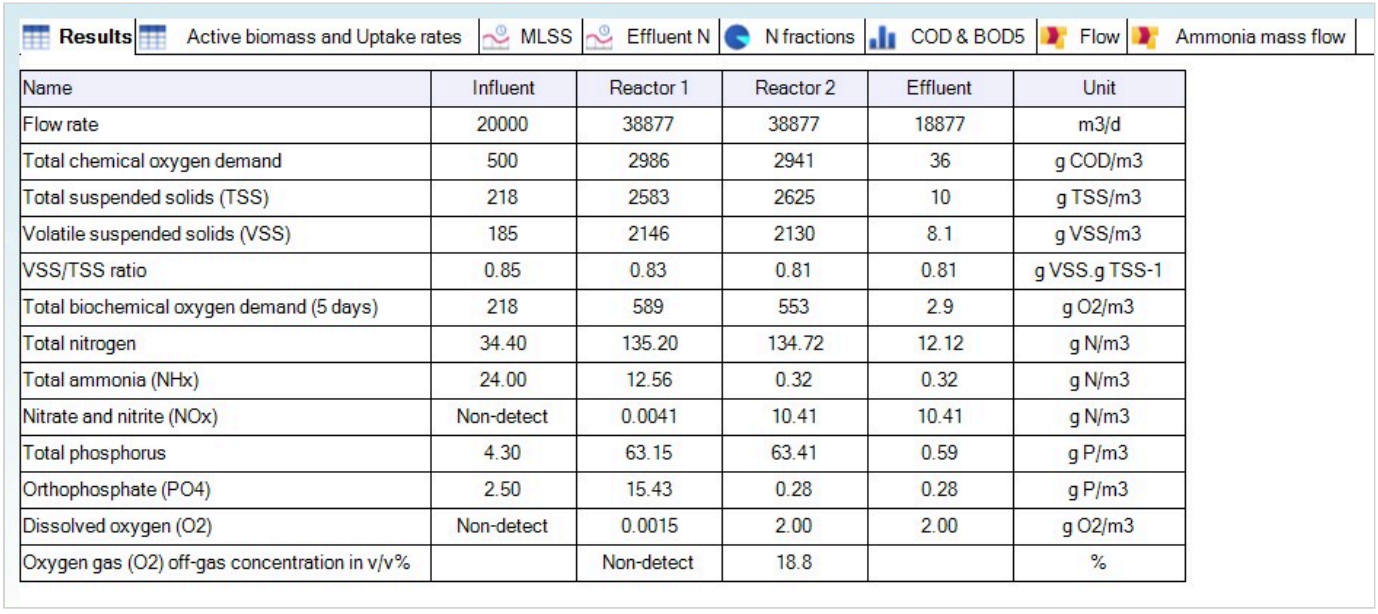


Figure 3.40 - Effluent ammonia and nitrate with denitrification



Results | Active biomass and Uptake rates | MLSS | Effluent N | N fractions | COD & BOD5 | Flow | Ammonia mass flow

Name	Influent	Reactor 1	Reactor 2	Effluent	Unit
Flow rate	20000	38877	38877	18877	m3/d
Total chemical oxygen demand	500	2986	2941	36	g COD/m3
Total suspended solids (TSS)	218	2583	2625	10	g TSS/m3
Volatile suspended solids (VSS)	185	2146	2130	8.1	g VSS/m3
VSS/TSS ratio	0.85	0.83	0.81	0.81	g VSS.g TSS-1
Total biochemical oxygen demand (5 days)	218	589	553	2.9	g O2/m3
Total nitrogen	34.40	135.20	134.72	12.12	g N/m3
Total ammonia (NHx)	24.00	12.56	0.32	0.32	g N/m3
Nitrate and nitrite (NOx)	Non-detect	0.0041	10.41	10.41	g N/m3
Total phosphorus	4.30	63.15	63.41	0.59	g P/m3
Orthophosphate (PO4)	2.50	15.43	0.28	0.28	g P/m3
Dissolved oxygen (O2)	Non-detect	0.0015	2.00	2.00	g O2/m3
Oxygen gas (O2) off-gas concentration in v/v%		Non-detect	18.8		%

Figure 3.41 - Tabular presentation of simulation results with a denitrifying plant

Results | **Active biomass and Uptake rates** | MLSS | Effluent N | N fractions | COD & BOD5 | Flow | Ammonia mass flow

Name	Reactor 1	Reactor 2	Unit
Ordinary heterotrophic organisms (OHO)	814.1	821.9	g COD/m3
Carbon storing organisms (CASTO)	243.9	251.5	g COD/m3
PAO (Phosphorus accumulating organisms) fraction of CASTO	215.4	221.3	g COD/m3
GAO (Glycogen accumulating organisms) fraction of CASTO	28.6	30.2	g COD/m3
Anoxic methanol utilizers (MEOLO)	0.65	0.65	g COD/m3
Aerobic nitrifying organisms (NITO)	48.6	50.2	g COD/m3
Acidoclastic methanogens (AMETO)	0.25	0.24	g COD/m3
Hydrogenotrophic methanogens (HMETO)	0.11	0.088	g COD/m3
Oxygen uptake rate (OUR)	1.4	24.3	mg O2/L/h
Carbonaceous oxygen uptake rate (COUR)	1.2	13.5	mg O2/L/h
Nitrification oxygen uptake rate (NOUR)	0.22	10.8	mg O2/L/h
Nitrate uptake rate (N3UR)	4.3	0.39	mg N/L/h
Ammonia uptake rate (AUR)	1.2	4.3	mg N/L/h
Phosphorus uptake rate (PUR)	2.0	3.6	mg P/L/h

Figure 3.42 - Tabular presentation of simulation results with a denitrifying plant

Besides calculating air flow from a defined input DO, Sumo also offers the possibility to calculate DO levels based on specified input air flow. To select this model option, go back to the *Configure* tab and select Reactor 1, then in the *Dissolved oxygen* process unit option, switch from *Input* to *Calculated* (Figure 3.43). The calculated DO option will provide a better estimate of expected effluent values. In an aerobic reactor, instead of DO setpoint, the air flow is defined in the *Inputs*, and the concentration of the DO is calculated based on a mass transfer model. In anoxic (and anaerobic) reactors, with zero airflow specified, only the DO introduced by their input flow is considered.

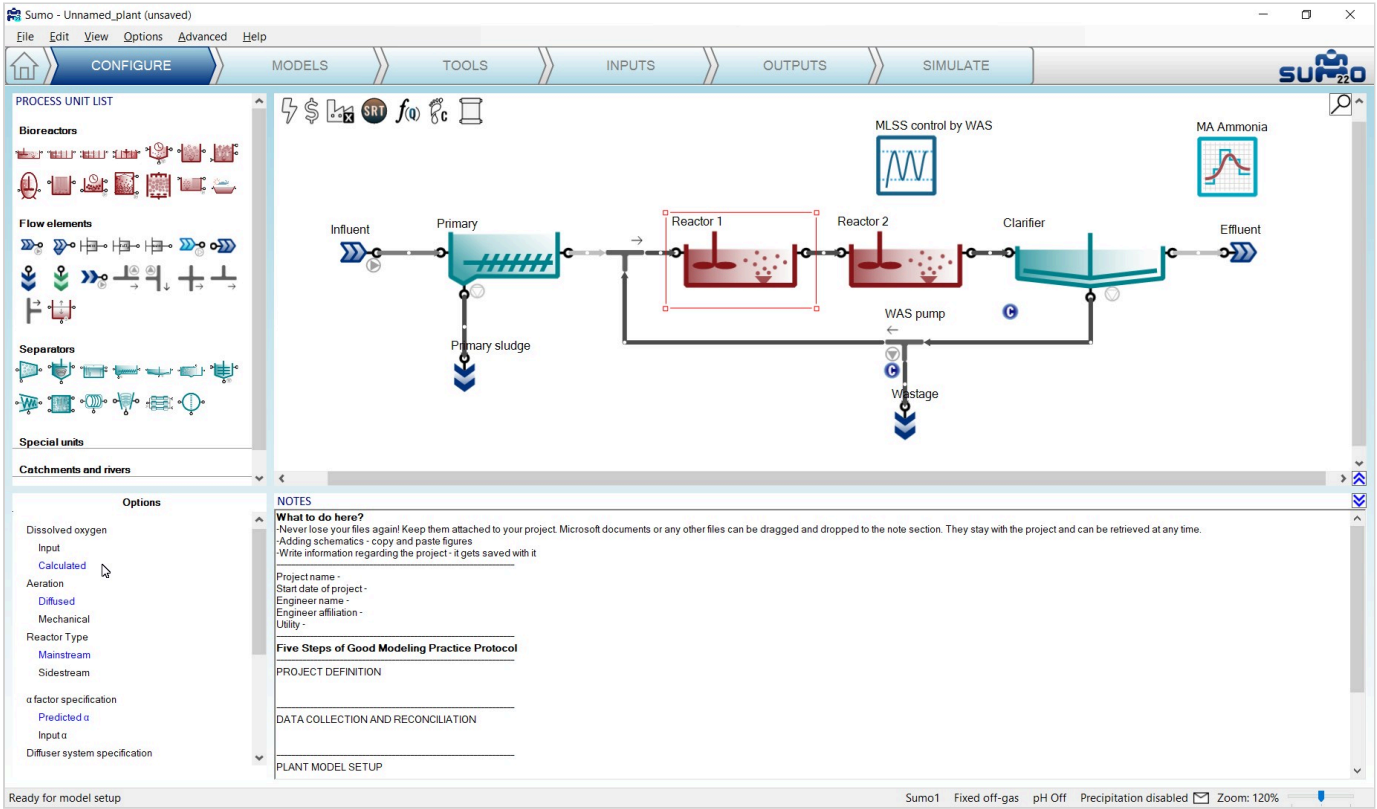
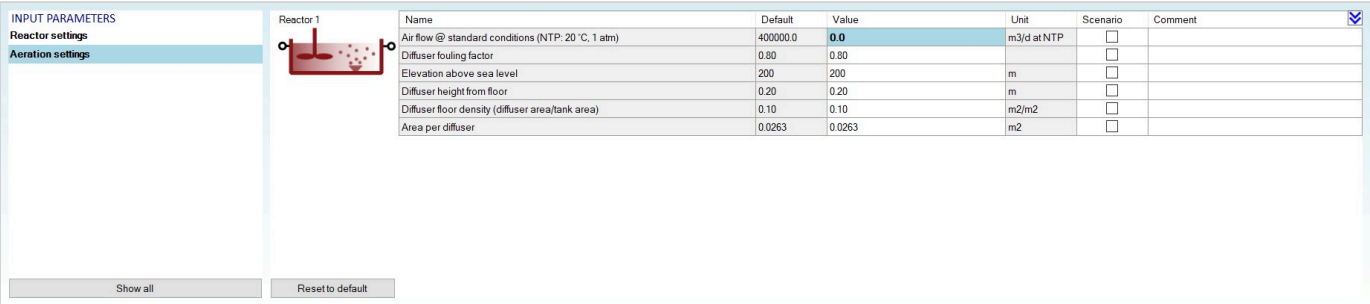


Figure 3.43 - Switching to “calculated DO” process unit option

The air flow can be provided on the *Inputs* tab. Let us change the blower airflow of Reactor 1 to 0 (Figure 3.44):



Name	Default	Value	Unit	Scenario	Comment
Air flow @ standard conditions (NTP: 20 °C, 1 atm)	400000.0	**0.0**	m3/d at NTP	☐	
Diffuser fouling factor	0.80	0.80		☐	
Elevation above sea level	200	200	m	☐	
Diffuser height from floor	0.20	0.20	m	☐	
Diffuser floor density (diffuser area/tank area)	0.10	0.10	m2/m2	☐	
Area per diffuser	0.0263	0.0263	m2	☐	

Figure 3.44 - Changing air flow in ‘Reactor 1’

After clicking on Reset, then running a 20-day simulation, you can compare the results of the plant operating with input DO (Figure 3.40, Figure 3.41 and Figure 3.42) and the plant operating with calculated DO (Figure 3.45, Figure 3.46 and Figure 3.47):

Results | Active biomass and Uptake rates | MLSS | Effluent N | N fractions | COD & BOD5 | Flow | Ammonia mass flow

Name	Influent	Reactor 1	Reactor 2	Effluent	Unit
Flow rate	20000	39327	39327	19327	m3/d
Total chemical oxygen demand	500	3054	2958	36	g COD/m3
Total suspended solids (TSS)	218	2711	2711	10	g TSS/m3
Volatile suspended solids (VSS)	185	2195	2140	7.9	g VSS/m3
VSS/TSS ratio	0.85	0.81	0.79	0.79	g VSS.g TSS-1
Total biochemical oxygen demand (5 days)	218	648	604	3.0	g O2/m3
Total nitrogen	34.40	140.52	137.93	12.04	g N/m3
Total ammonia (NHx)	24.00	12.43	0.31	0.31	g N/m3
Nitrate and nitrite (NOx)	Non-detect	0.0042	10.39	10.39	g N/m3
Total phosphorus	4.30	87.27	86.58	0.67	g P/m3
Orthophosphate (PO4)	2.50	17.02	0.29	0.29	g P/m3
Dissolved oxygen (O2)	Non-detect	0.0015	2.00	2.00	g O2/m3
Oxygen gas (O2) off-gas concentration in v/v%		Non-detect	18.8		%

Figure 3.45 - Tabular presentation of simulation results with a denitrifying plant with calculated DO

Results | Active biomass and Uptake rates | MLSS | Effluent N | N fractions | COD & BOD5 | Flow | Ammonia mass flow

Name	Reactor 1	Reactor 2	Unit
Ordinary heterotrophic organisms (OHO)	839.0	832.0	g COD/m3
Carbon storing organisms (CASTO)	344.3	347.5	g COD/m3
PAO (Phosphorus accumulating organisms) fraction of CASTO	305.4	307.0	g COD/m3
GAO (Glycogen accumulating organisms) fraction of CASTO	39.0	40.5	g COD/m3
Anoxic methanol utilizers (MEOLO)	0.69	0.68	g COD/m3
Aerobic nitrifying organisms (NITO)	51.1	51.8	g COD/m3
Acidoclastic methanogens (AMETO)	0.26	0.24	g COD/m3
Hydrogenotrophic methanogens (HMETO)	0.12	0.092	g COD/m3
Oxygen uptake rate (OUR)	1.4	24.8	mg O2/L/h
Carbonaceous oxygen uptake rate (COUR)	1.2	13.8	mg O2/L/h
Nitrification oxygen uptake rate (NOUR)	0.23	10.9	mg O2/L/h
Nitrate uptake rate (N3UR)	4.3	0.40	mg N/L/h
Ammonia uptake rate (AUR)	1.2	4.4	mg N/L/h
Phosphorus uptake rate (PUR)	1.7	4.0	mg P/L/h

Figure 3.46 - Tabular presentation of simulation results with a denitrifying plant with calculated DO

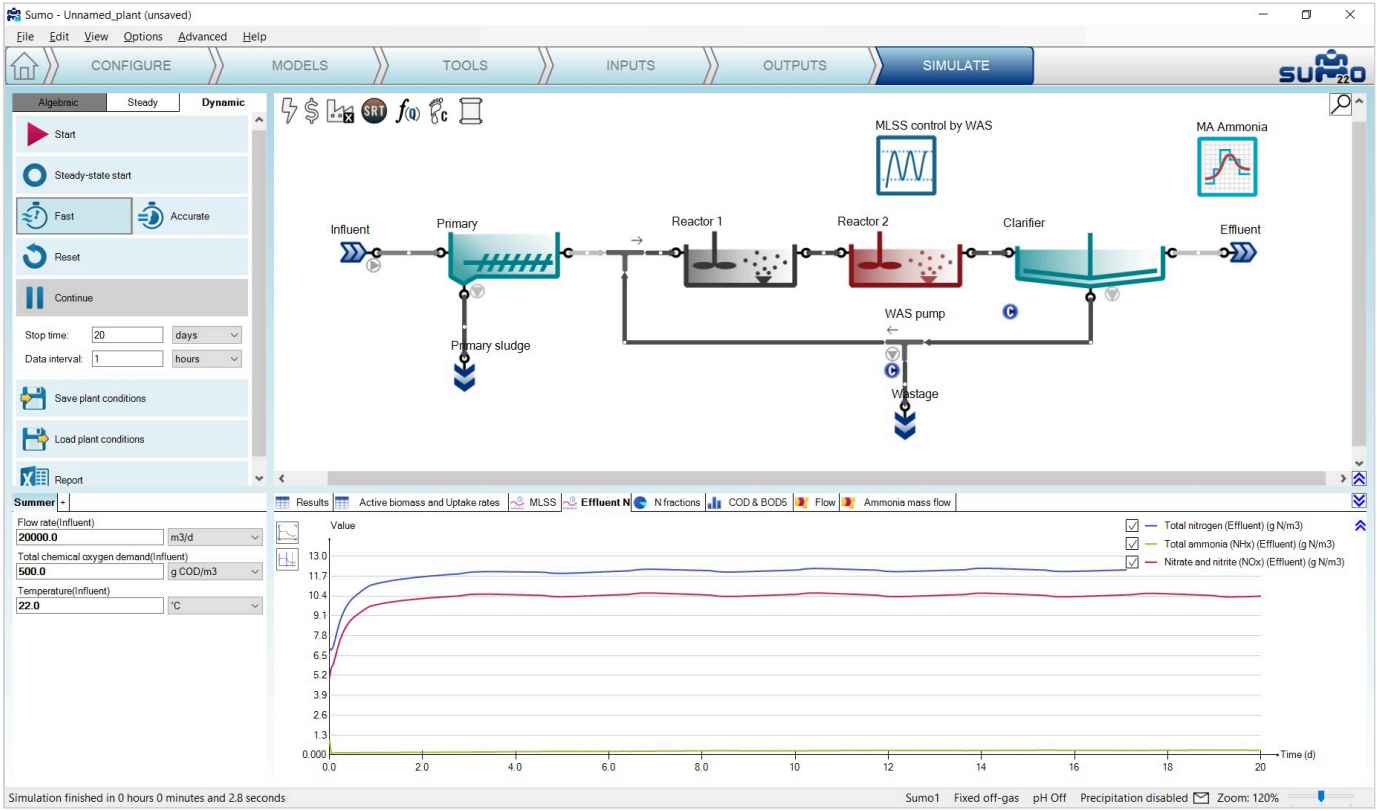


Figure 3.47 - Effluent ammonia and nitrate with calculated DO

Subjecting the plant to dynamics

Plants are usually subjected to diurnal variation and we might be interested not only in the average, but the peak effluent concentrations as well (e.g. in certain jurisdictions the effluent limits are based on grab samples

never to exceed, daily maximum, etc.). This requires a dynamic simulation to investigate potential peaks during the day.

Select the *Inputs* tab, and the Influent process unit, where we will provide diurnal flow variation. In *Constants* mode, the *Influent tool* is available for Sumo models as an Excel file, containing typical fractions and diurnal variations with different plant sizes. Click on the button (located in the bottom right screen panel) to open this tool and copy the “medium plant” table from the *Diurnal flow* sheet to the clipboard (Figure 3.48):

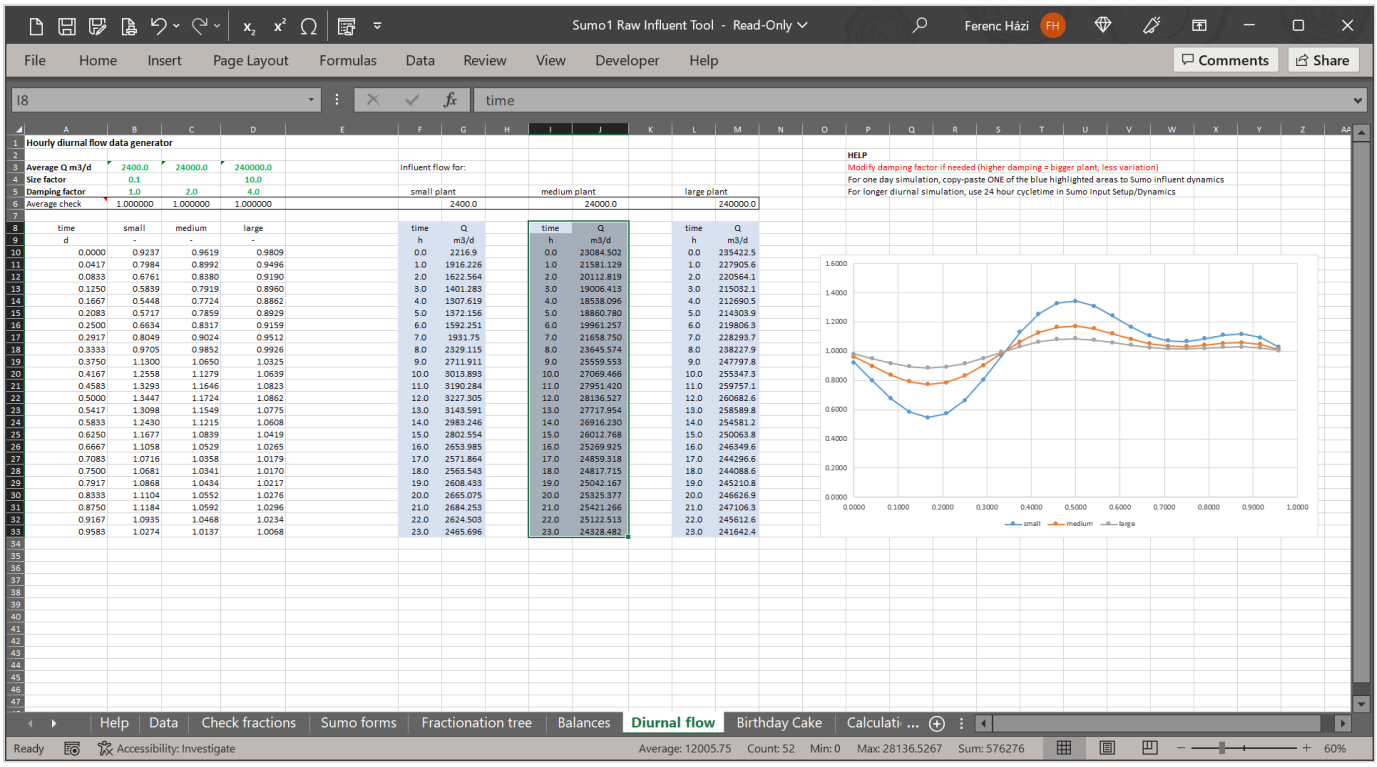


Figure 3.48 - Sumo1 Influent tool

Now switch to *Dynamics* mode in Sumo and paste your table by clicking on the *Paste table form clipboard* button (after this, you can close the *Influent tool* Excel file). On the drawing board, a small sign will appear below the Influent, showing that dynamic parameter input is used. These tables can be disabled/enabled or deleted by right-clicking on the name in the bottom left screen panel. Note that for a certain variable/parameter, only one dynamic table can remain enabled (Sumo will give you a warning if more than one tables are enabled for the same subject). The names of disabled tables (which are editable in the bottom right screen panel) will show up in grey, and in case all dynamic input tables are disabled, the sign beside the process unit will also turn to grey (indicating that there are dynamic inputs available, but not used). Linear interpolation and cycle repeat can also be set for dynamic input tables. Rename the newly inserted dynamic input table in the example to “Diurnal flow”, check the box to repeat the contents of the table and provide the repeat frequency as 24 hours in this example, as depicted on Figure 3.49.

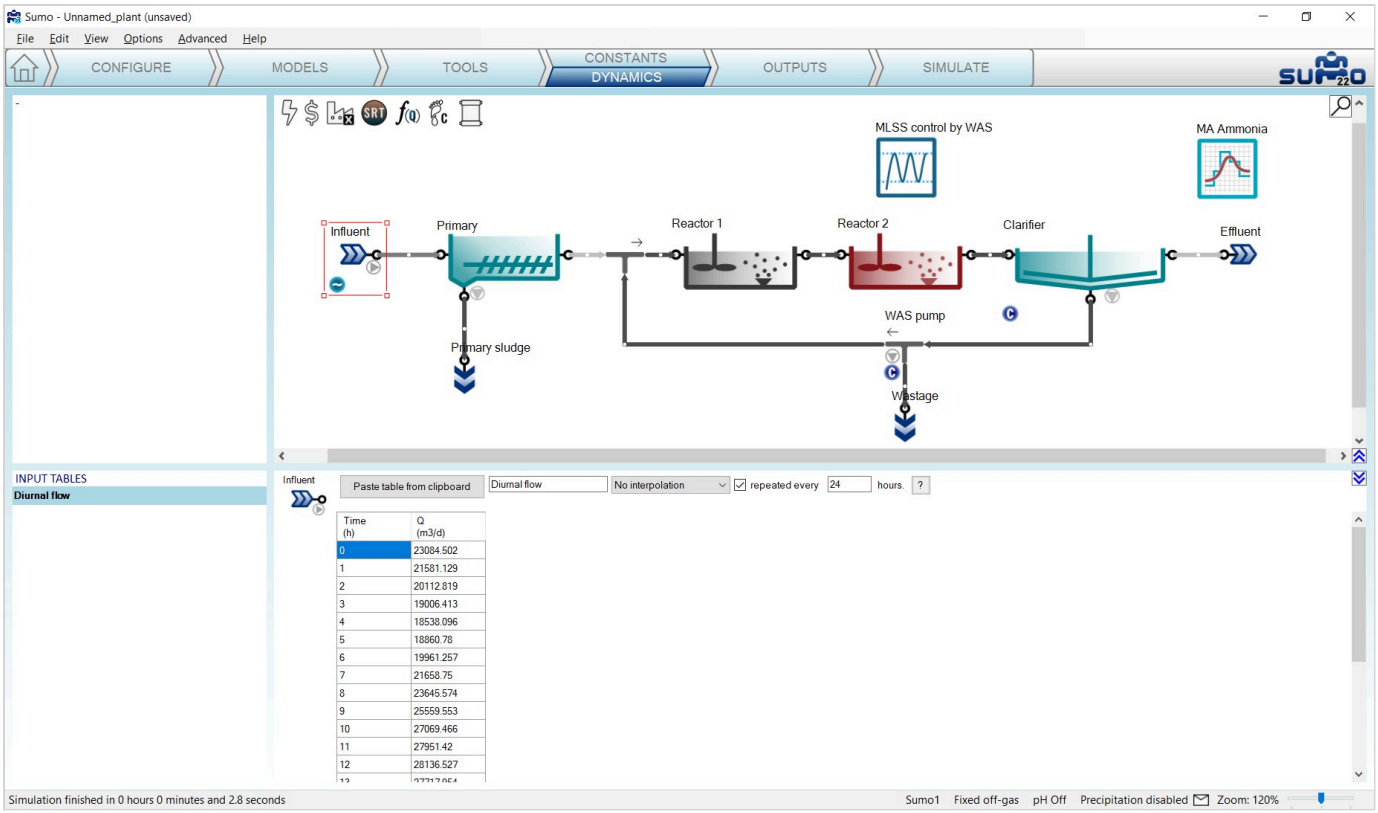


Figure 3.49 - Configuring dynamic input

If you can provide data from measurement, your input data (flow variation in this case) should be in Excel, in the following format: the header should be “Time” (“time” is also accepted) and the selected variable name as it is used by Sumo, in this case “Q” (denoting flow), with the respective units (“h” and “m3/d”) in the second row, as illustrated by Table 3.6.

Table 3.6 – Dynamic input of influent flow pattern

time	Q
h	m3/d
0.0	23084.502
1.0	21581.129
2.0	20112.819
3.0	19006.413
4.0	18538.096
5.0	18860.780
6.0	19961.257

time	Q
7.0	21658.750
8.0	23645.574
9.0	25559.553
10.0	27069.466
11.0	27951.420
12.0	28136.527
13.0	27717.954
14.0	26916.230
15.0	26012.768
16.0	25269.925
17.0	24859.318
18.0	24817.715
19.0	25042.167
20.0	25325.377
21.0	25421.266
22.0	25122.513
23.0	24328.482

To find out what is the internal identifier for a certain variable (or model parameter), you can just hover the mouse above the name of the specific item in the parameter tables of *Inputs – Constants* (or in the case of model parameters, the *Models*), and a popup will show you the cryptic name of your input variable that has to be used in the dynamic table (see Figure 3.50). For your comfort, right-clicking here offers an option to copy this symbol directly to the clipboard (and the same goes for units), from where you can paste it into your table.

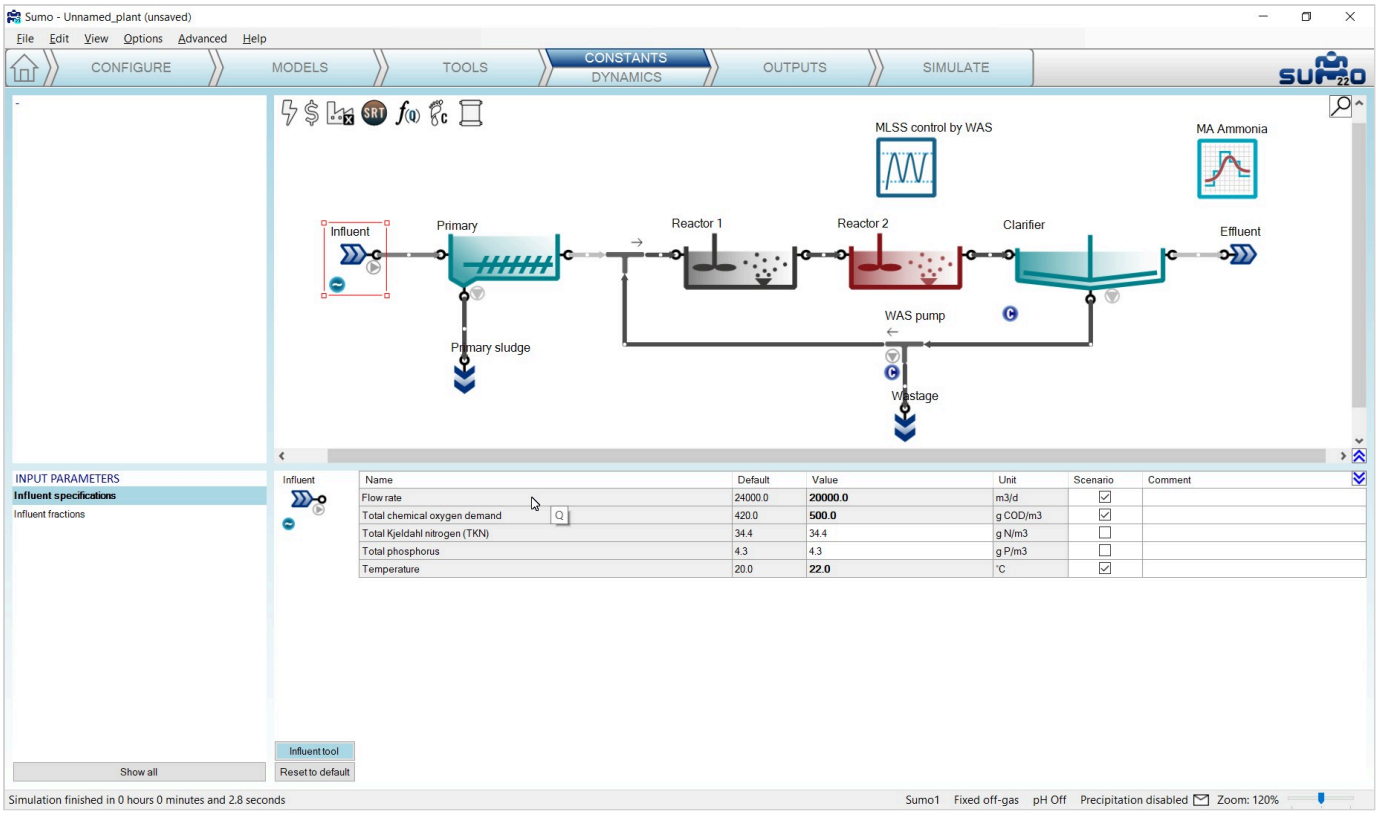


Figure 3.50 – Variable name pop-up message at the Input setup

Having set up the diurnal flow, go to the *Simulate* tab and start a new dynamic simulation of 5 days duration: In this case, the result of the last simulation will be used as initial values. The variation in loading should have an effect on effluent quality, as shown by Figure 3.51.

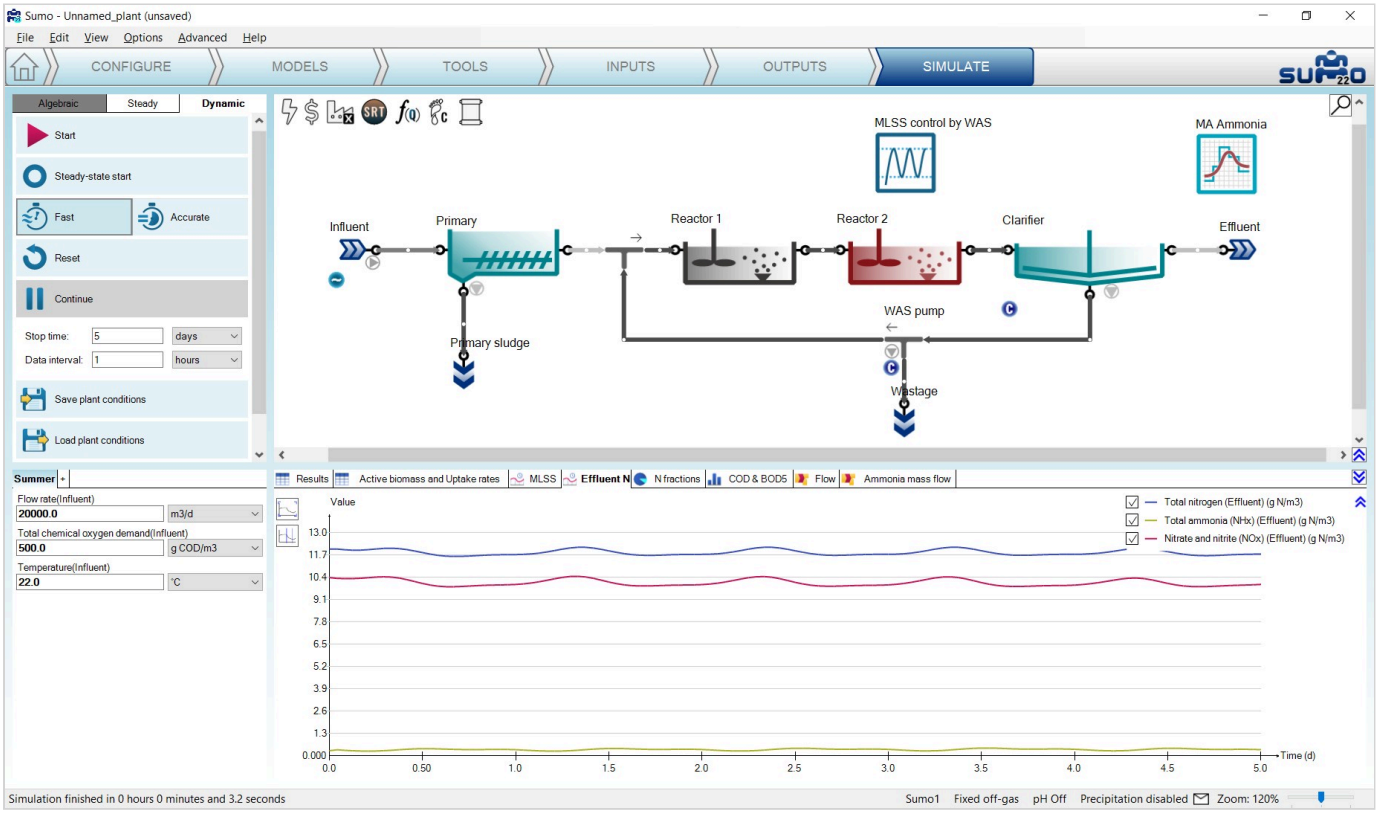


Figure 3.51 - Effluent ammonia and nitrate variation with changing influent flow

We can observe higher ammonia concentrations during the high loaded periods, and lower nitrate concentrations, due to lower nitrification and the abundance of organic substrate for denitrification.

We can of course always turn on our aerators in the first reactor (not so easy in an actual plant) by going to the *Inputs* tab, selecting Reactor 1 and changing the air flow to 150000 Nm^3/d. In the *Simulate* tab, we can extend the length of the run for 10 days and hit *Continue*.

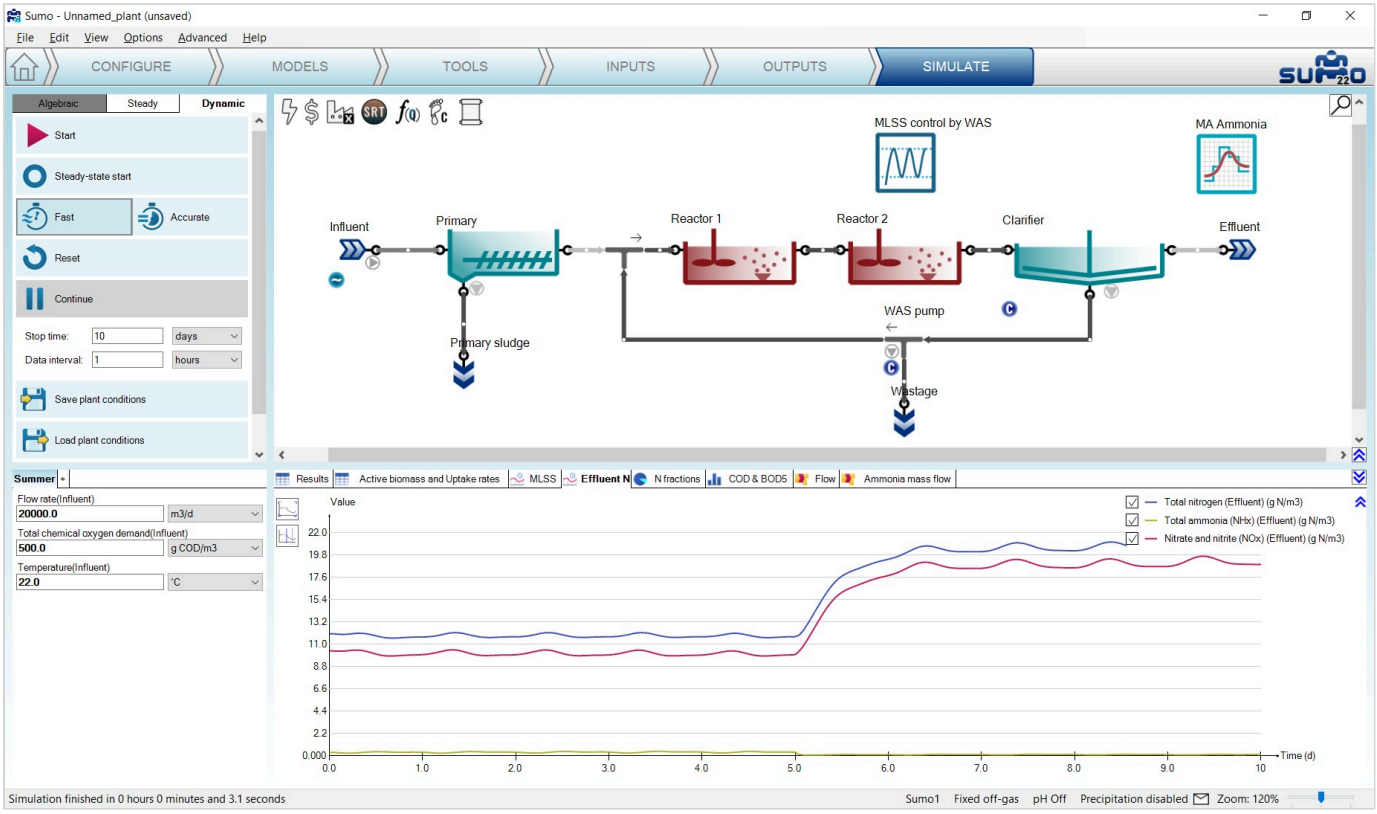


Figure 3.52 - Effluent ammonia and nitrate variation – aeration switched back in 'Reactor1'

Nitrate concentration will increase, and the ammonia peaks will get much reduced from day 5, when the aerators were turned back on. After this exercise, reset the air flow in Reactor 1 to 0 Nm^3/d and run a 10 d simulation to get back to denitrifying plant.

Model parameter dynamic input

Model parameters and plantwide parameters can be added as dynamic inputs as well – in these cases, the plantwide (factory) icon should be selected on the drawing board in the *Inputs – Dynamics* tab, and extended descriptions of the model parameters are to be used in the dynamic input tables, as described below.

The incode name of model parameters can be found as popup by hovering the mouse over the desired parameter on the *Models* tab. See the example of *Maximum specific growth rate of the NITOs* (nitrifier

organisms) on Figure 3.53: **µNITO** is the name of the parameter in the active model, which is the Sumo1 model in this tutorial.

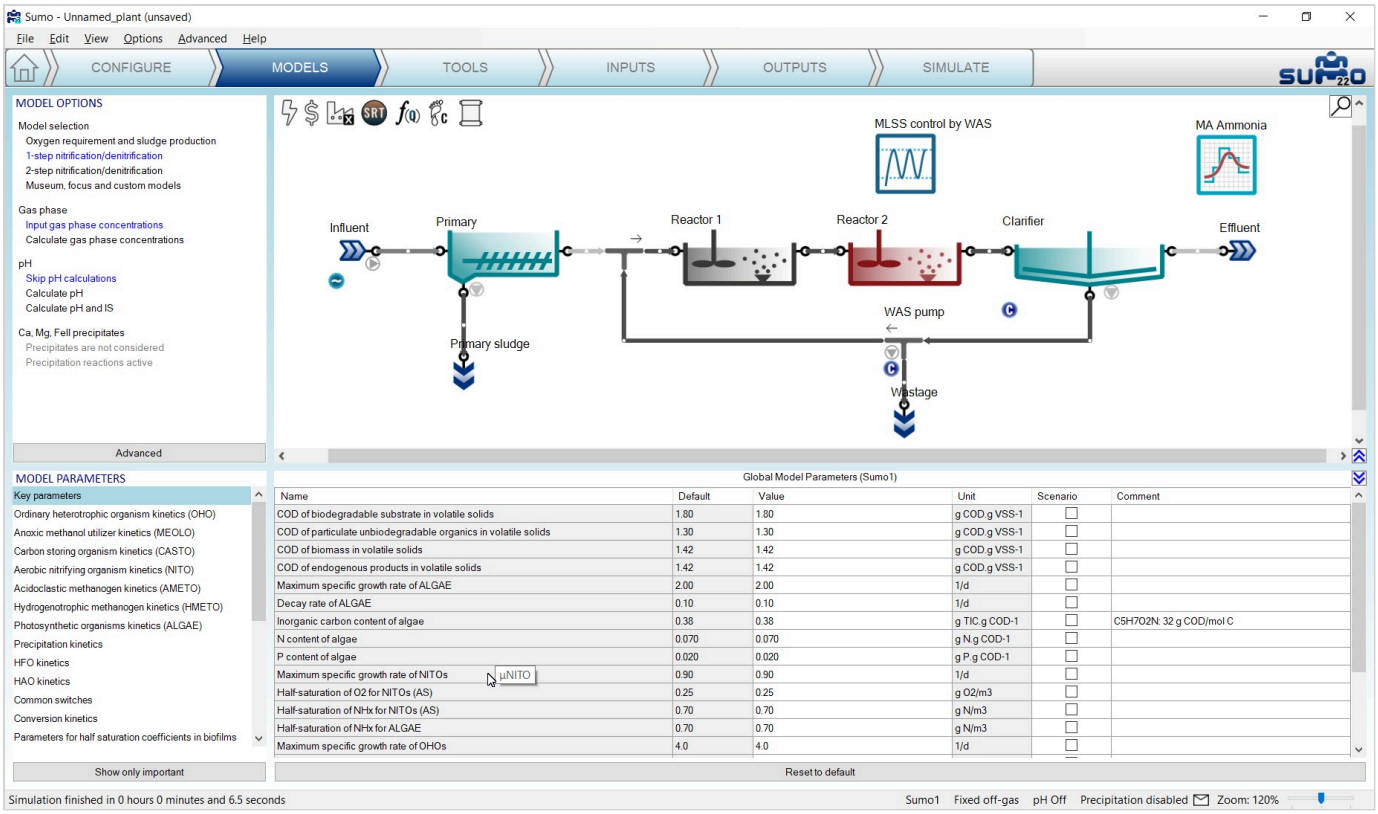


Figure 3.53 – Model parameter name

The model name of the parameter is the compound of the model name and the parameter name, separated by two dots. So in our example, **Sumo1..µNITO** will be the correct model parameter name to be used in the dynamic input table (Table 3.7).

Table 3.7 – Model parameter dynamic input table

time	Sumo1..µNITO
h	1/d
0.0	0.9
6.0	0.4

Inserting the dynamic input table is done the same way as it was done in the diurnal flow – just copy the prepared table from Excel and paste using the button in the *Inputs – Dynamics* tab (remember that the factory icon shall be selected for showing this functionality). The presence of the dynamic global model parameter input will be indicated by a blue circle with a wave inside on the drawing board, below the factory icon (see Figure 3.54).

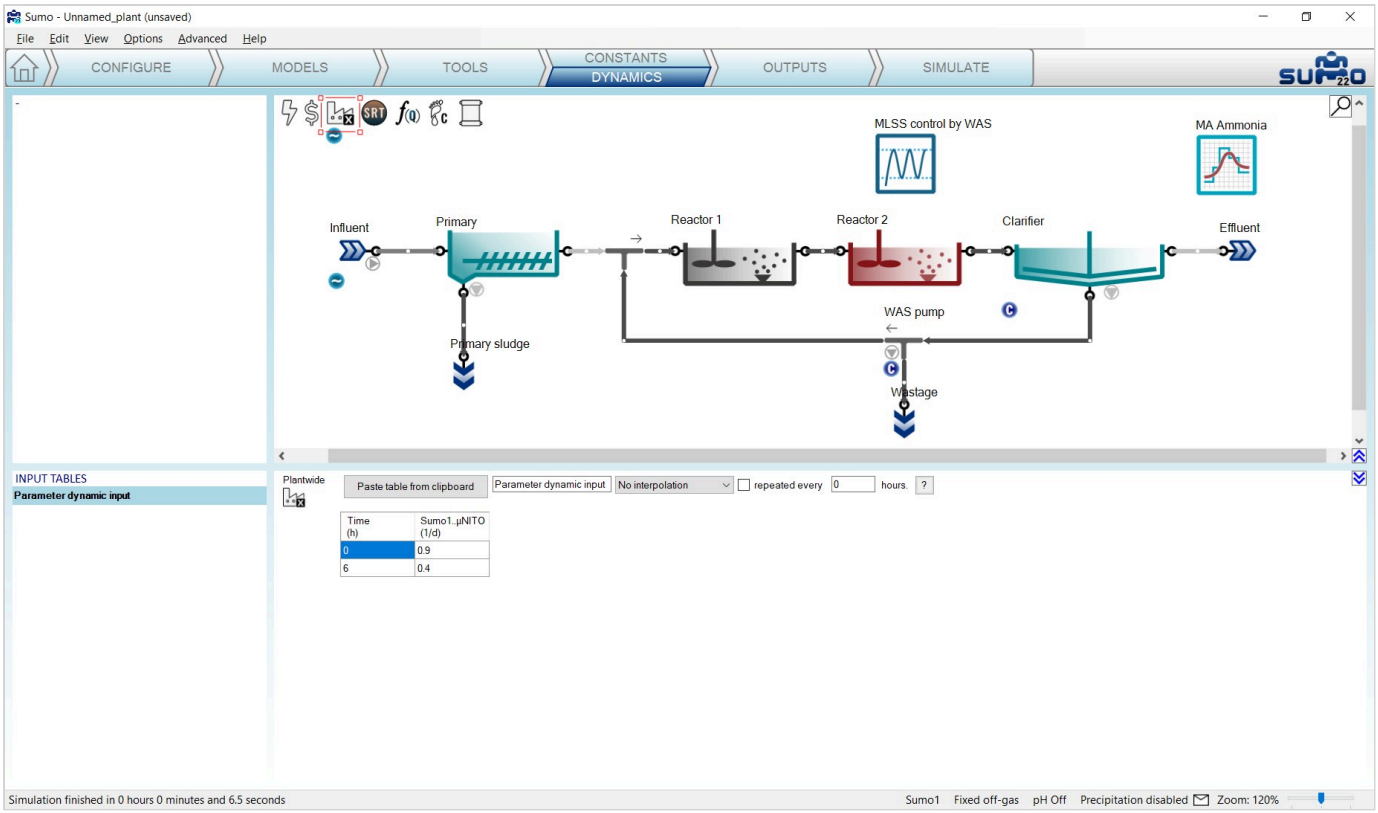


Figure 3.54 – Dynamic global model parameter input

Now let us go to the *Simulate* tab and start a 2-day simulation with an hourly data interval. The decrease in nitrifier maximum growth rate (caused by i.e. a toxic substance in the influent) should have an effect on effluent quality as shown in Figure 3.55: we can observe higher ammonia concentrations after the decrease in the NITO growth rate.

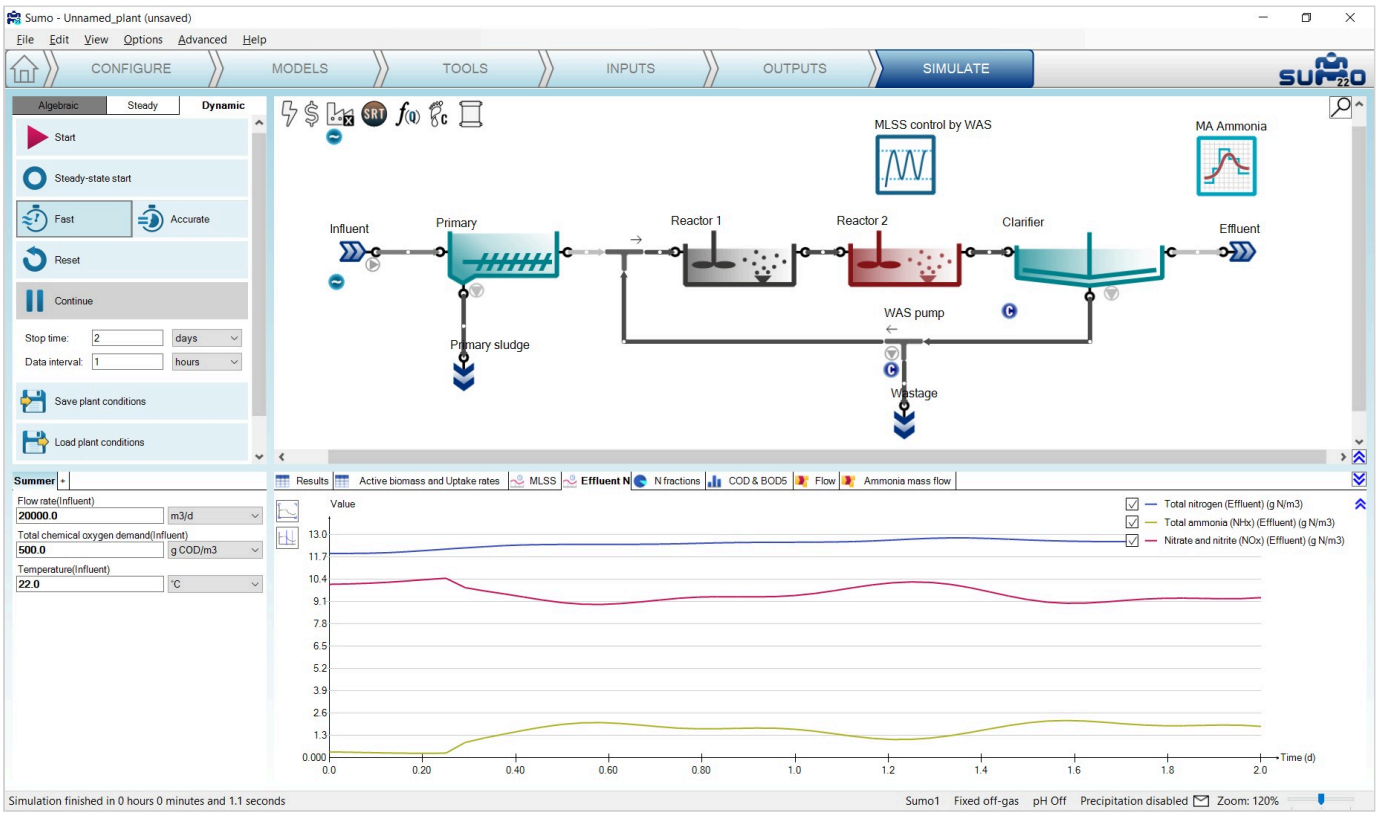


Figure 3.55 - Effluent ammonia and nitrate variation with NITO growth rate decrease

During the following exercises, we will not use the dynamic input for model parameters any more. In the bottom left screen panel of the *Inputs/Dynamics* tab, right click on the name of this table and choose *Delete table* to remove the table. Alternatively, you can just use the *Disable table* option as well, in order to keep the table but not to use it during the subsequent simulation. Let us try this option for switching off the diurnal flow (the indicator below the Influent icon will turn to light grey).

Adding measured data to the charts

Plants do collect information and one important task in process simulation is to compare measured data with simulation results (and potentially using the information to calibrate the model). Let us assume that this plant has MLSS grab samples once a day in Reactor 2 (TSS Reactor 2). The collected data is shown in Table 3.8 below.

Table 3.8 – Measured TSS data for the example plant

Time	XTSS (Reactor2)
d	g/m3
0	2800
1	2700
2	2600
3	2700
4	2780
5	2700
6	2750
7	2725
8	2775
9	2600
10	2750

Copy this table into an Excel sheet (e.g. named Plant Data.xlsx) and rename the sheet “Measured TSS” (Actual names are irrelevant and flexible).

Switch Sumo to *Simulate* mode, click on *Reset*, then run a 10-day simulation to let the system settle into stable condition. Then run another 10-day simulation for evaluating the MLSS trend due to the deadband controller.

Switch Sumo to *Outputs* mode, right click on the MLSS timechart tab and select *Import data*. The data import is carried out the same way as the dynamic input table: simply paste from the clipboard (Figure 3.56).

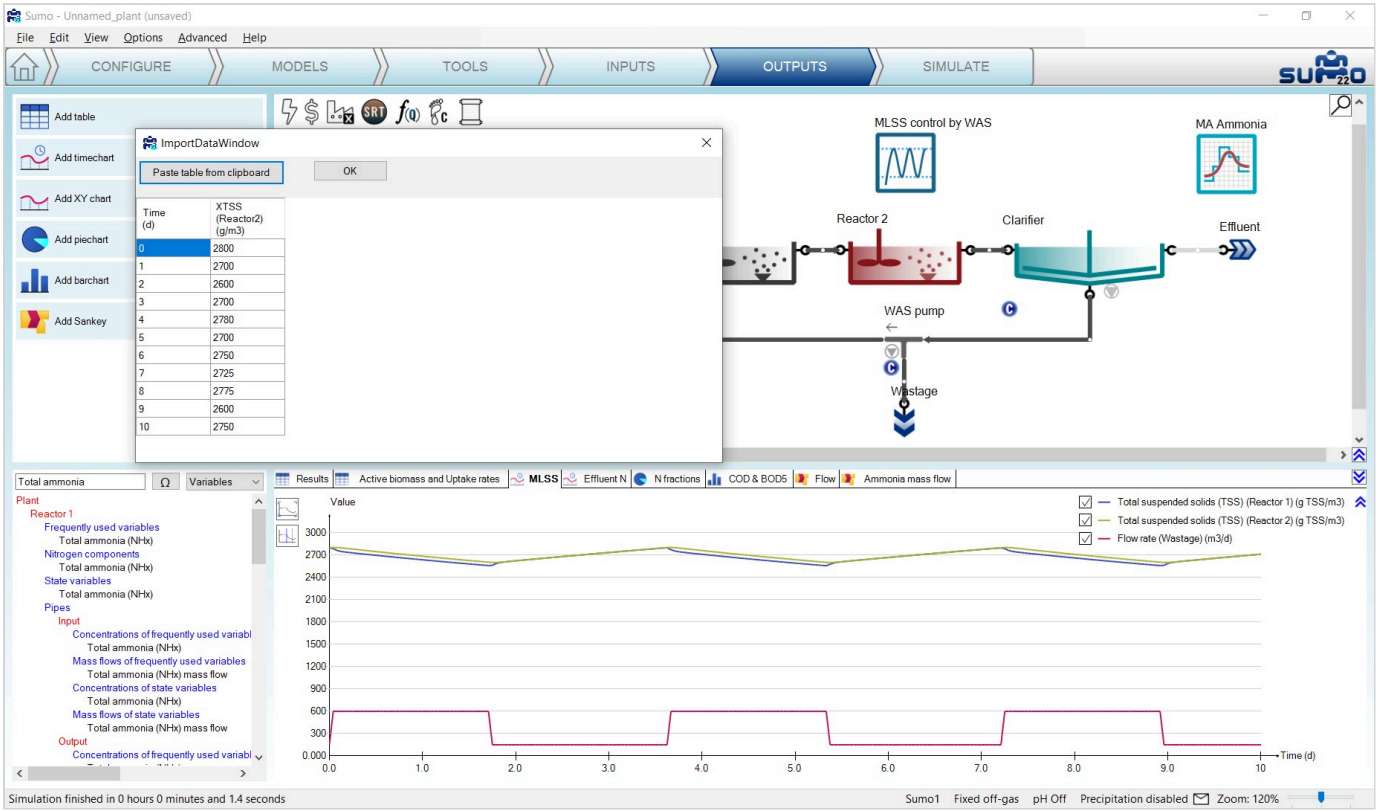


Figure 3.56 - The data import dialog

Pressing *OK* the data is plotted along the simulation results (Figure 3.57):

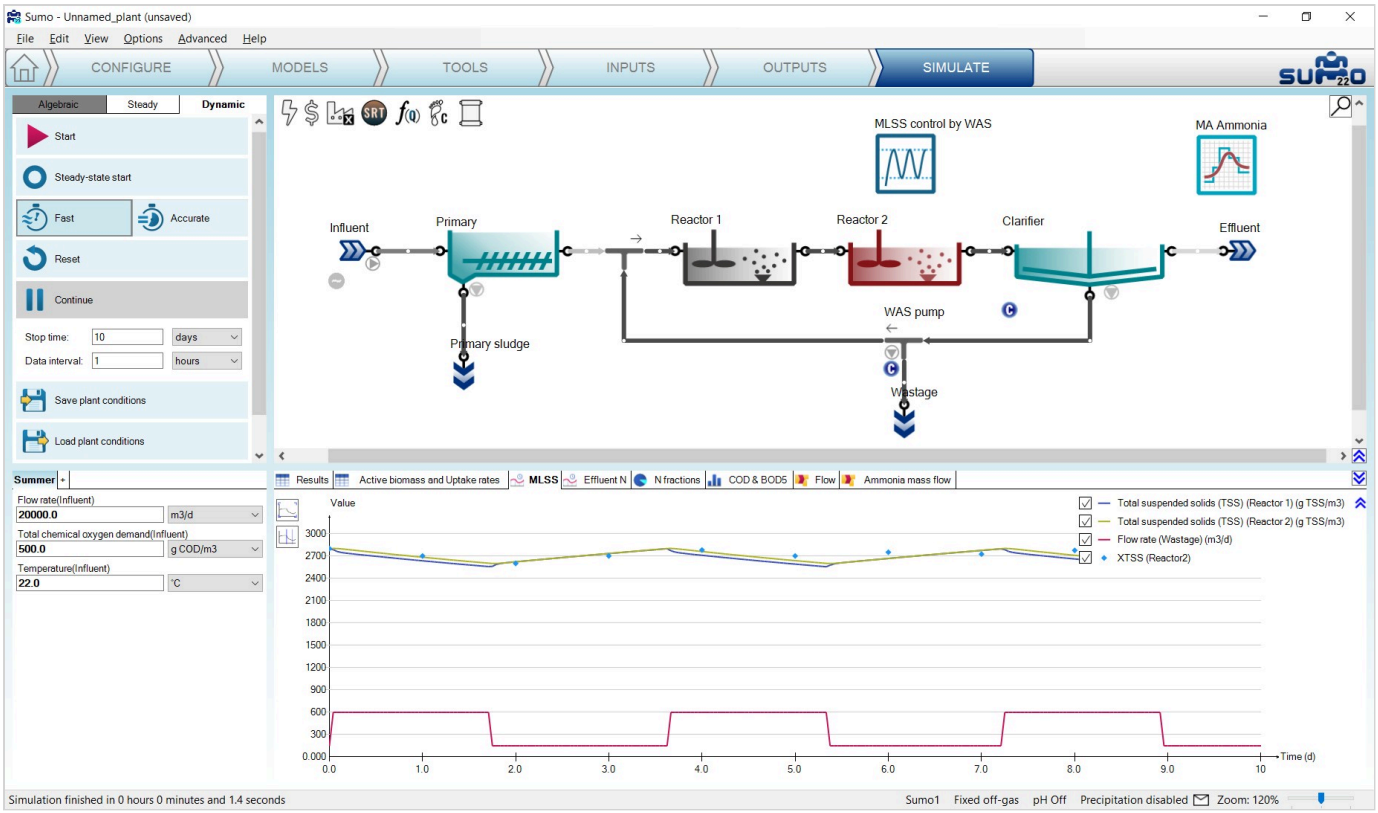


Figure 3.57 - Measured and simulated data in the same chart

The project can be saved any time during the configuration and project development using the *File* menu and reloaded at a later point in time to continue the work.

Many other operational scenarios can be simulated with Sumo, including more complex reactor configurations and more elaborate operational scenarios. Please see *Examples* under the *Help* menu and for further description check out the Examples chapter of this manual.

Scenarios

By default, the simulation is using the input parameters defined in *Inputs*, such as the influent flow rate, the influent Total Chemical Oxygen Demand and the influent temperature, which we have also selected for scenario analysis at an earlier stage. On the bottom left screen panel of the *Simulate* tab, further scenarios can be defined by clicking on the Add Scenario (+) tab. Add a new scenario, rename it to *Winter* and set 14°C, 26000 m^3/d flow rate and 460 mg O_2/l COD as input parameters instead of the default parameter set provided in the Summer tab. (Figure 3.58). With this simple setup the simulation will now use (as long as the *Winter* tab is active) 14°C as influent wastewater temperature, modified influent flow and COD composition and the results can be compared.

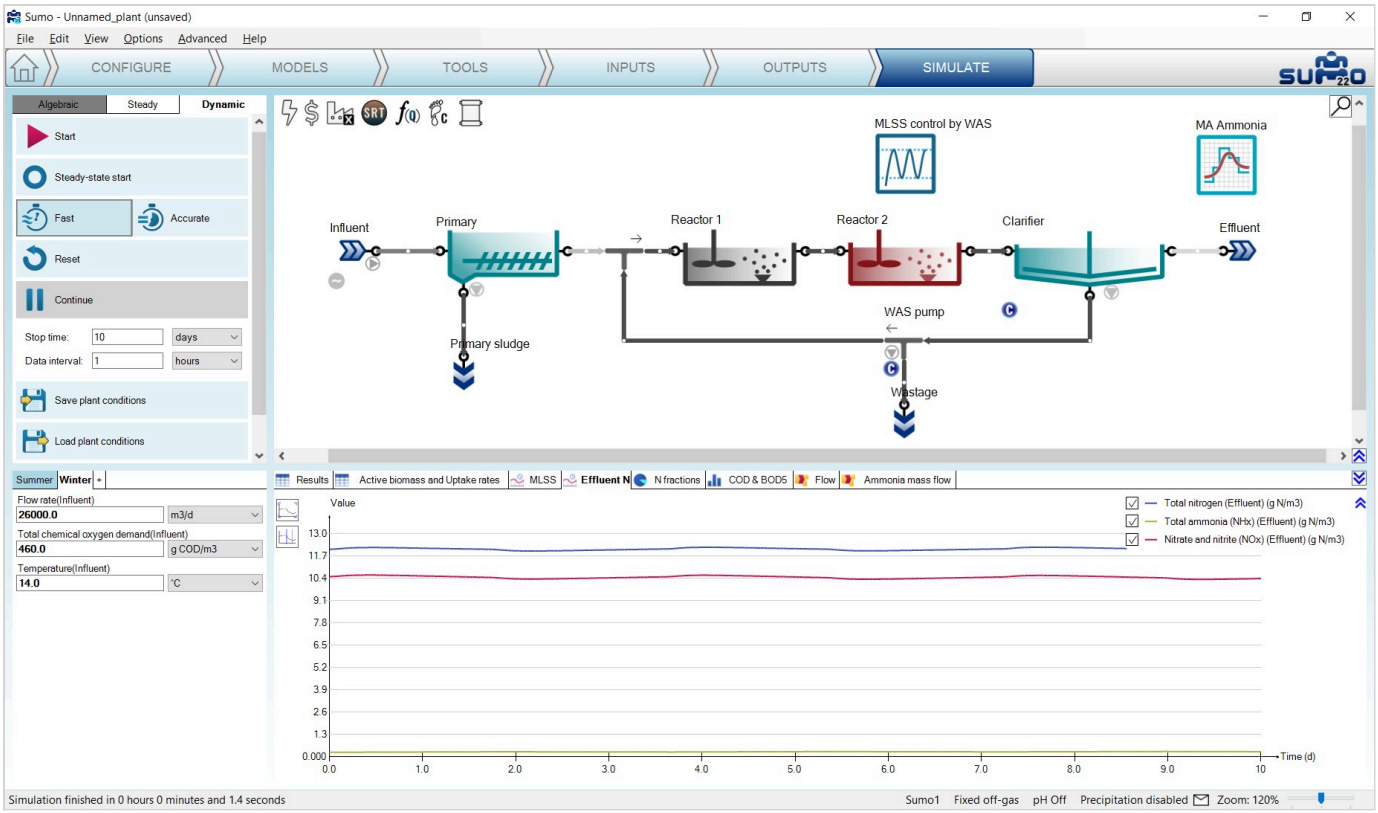


Figure 3.58 – Scenario definition for Winter conditions

After clicking on *Reset* and running two consecutive 10-day dynamic simulations (in order to get the system to a characteristic winter operation), activate the *Summer* scenario by clicking on its tab, modify the simulation stop time to 20 day and hit *Continue*. The change due to new influent conditions can be seen quickly (Figure 3.59):

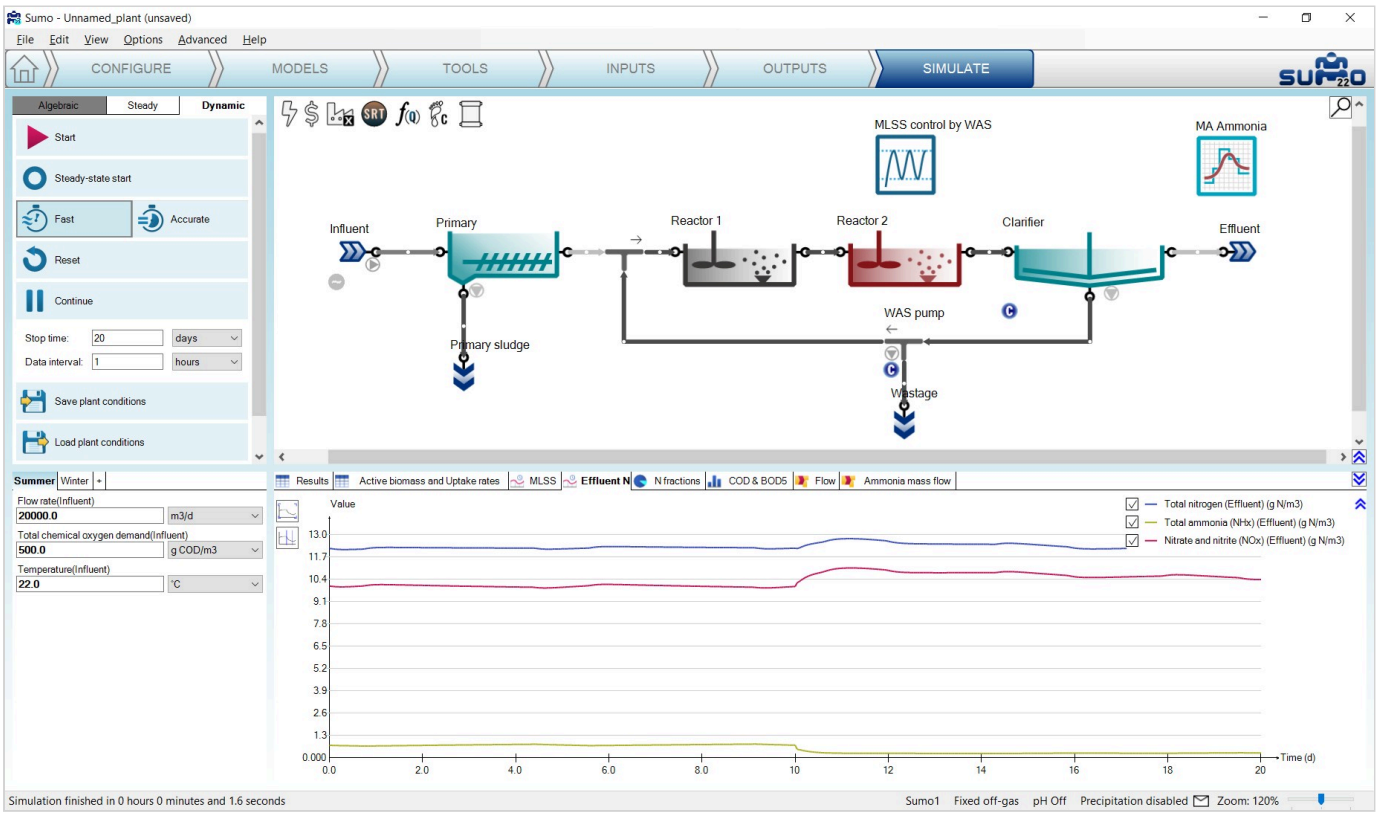


Figure 3.59 – Low temperature scenario results followed by summer conditions at 10 days

If you want to add further parameters, just go back to the *Inputs* tab and select the desired parameters of the desired process unit. Model parameters can be selected as well for scenario analysis and the *Models* tab.

Adding popups

If you hover above any process unit on the *Simulate* tab with the mouse and leave it there for a second, a yellow popup will appear with a summary table of the most important variables related to that process unit type (Figure 3.60). Moving the mouse elsewhere will make the popup disappear soon after. However, if you grab it with the mouse while it is active and place it somewhere in the layout, it will remain there as a sticky note as long as you don't close it with the *X* in the top right corner. Most popups will have a few tabs in the bottom which you can toggle when the popup is active, in order to reveal more information.

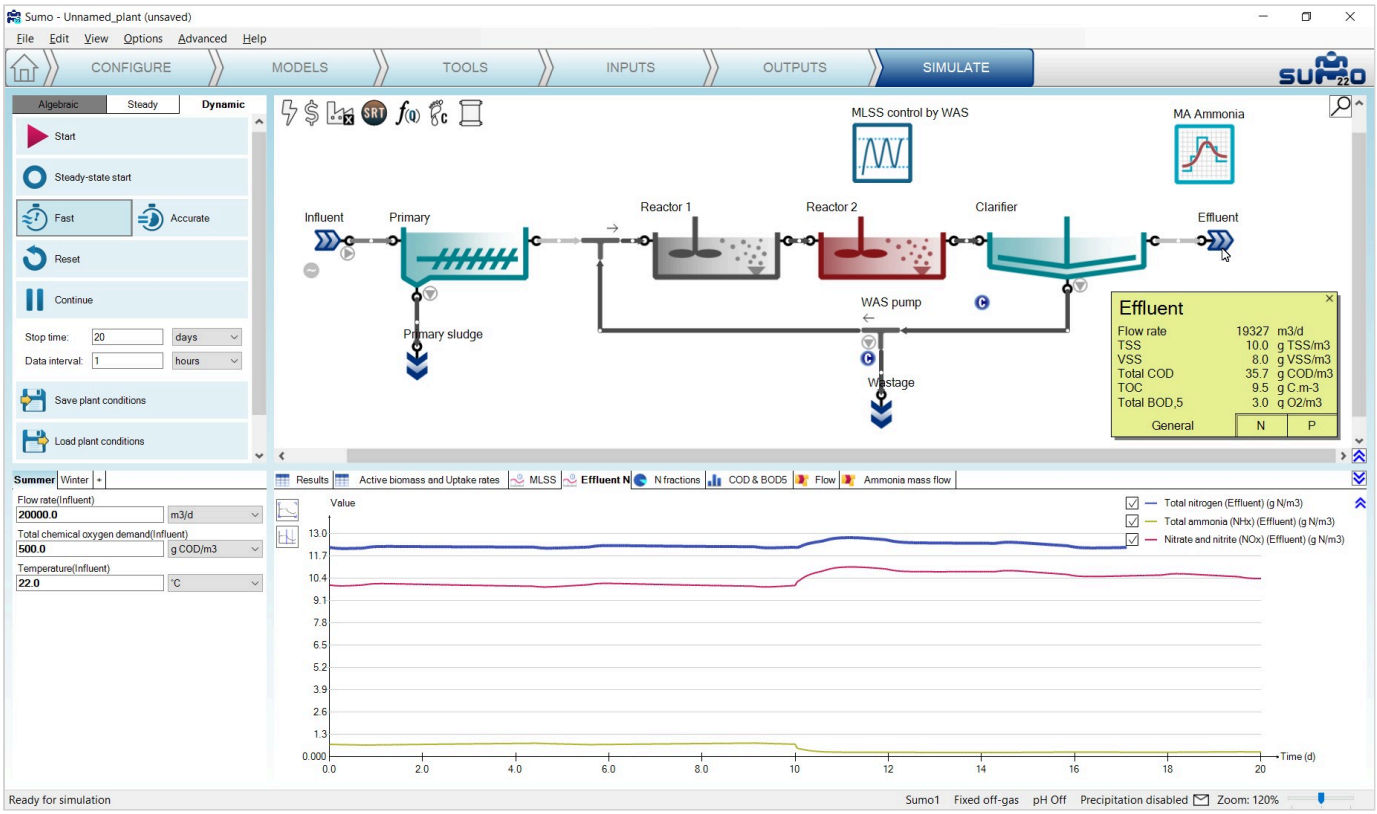


Figure 3.60 - Adding popup table to the layout

Adding pipe info tables

Data from any table can be set to be shown on the pipes of the layout. For an excercise, let's go back to the *Outputs* tab and add a table with the *Flow rate* of the *Influent* process unit (can be found under *Frequently used variables*). Rename the table to *Pipe info table* and right click on the name tab, then click the *Show values on pipes* option (Figure 3.61).

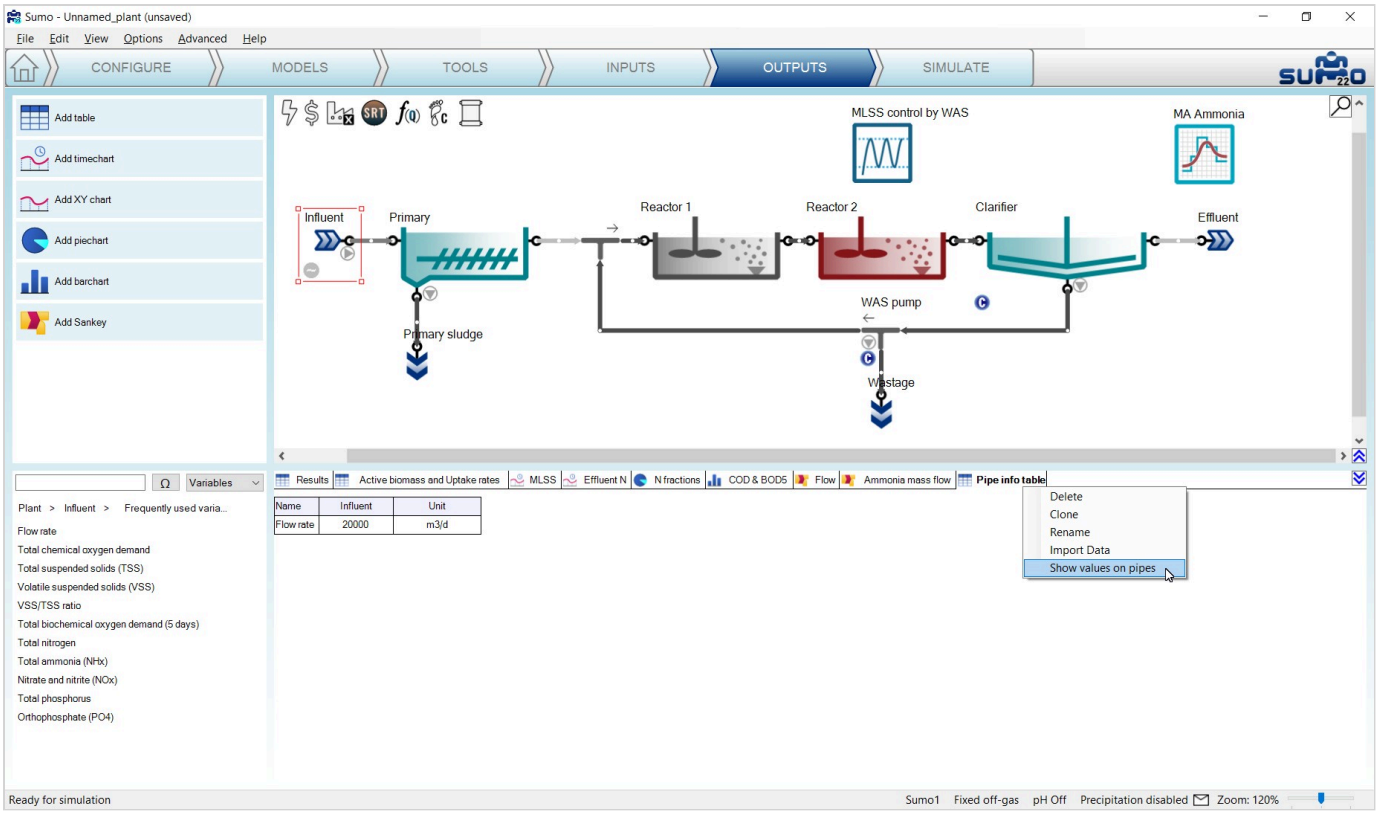


Figure 3.61 - Setting up table to show values on pipes

This will add a transparent popup nearby ALL pipes of the configuration. In most cases you will only need a handful of them, so you can remove the unnecessary ones by clicking the *X* in the top right corner of the unwanted popups. For the excercise, keep only the ones belonging to Influent, Effluent, Primary sludge and Wastage. By dragging and dropping, you can reposition the pipe info popups for better readability. If you add further variables to the source table, you will see that they will be shown on the popups as well (Figure 3.62). Along the same line, removing variables from the source table will remove them from the pipe info, too.

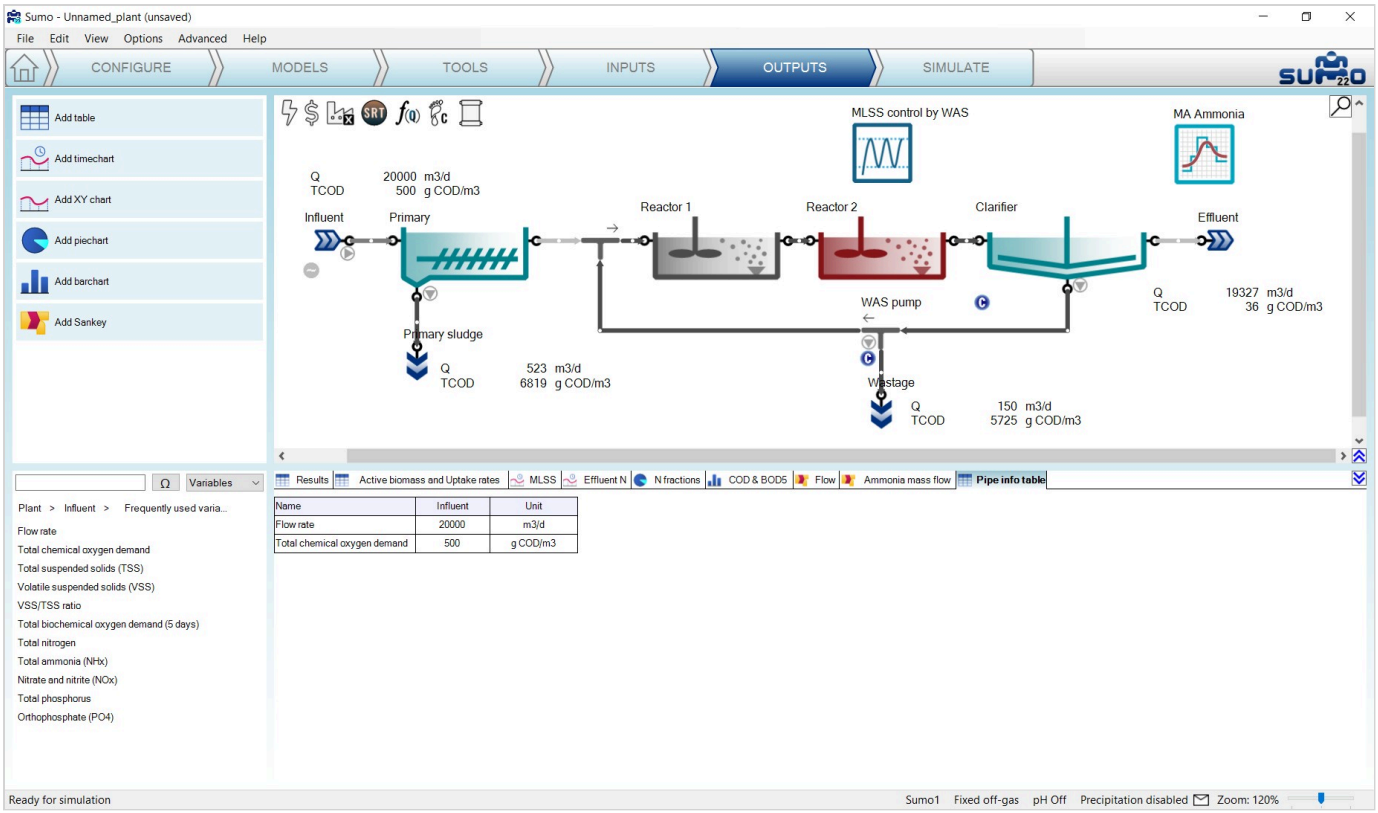


Figure 3.62 - Adding additional variables to pipe info

Writing a report

On the Control panel of the *Simulate* tab, a *Report* button is available. When clicked, results will be written to an Excel file, available for further processing. The resulting Excel file is named the same as the sumo project file by default (Figure 3.63). This function creates an Excel file with the following sheets:

- Project overview: contains the configuration layout and basic project information
- Notes: the contents of the *Notes* screen panel from the *Configuration* tab
- Modified parameters: values of all parameters in the project that were changed from default
- Scenarios: values of parameters in the scenarios
- Simulation results: all results of the output tabs get saved to separate sheets, including data tables for the diagrams
- Model: contains all parameter values for the used model (in this example: Sumo1)
- Plantwide calculations: Plantwide, Energy center, Cost center, SRT and Flow dependence settings are saved on separate sheets
- Process Units: all settings and PU parameters are displayed on separate sheets for each unit, including pipes.
- Controllers: all settings and parameters of the controllers employed in the project (if any).

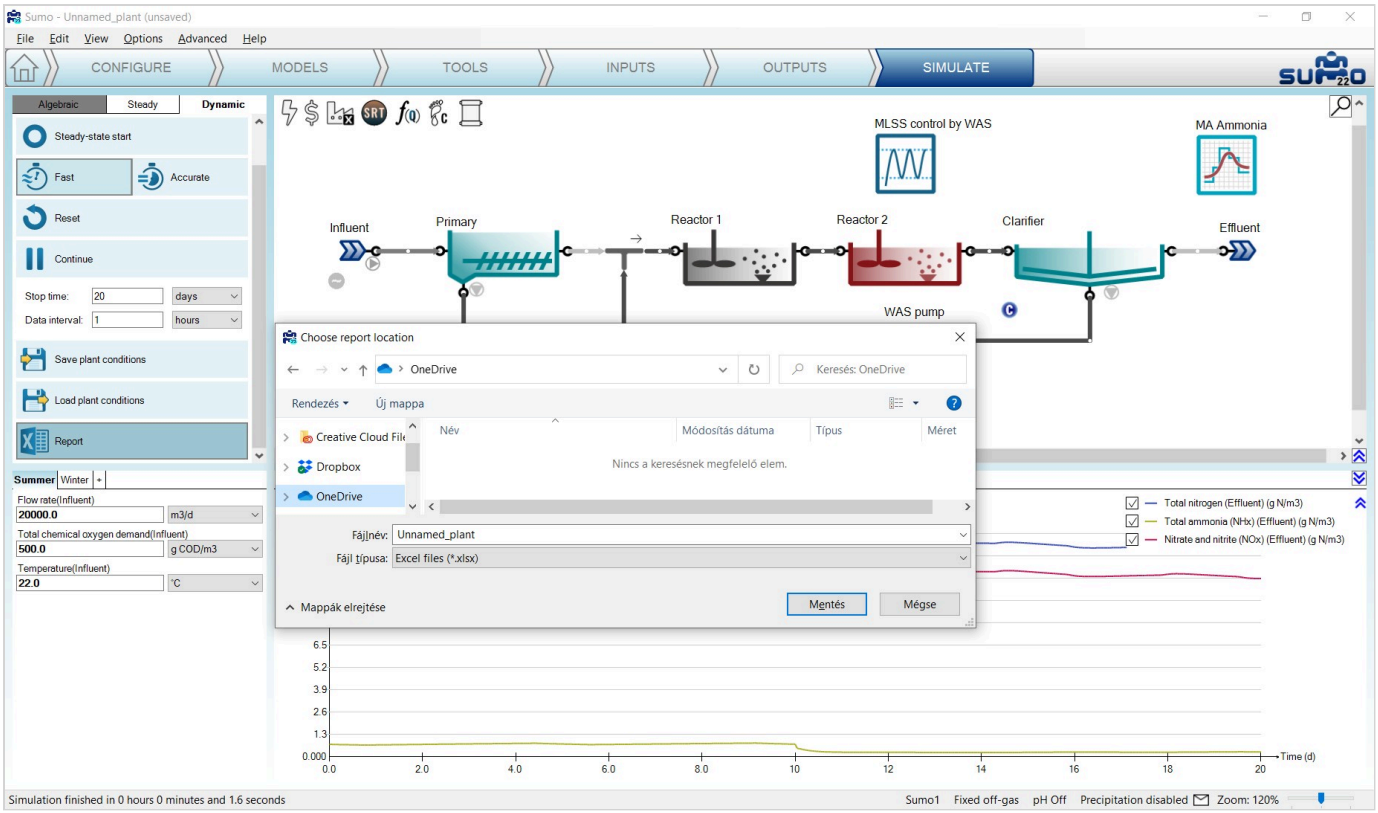


Figure 3.63 - Saving the Report

Controllers

Controllers are used to set operational parameters based on measured values during the operation of the plant. In Sumo, the controlled values are calculated variables from the simulation. The on-off controller has no controlled variable. The manipulated parameters are input values for the controlled process unit. For example, this way the reactor MLSS can be automatically controlled by manipulating the wastage sludge flow. Another example is setting the air flow into the aerated reactor to maintain a certain dissolved oxygen level.

There are 6 different type of controllers implemented in Sumo, which can be added on the *Tools* tab (Figure 4.1):

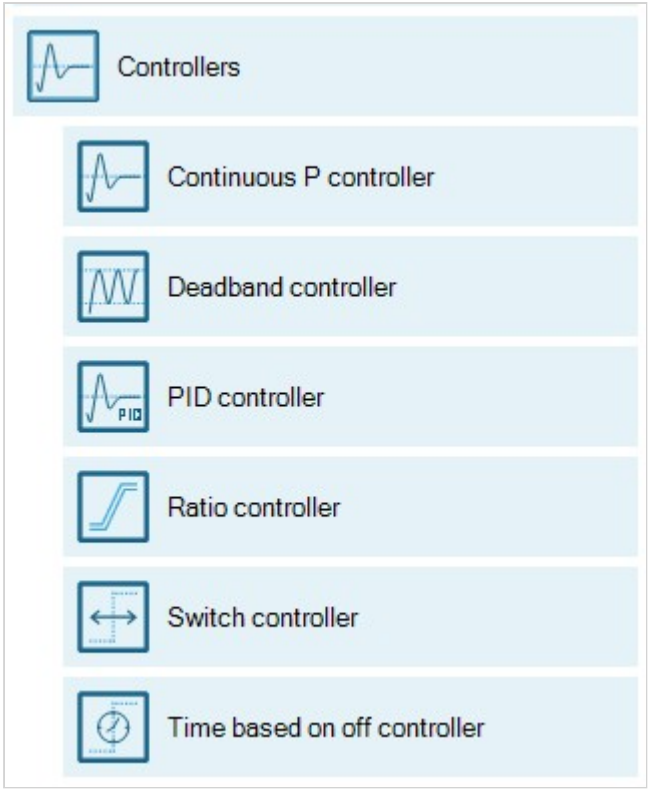


Figure 4.1 – Available controllers

Clicking the *Controllers* button on the *Tools* tab will open this dropdown list of controllers, where you can pick the desired one and configure the control variable (CV) and the manipulated variable (MV) which is a parameter in the model; while on the *Inputs* tab you can fine tune the controller settings. In this chapter, the setup possibilities will be presented for each available controller one by one, based on the example project built in the previous chapter (How to use Sumo for simulations).

Continuous P controller

The Continuous P controller is a model controller that continuously sets (integrates) the input parameter (Manipulated variable) of the desired unit to meet the control variable value setpoint (as opposed to discrete controllers).

Add this controller to the layout from the *Tools* and configure it as follows. First drag and drop the manipulated process unit (Reactor 2) to the left side of the equation in the bottom right screen panel and the controlled unit (Effluent) to the right side of the equation. On the bottom left screen panel, you can now select the control variable and the manipulated variable in the respective units. In this example, we will manipulate the requested DO setpoint to maintain the desired ammonium concentration in the effluent. Rename the unit (using F2 or right click) to “Ammonia control” (Figure 4.2).

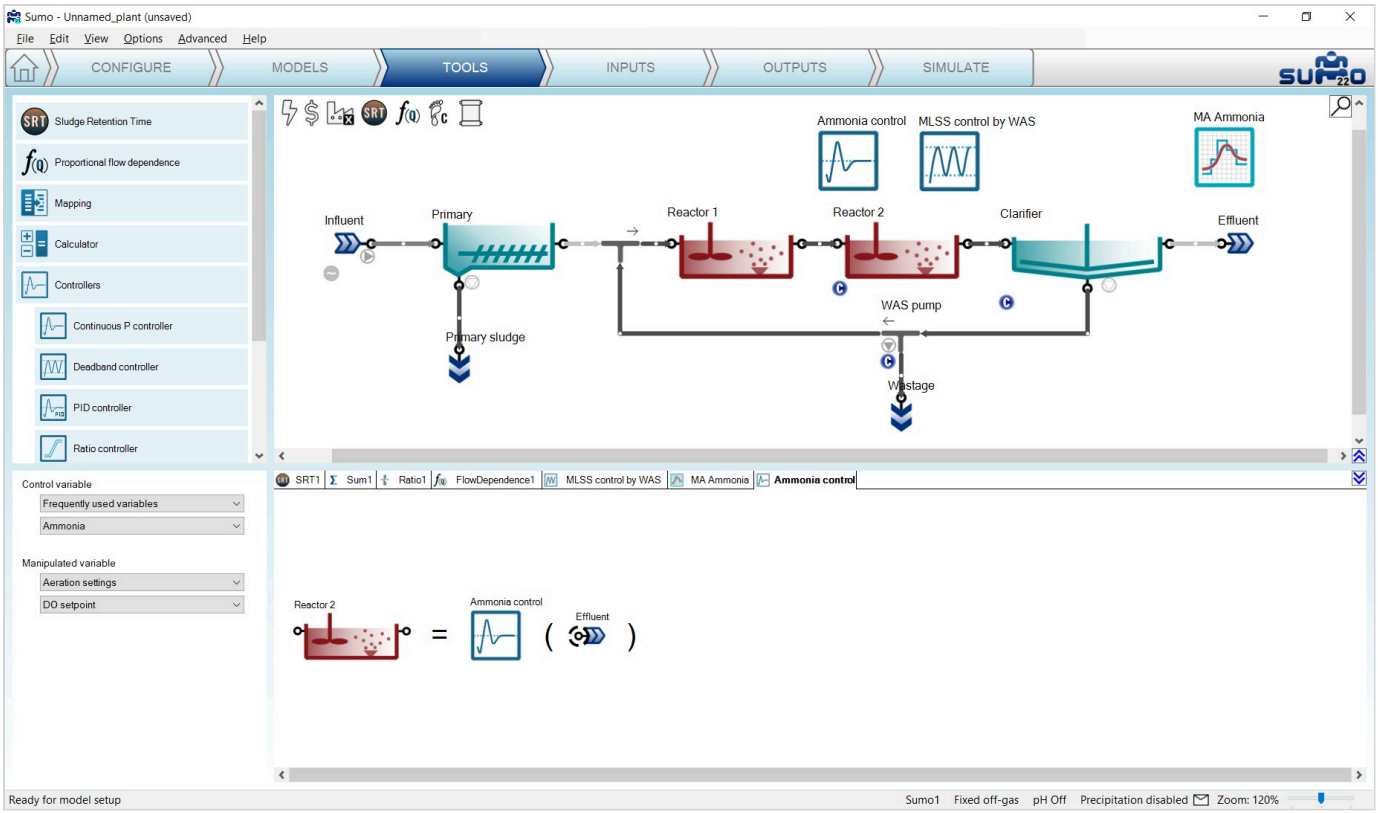


Figure 4.2 – Configuration of the continuous P controller

Proceed to the *Inputs* tab and select the newly added controller. Once the project compiled, in the *Controller parameters* table, enter the following settings:

- *Controlled variable setpoint* to 0.5 g N/m^3 (target effluent ammonia concentration);
- the *Maximum of the manipulated variable* value to 3 g O_2/m^3;
- the *Controller direction* to -1, because it is an inverse controller (to decrease the ammonia concentration the DO setpoint has to be increased).

At the *Controller initialization* table, set the *Initial value of manipulated variable* to 2 g O_2/m^3 (Input DO setpoint in Reactor 2). Leave the other parameters default (Figure 4.3).

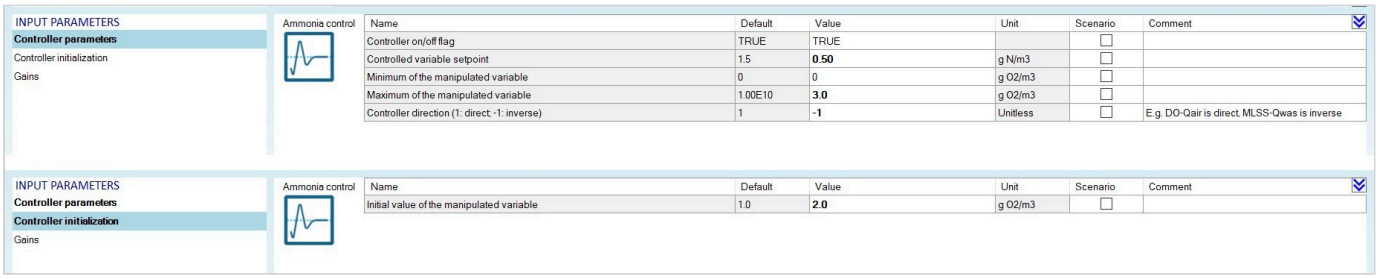


Figure 4.3 – Setting continuous P controller input parameters

To follow the effect of the controller, you can add the setpoint to the *Effluent N* timechart on the *Outputs* tab: select the *Ammonia control* controller and from the bottom left screen panel, go to *Parameters* > *Controller*

parameters menu and add *Controlled variable setpoint* to the timechart. (Figure 4.4).

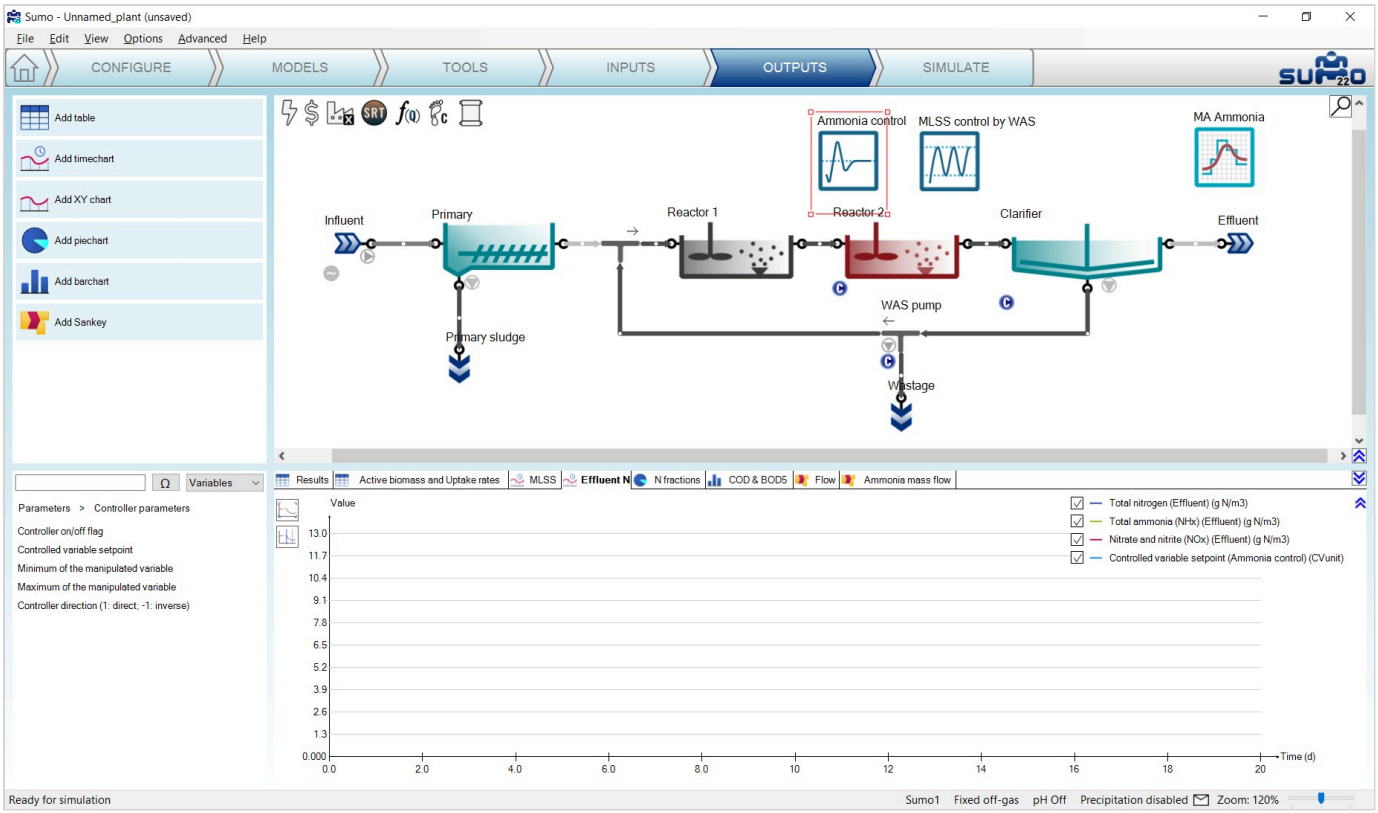


Figure 4.4 – Adding controlled variable setpoint to timechart

Before starting the simulation, go to the *Inputs*/*Dynamics* tab and enable the Diurnal flow dynamic input table of the Influent to have changes in the ammonia load (see Figure 4.5).

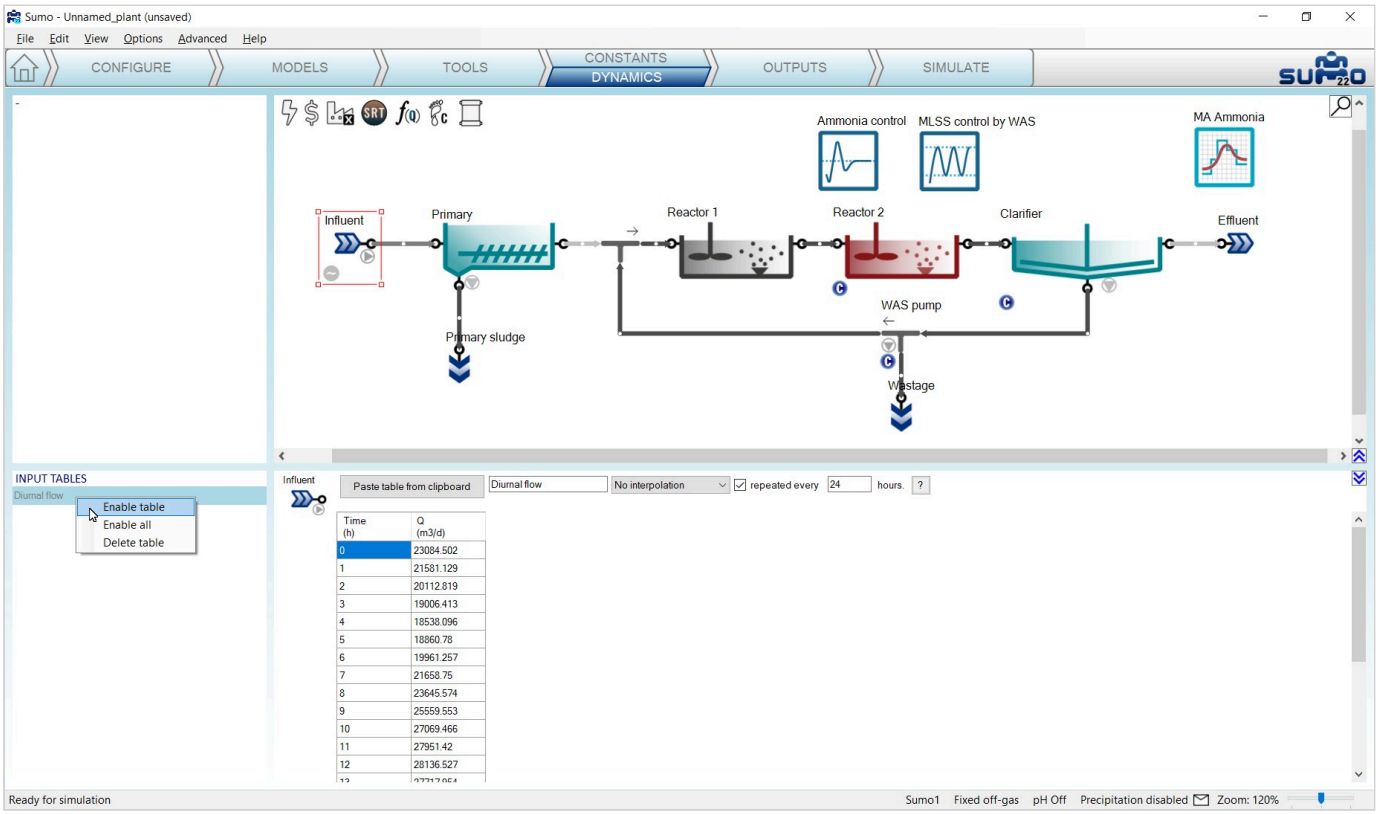


Figure 4.5 – Enabling diurnal flow dynamic input for the influent

Finally go to the *Simulate* tab, set the *Stop time* to 1 day and the *Data interval* to 1 minute (to see finer details of the operation of the controller) and run the simulation. During the calculation, you can follow the change of the effluent ammonium along with nitrate and nitrite on the previously extended chart (Figure 4.6).

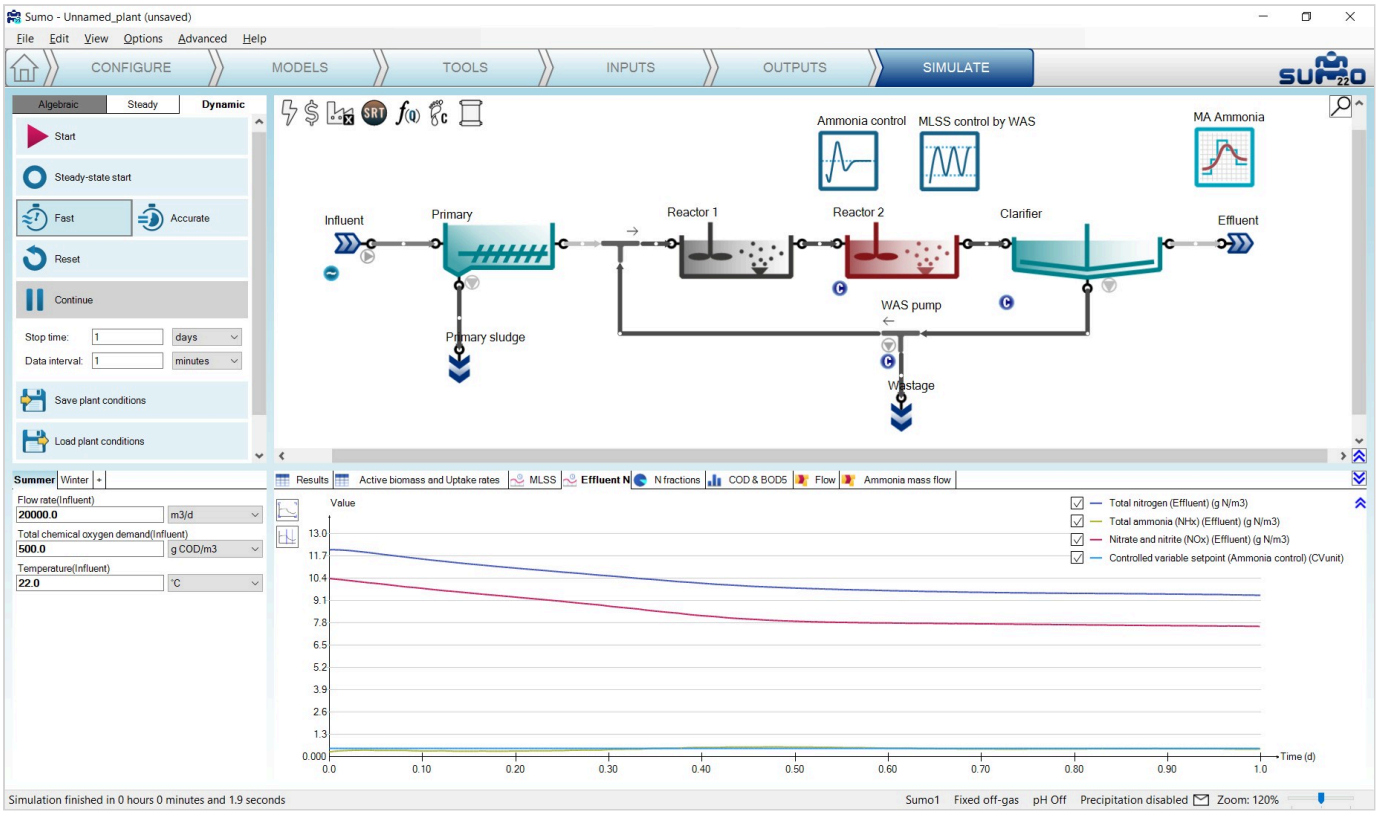


Figure 4.6 - Simulation results with DO setpoint based on effluent ammonium continuous P control

To modify the setpoint of the controller, go to the *Inputs* tab, select the *Ammonia control* controller and modify the setpoint to 1.0 g/m^3 (effluent ammonia concentration). On the *Simulate* tab increase the *Stop time* for 2 days and continue the simulation (Figure 4.7).

Note: Keep in mind that the effluent fluctuation is caused by the influent diurnal flow and the MLSS deadband controller, which are independent of the continuous P controller.

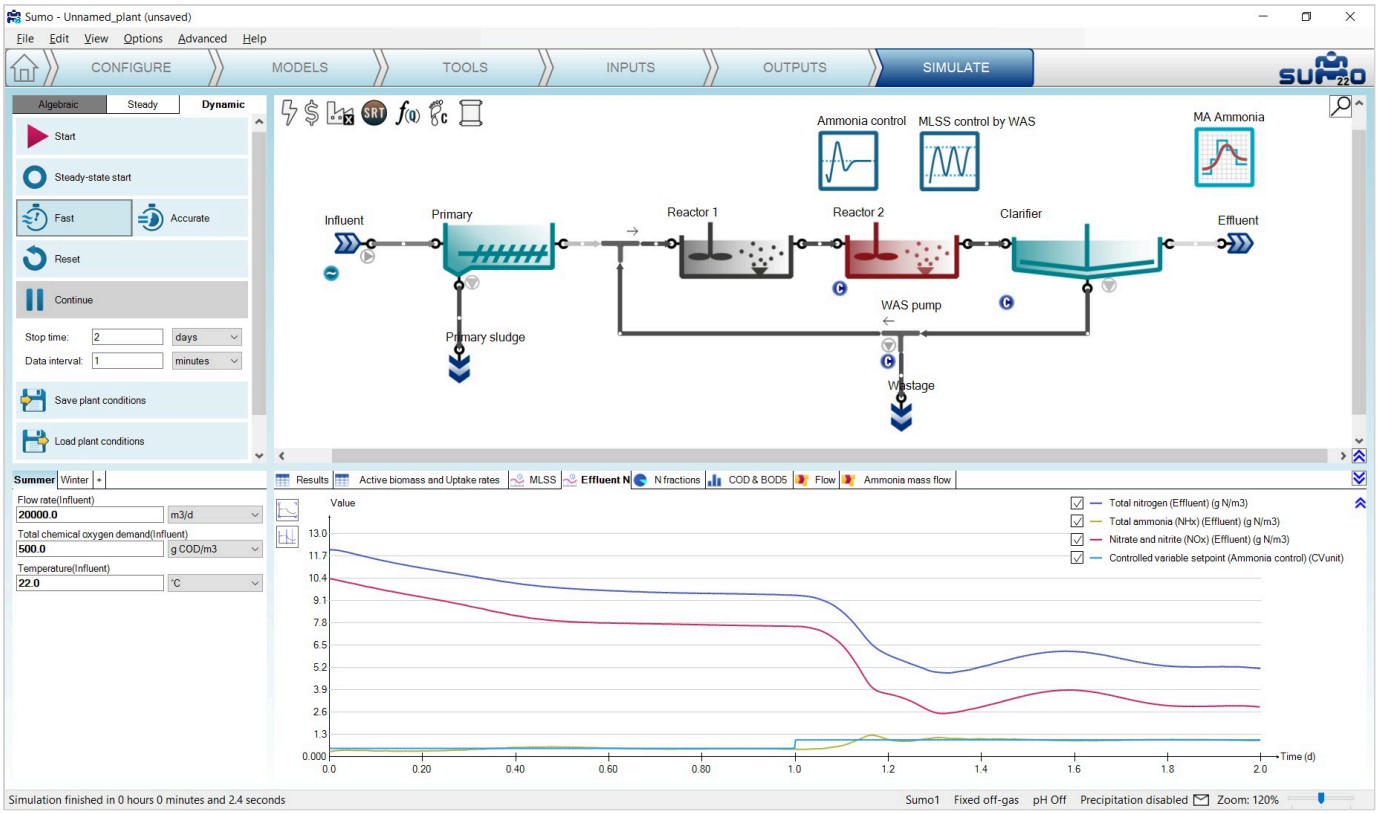


Figure 4.7 - Effect of Controller setpoint modification

The *Total nitrogen* and the *Nitrate and nitrite* (NO_x) curves can be unchecked in the graph legend, thus the smooth changes in the effluent caused by the controller DO setpoint modification can be seen in detail. (Figure 4.8)

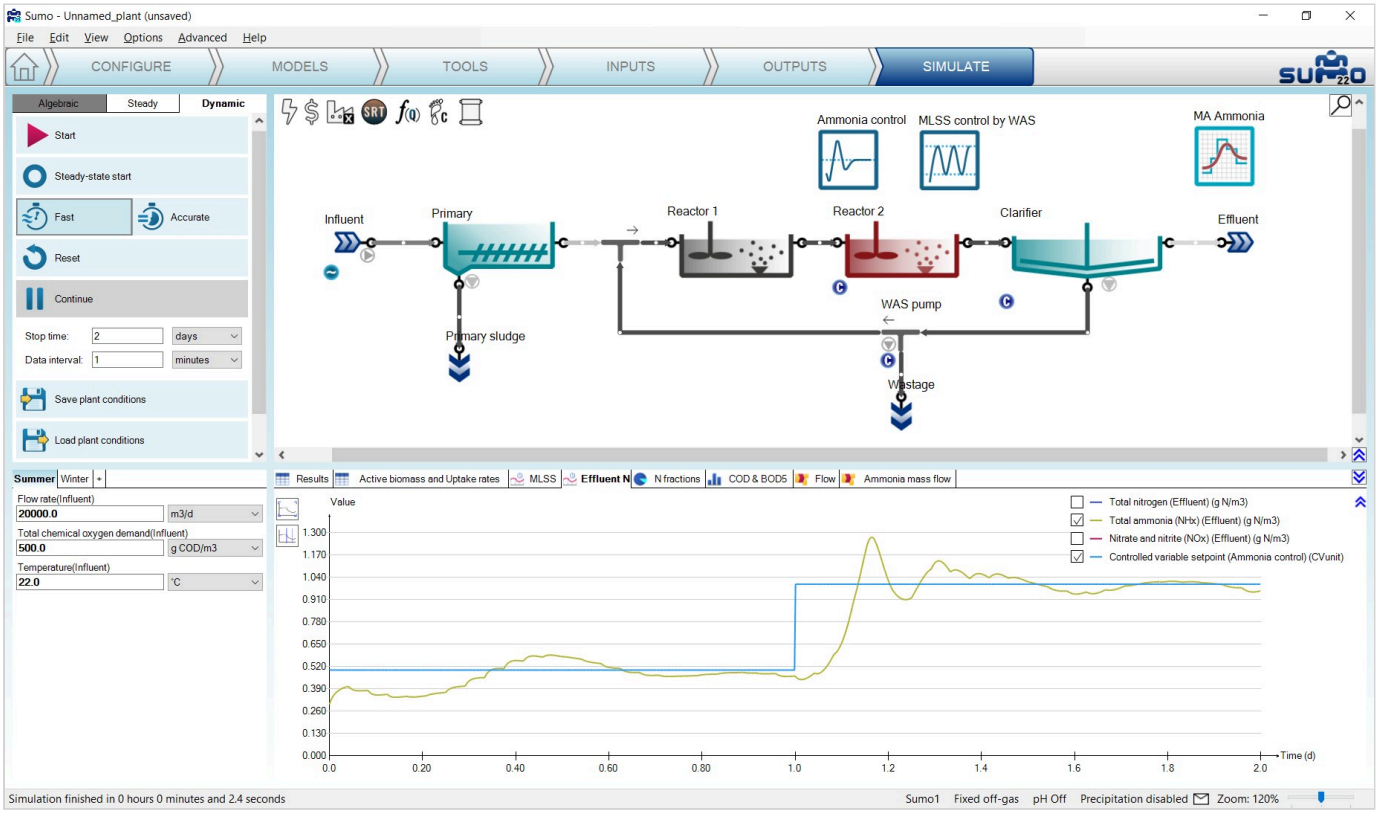


Figure 4.8 - Simulation results with DO setpoint Continuous P controller based on effluent ammonium (without NO_x)

Deadband controller

In an earlier chapter we added a Deadband controller to manage the MLSS in the reactors.

PID controller

The PID controller is using a discrete time step to set the input parameter (manipulated variable) of the desired unit to meet the controlled variable setpoint.

To demonstrate the capabilities of this controller, let us set Reactor 2 of the example project to use the *Calculated* option for Dissolved oxygen (*Configure* tab). Then add the controller and configure on the *Tools* tab as follows. First drag and drop the manipulated unit (Reactor 2) to the left side of the equation in the bottom right screen panel and the control unit (also Reactor 2) to the right side of the equation. In the bottom left screen panel, you can now select the control variable and the manipulated variable of the selected unit. In this example, we are going to control the requested air flow rate to maintain the desired dissolved oxygen concentration. Rename the controller unit (using F2 or right click) to “DO control by Air flow” – this will rename the tab as well (see Figure 4.9).

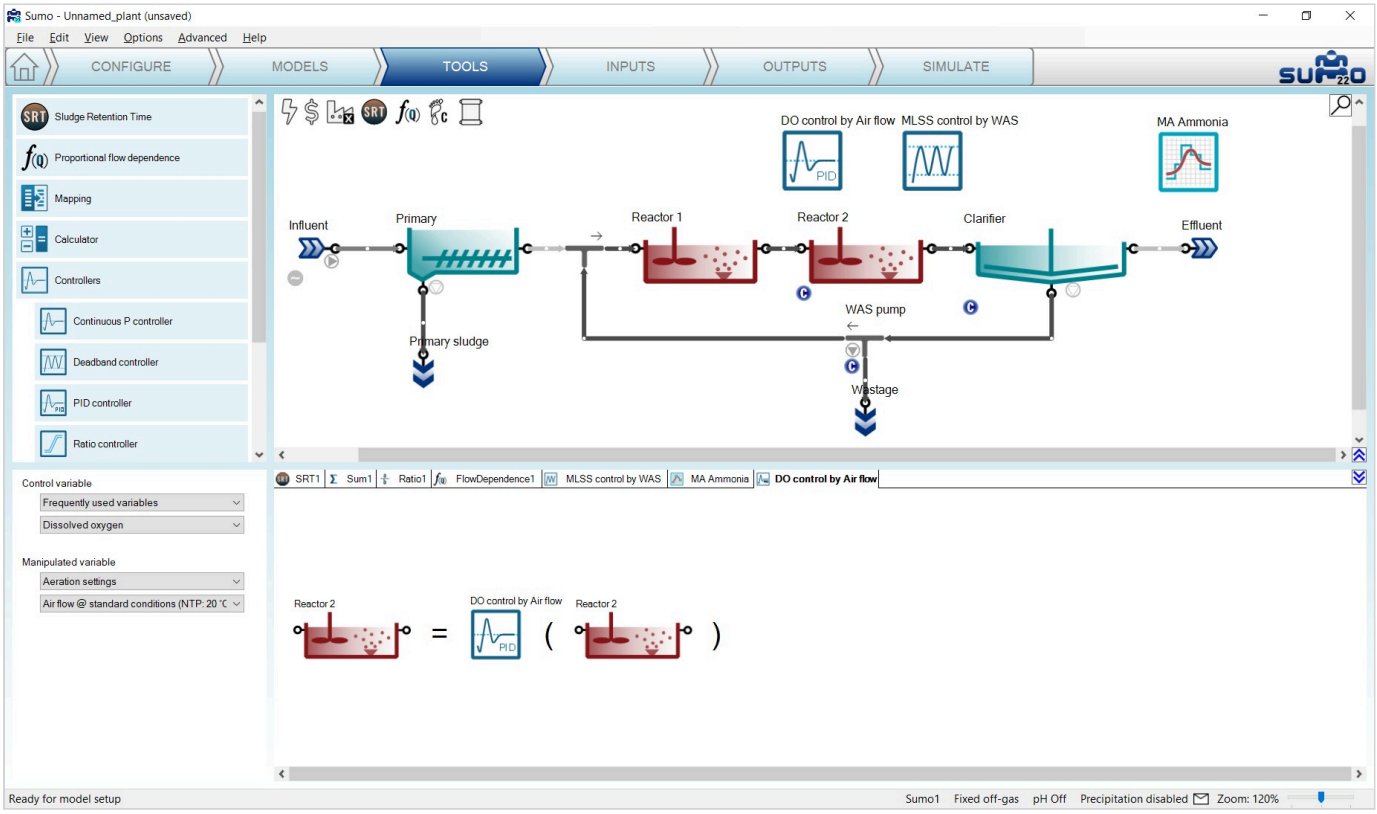


Figure 4.9 – PID controller configuration

On the *Inputs* tab, select the newly added *DO control by Air flow* controller. Once the project compiled, in the *Controller parameters* menu set the following:

- the *Controlled variable setpoint* to 2.0 g O_2/m^3 (maintained DO concentration),
- the *Initial value of manipulated variable* to 75000 Nm^3/d (Input air flow of Reactor 2),
- the *Minimum of manipulated variable* to 30000 Nm^3/d, and
- the *Maximum of manipulated variable* to 200000 Nm^3/d.

Within the *Gains* menu set the *Proportional gain* to 50000, the *Integral gain* to 1000 and the *Derivative gain* to 125 (Figure 4.10).

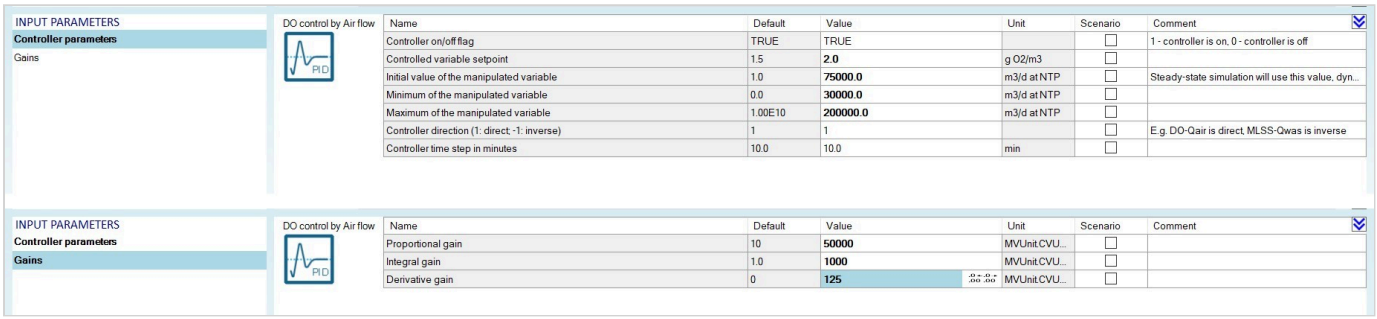


Figure 4.10 - Setup PID controller parameters

Note: The proper tuning of the controller needs attention. In every situation, the best gains for the controller depend on the combination of the controlled and manipulated variable. In this case, the controlled variable is set to 2, while the manipulated variable can change between 30,000 and 200,000. Properly operated controllers react quickly to the change of the controlled variable, depending on the inertia of the system. As a rule of thumb, the gain is related to the MV/CV ratio. The proportional gain in this specific case should turn the error derived from small numbers (DO) into large air flow ranges. As it was seen at the Continuous P controller, if both the controlled and the manipulated variables are in the same range, the most suitable proportional gain will be a small number.

Note: Controllers use units for the controlled and manipulated variable from the internal code of the system (called “in code unit”). To make sure that the controller is set up properly, change the *Unit system*s in the *Options* menu to “in code”, so that on the *Inputs* tab the respective units for the controlled and the manipulated variables can be verified.

To follow the changes in the aeration of Reactor 2, add a timechart in the *Outputs* tab and rename it to “Air flow and DO”. Select Reactor 2 and drop *Dissolved oxygen* and *Air flow @ standard conditions* from *Operational* menu (Figure 4.11). Then select the *DO control by Air flow* controller and add the *Controlled variable setpoint* from the *Controller parameters* menu under the *Parameters* group (Figure 4.12).

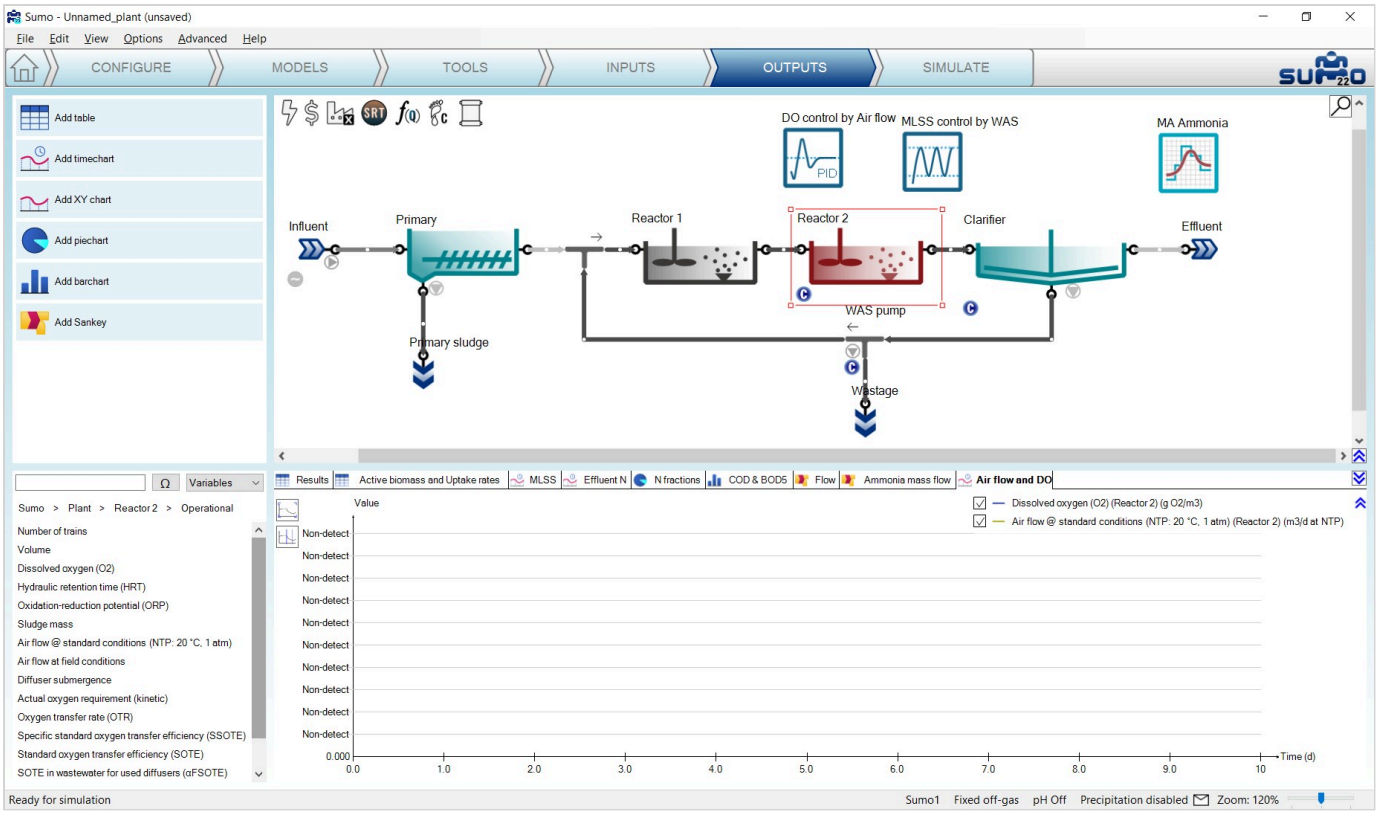


Figure 4.11 – Timechart setup for Input air flow and Dissolved oxygen

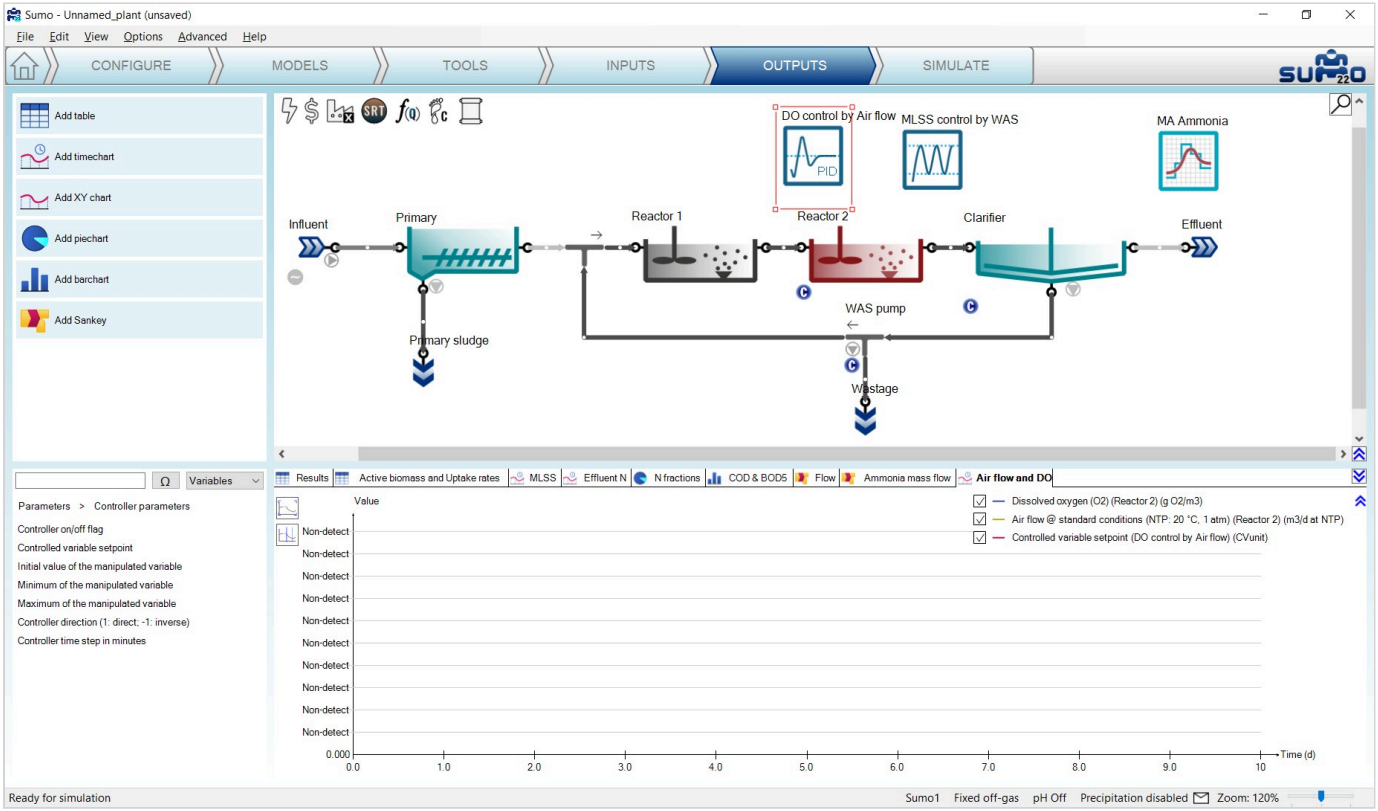


Figure 4.12 – Timechart setup for Controlled variable setpoint

Switch on the diurnal flow dynamic input table for the influent on the *Inputs/Dynamics* tab, then go to the *Simulate* tab and set the stop time to 2 day, then run a dynamic simulation. During the calculation, you can follow the change of the air flow on the *Air flow and DO* timechart (Figure 4.13). Unchecking the *Air flow* item on the timechart, only the dissolved oxygen setpoint and the predicted DO will be shown (Figure 4.14). Using these gain settings, the controller can keep a strict fit to the setpoint without oscillation or overshoot (this can be verified by hovering the mouse on the graph and checking the values on the popup that appears on the timechart).

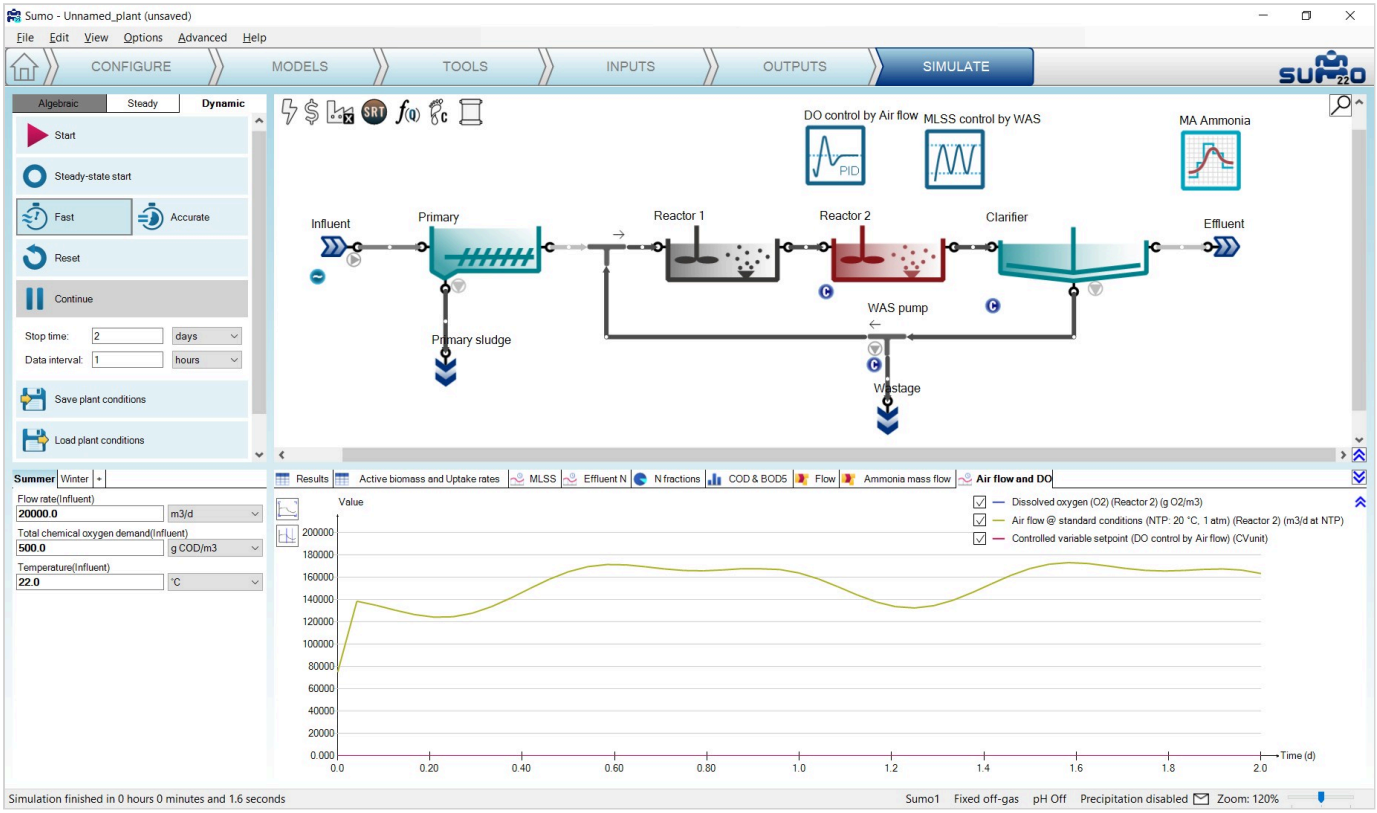


Figure 4.13 - Change of Input air flow PID controller set for DO control

Note: It is good to keep in mind that this plant is subjected to dynamic influent load and a *Deadband MLSS* controller, thus the system never reaches steady state conditions.

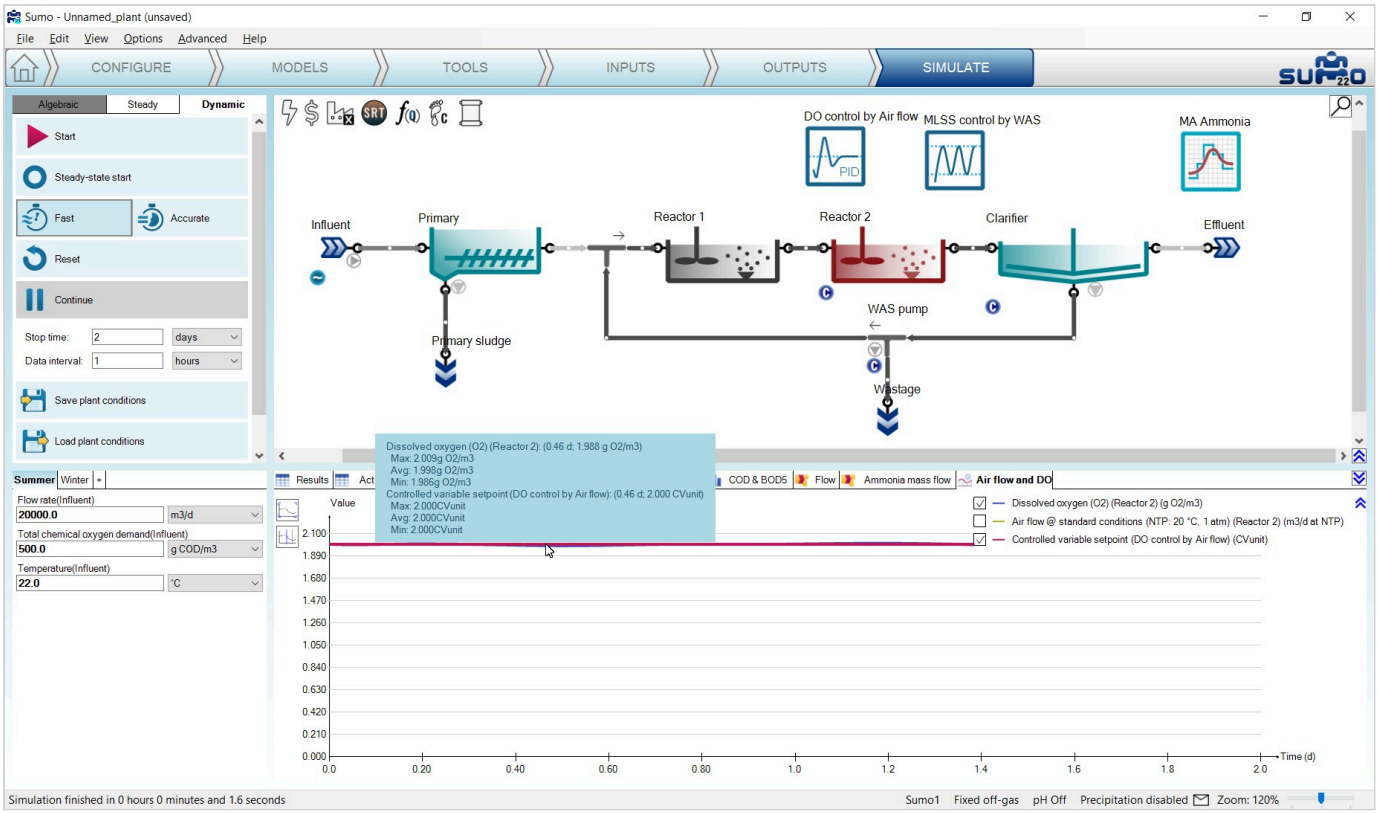


Figure 4.14 - Simulation results with Input air flow PID controller set for DO control

Ratio controller

The Ratio controller is using a ratio as multiplier for the manipulated variable, thus keeping the ratio of the manipulated and the control variable constant during the operation of the facility. To test this function, add a *Carbon dosage* unit (choose the mass flow based & methanol options) using a flow combiner before Reactor 1 of the example project, as shown by Figure 4.15 (renaming the new unit to “Methanol dosage”).

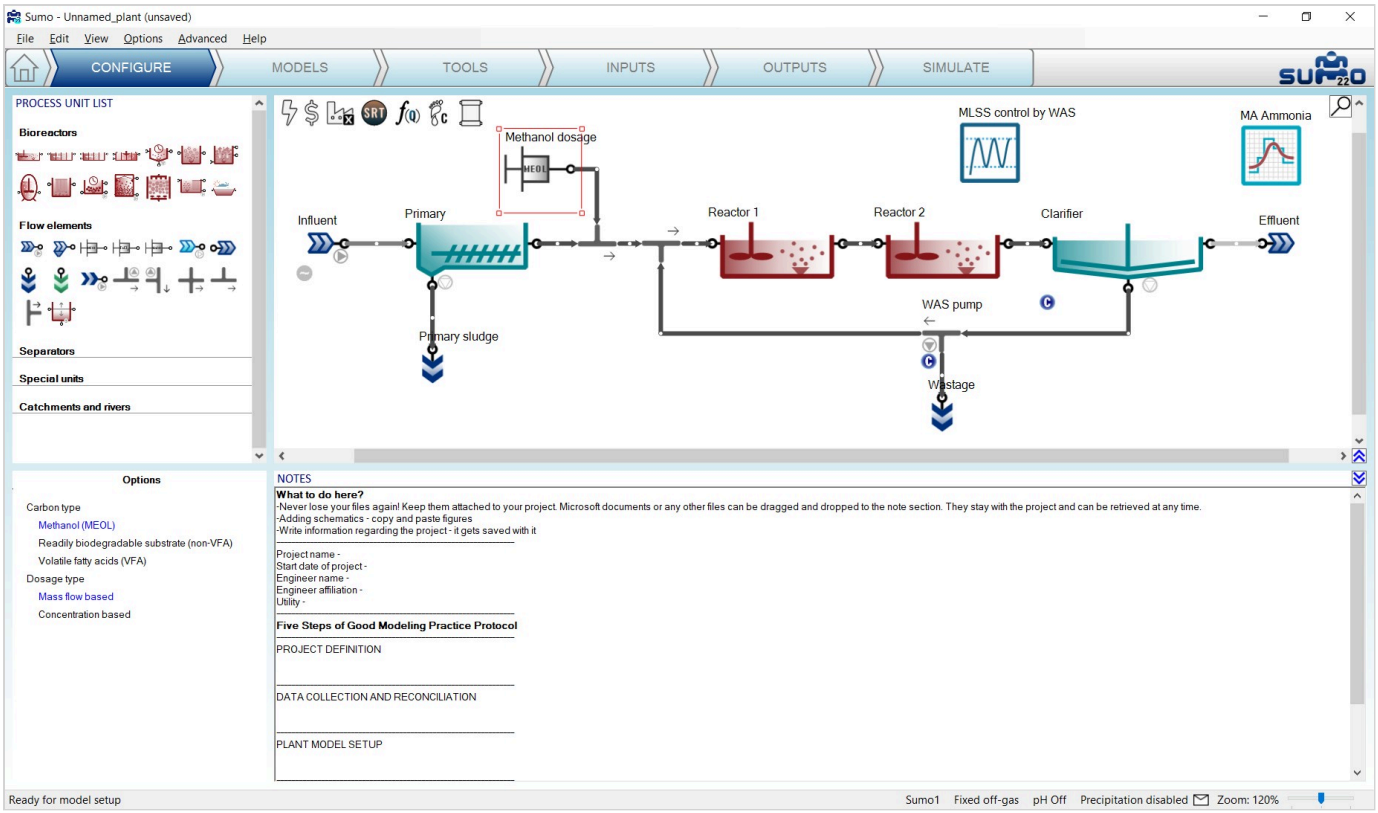


Figure 4.15 – Adding Carbon dosage to the layout

Now add the controller on the *Tools* tab as follows: first drag and drop the manipulated unit to the left side of the equation on the bottom right screen panel and the control unit to the right side of the of the equation. On the bottom left screen panel, you can now select the control variable and the manipulated variable of the selected units. In this example, we will manipulate the methanol dosage unit mass flow rate, depending on the ratio to the influent flow rate. Rename the controller (using F2 or right click) to “Methanol dosage control” (Figure 4.16).

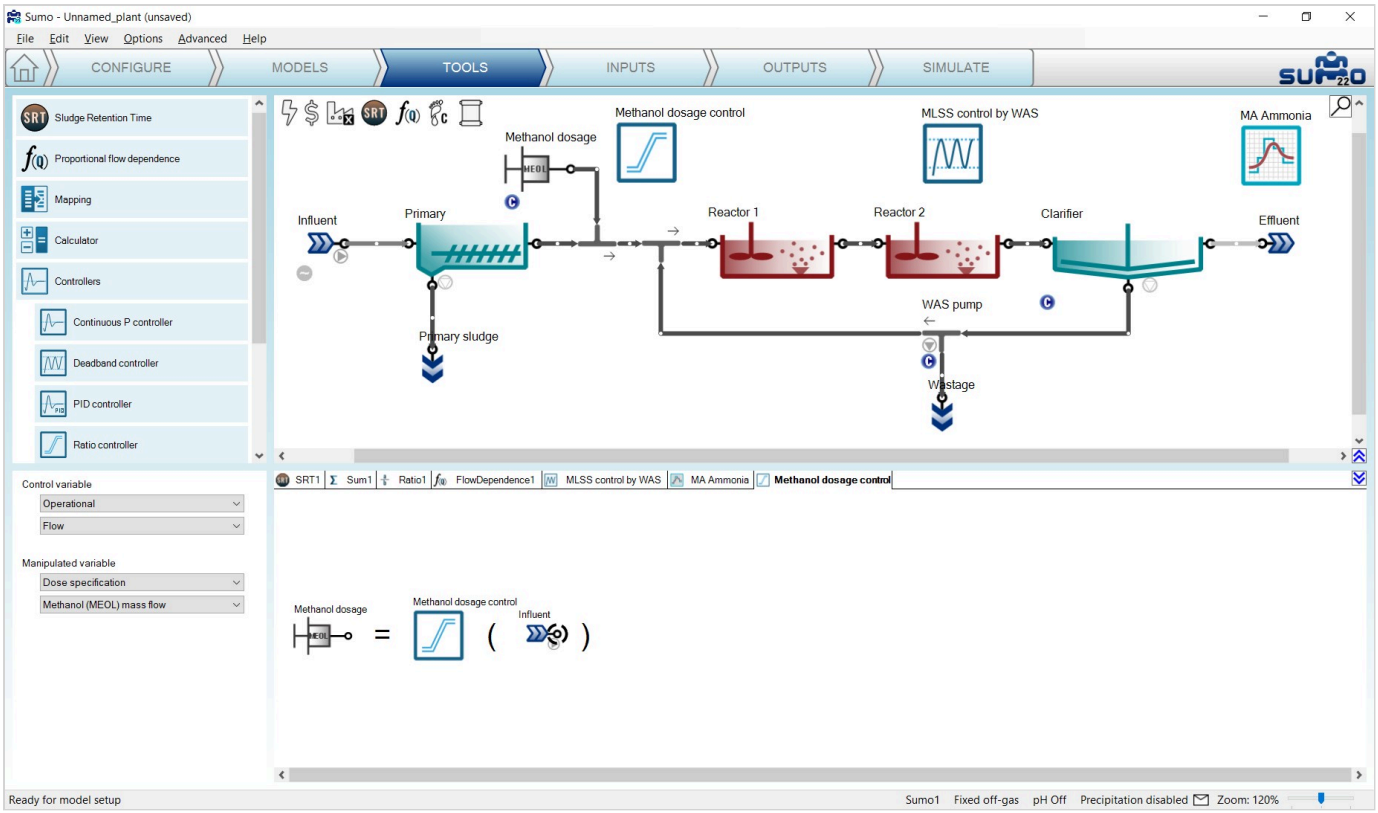


Figure 4.16 – Adding Ratio controller for Methanol dosage control

To properly set the controller parameters, the Unit system selection should be turned to “in code” in the *Options* menu > *Unit systems*. On the *Inputs* tab select the *Methanol dosage* and check the Unit of the mass flow – it is g COD/d (Figure 4.17). Select the new *Methanol dosage controller*. In the *Ratio controller parameters* table set the *Ratio* to 50, thus every influent m^3 wastewater triggers 50 g of COD equivalent methanol dosage. Set the *Minimum value of manipulated variable* to 0, the *Maximum value* to 2.844E07 (equals the capacity of a dosage pump of 1 m^3/h) and the *Initial value* to 1000000 (Figure 4.17). Turn on the dynamic input table for the Influent and leave other settings as they were set previously (Figure 4.17).

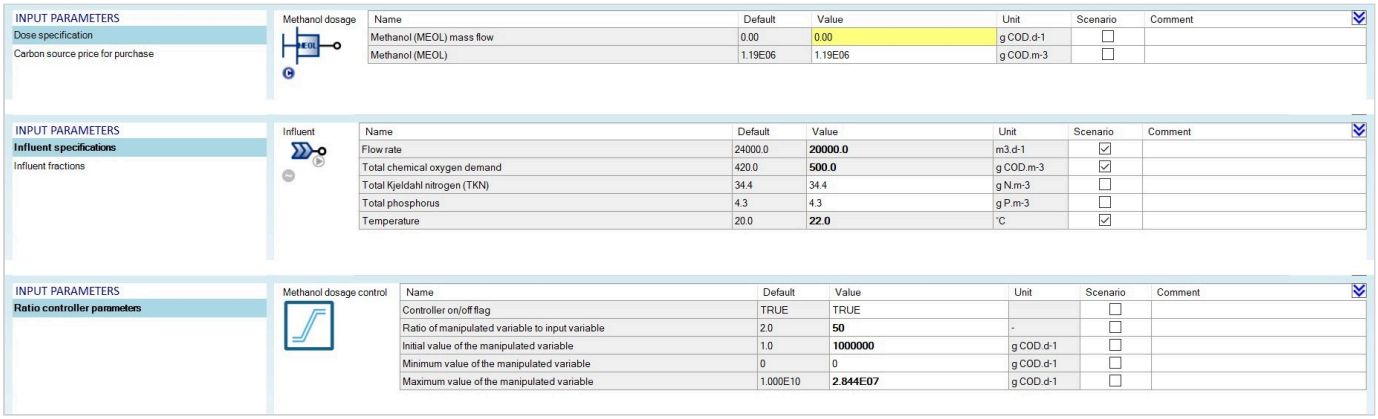


Figure 4.17 - Setup Ratio controller parameters with Unit check

To follow the change of the Methanol dosage before Reactor 1, add a timechart on the *Outputs* tab and name it as “Methanol dosage”. Select the *Methanol dosage* process unit and drop *Flow rate* from the *Operational*

parameters group (Figure 4.18).

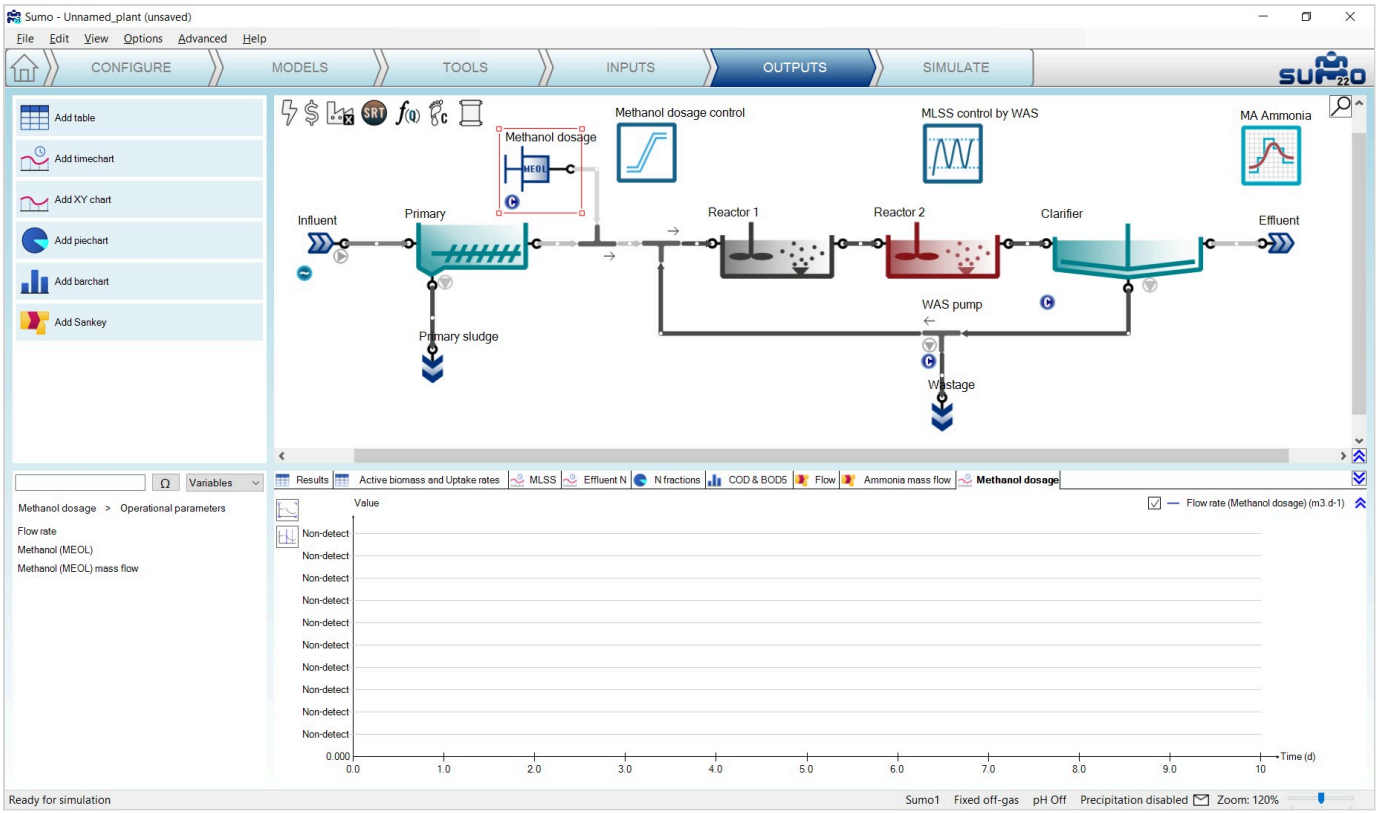


Figure 4.18 – Timechart setup for Methanol dosage flow rate

Go to the *Simulate* tab, set the stop time to 1 day with a data interval of 10 min and run a dynamic simulation. You can follow on the *Methanol dosage* timechart how the methanol dosage flow rate changes during the calculation, responding to the diurnal flow (Figure 4.19).

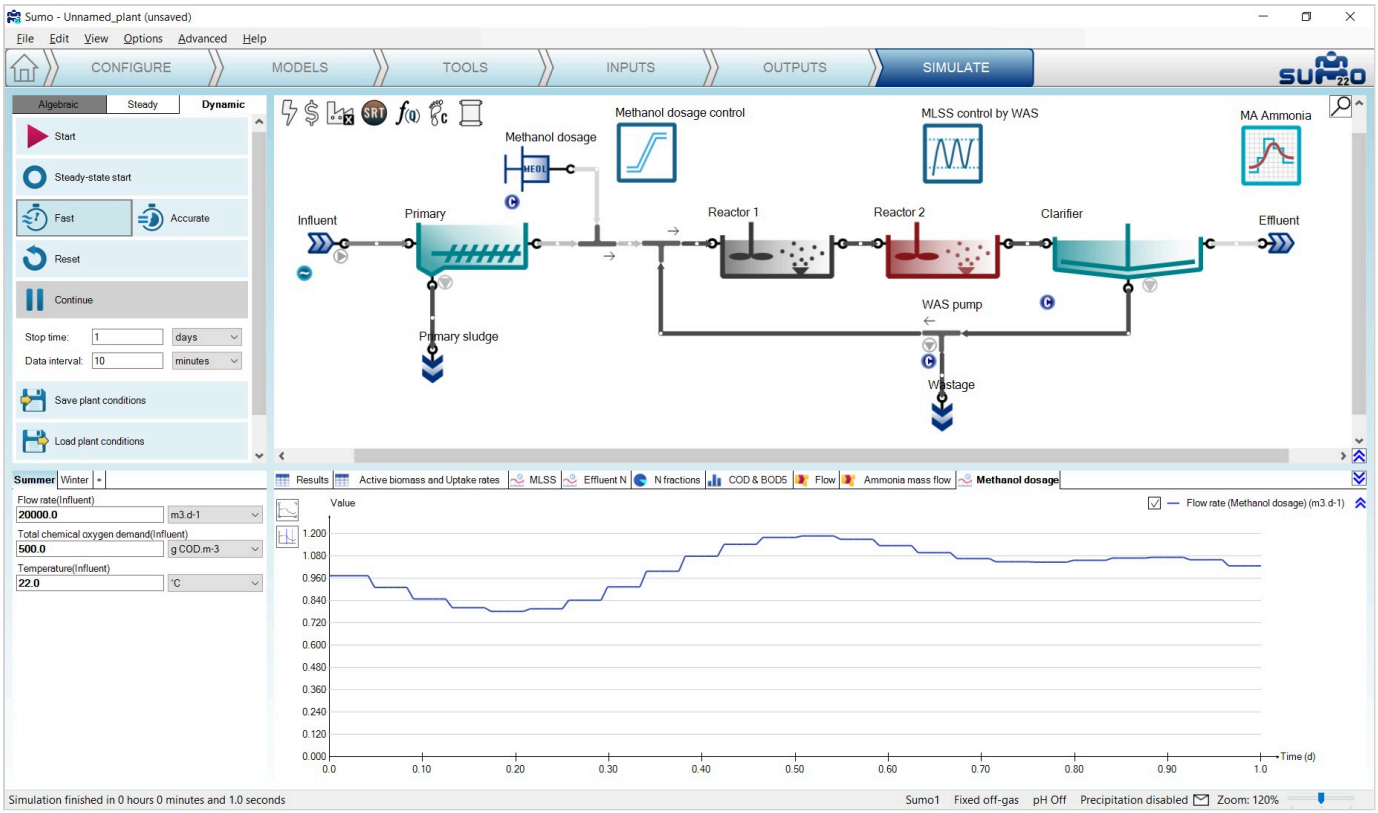
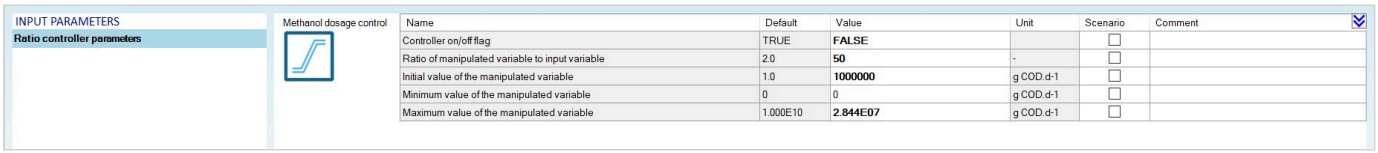


Figure 4.19 - Change of Methanol dosage set by Ratio controller based on Influent flow rate

Now go to the *Inputs* and set the *Controller on-off flag* to 0 for the *Methanol dosage control* unit (Figure 4.20).



Name	Default	Value	Unit	Scenario	Comment
Controller on/off flag	TRUE	**FALSE**		☐	
Ratio of manipulated variable to input variable	2.0	**50**	-	☐	
Initial value of the manipulated variable	1.0	**1000000**	g COD.d-1	☐	
Minimum value of the manipulated variable	0	0	g COD.d-1	☐	
Maximum value of the manipulated variable	1.000E10	**2.844E07**	g COD.d-1	☐	

Figure 4.20 - Turn off Methanol dosage control

Go to the *Simulate* tab, set the stop time 2 days and hit *Continue*. The flow rate of the methanol dosage pump will drop to 0 m^3/d (Figure 4.21), which corresponds to the value given at the *Inputs/Constants* tab as 0 g COD/d dosage rate. Note that the GUI turns the controller color to grey in order to inform the user that it is turned off.

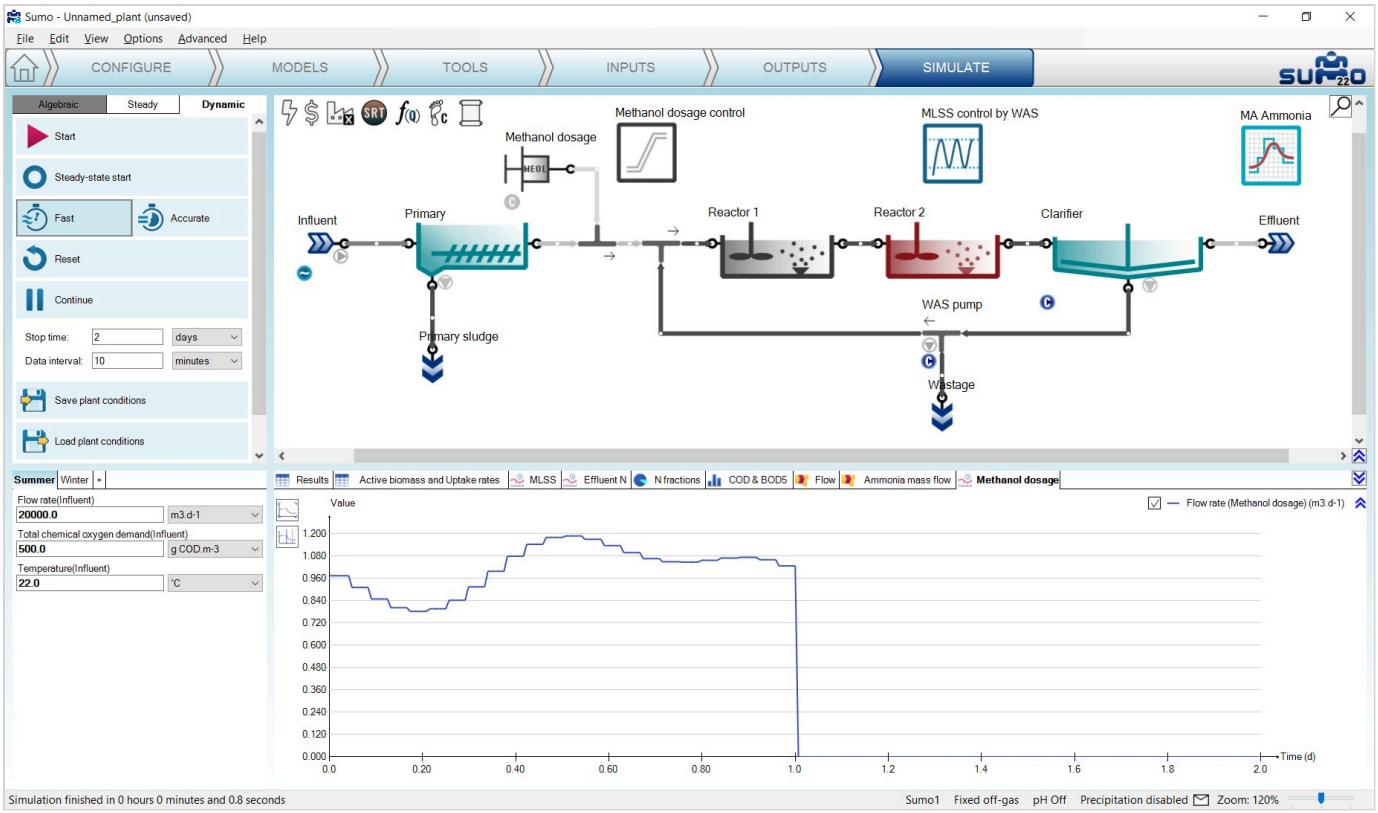


Figure 4.21 - Methanol dosage control shut down

Time based on-off controller

The Time based on-off controller is a controller that sets the input parameter (manipulated variable) of the desired process unit based on a time step between a defined high and low value. This controller has no measured variable input (no control variable).

To demonstrate the capabilities of this controller, let us set Reactor 2 to use the *Calculated* option for Dissolved oxygen (*Configure* tab). Then add the controller and configure on the *Tools* tab as follows. First drag and drop the manipulated process unit (Reactor 2) to the left side of the equation in the bottom right screen panel. On the bottom left screen panel, you can now select the manipulated parameter of the selected unit. In this example, we will generate intermittent aeration in the chosen reactor by changing the air flow (located under *Aeration settings*). Rename the controller (using F2 or right click) to “Intermittent aeration” (Figure 4.22). This will rename the tab as well.

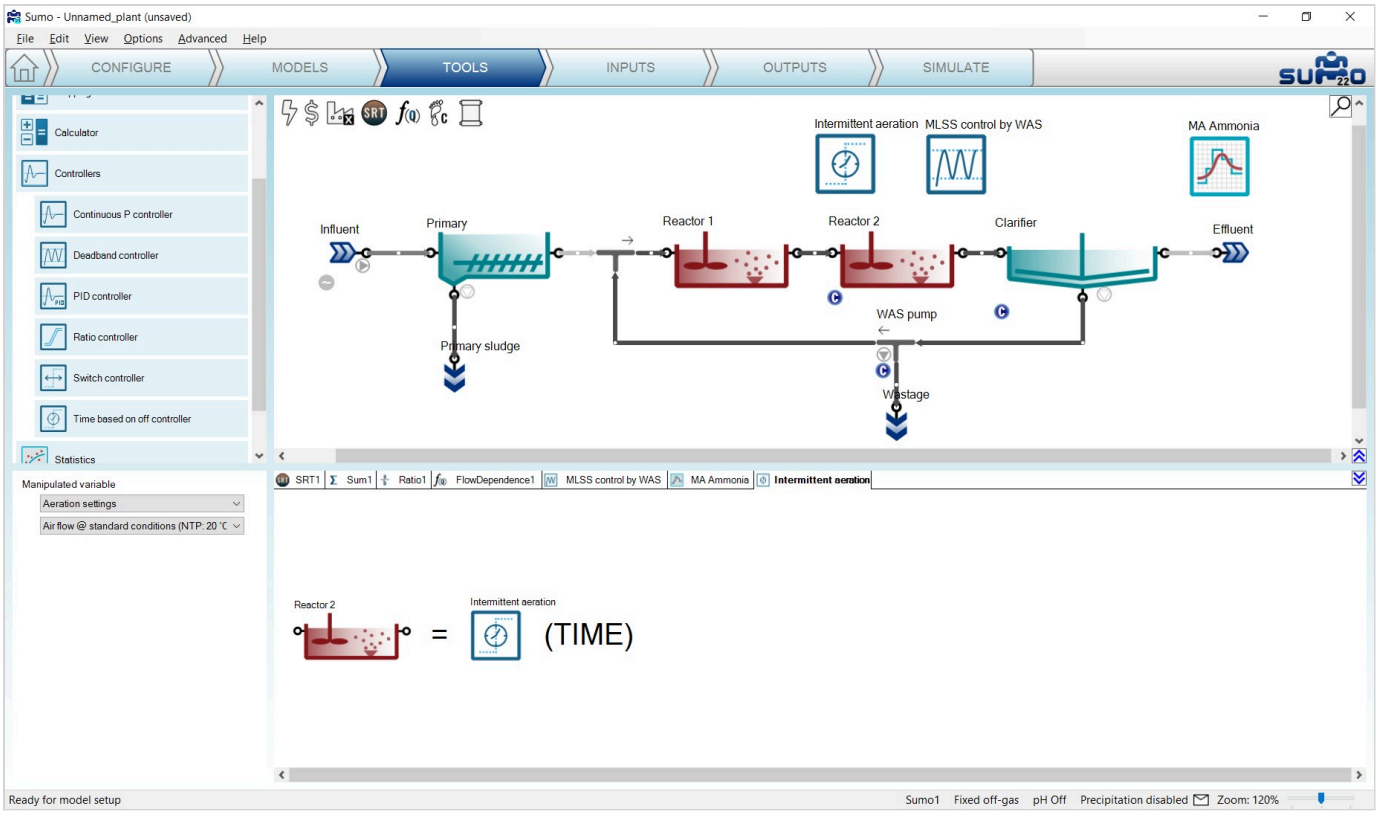
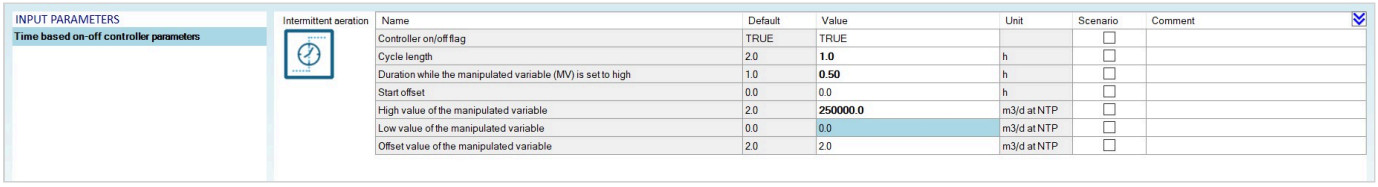


Figure 4.22 – Adding a Time based on-off controller

On the *Inputs* tab, select the new *Intermittent aeration* controller and review the *Time based on-off controller parameters* table. Set the *Cycle length* to 1 h, the *Duration while the manipulated variable is set to high* parameter to 0.5 h (aeration will be turned on for 30 min) and the *High value of the manipulated variable parameter* to 250000 m^3/d, leaving the other parameters at default (Figure 4.23).



Name	Default	Value	Unit	Scenario	Comment
Controller on/off flag	TRUE	TRUE			
Cycle length	2.0	**1.0**	h		
Duration while the manipulated variable (MV) is set to high	1.0	**0.50**	h		
Start offset	0.0	0.0	h		
High value of the manipulated variable	2.0	**250000.0**	m3/d at NTP		
Low value of the manipulated variable	0.0	0.0	m3/d at NTP		
Offset value of the manipulated variable	2.0	2.0	m3/d at NTP		

Figure 4.23 - Setup Time based on-off controller parameters

Before moving on, also make sure that the diurnal flow dynamic input table is turned on for the influent.

To follow the changes in the aeration of Reactor 2, add a timechart on the *Outputs* tab and rename it to “Air flow and DO”. Select Reactor 2 and drop *Dissolved oxygen* and *Input air flow* from *Operational* menu (same method as described in the PID controller chapter, see Figure 4.11).

Now go to the *Simulate* tab, set the stop time to 1 day with 1 minute data interval and run a dynamic simulation from steady state. During the calculation, you can follow the periodic changes in the air flow on the timechart (Figure 4.24).

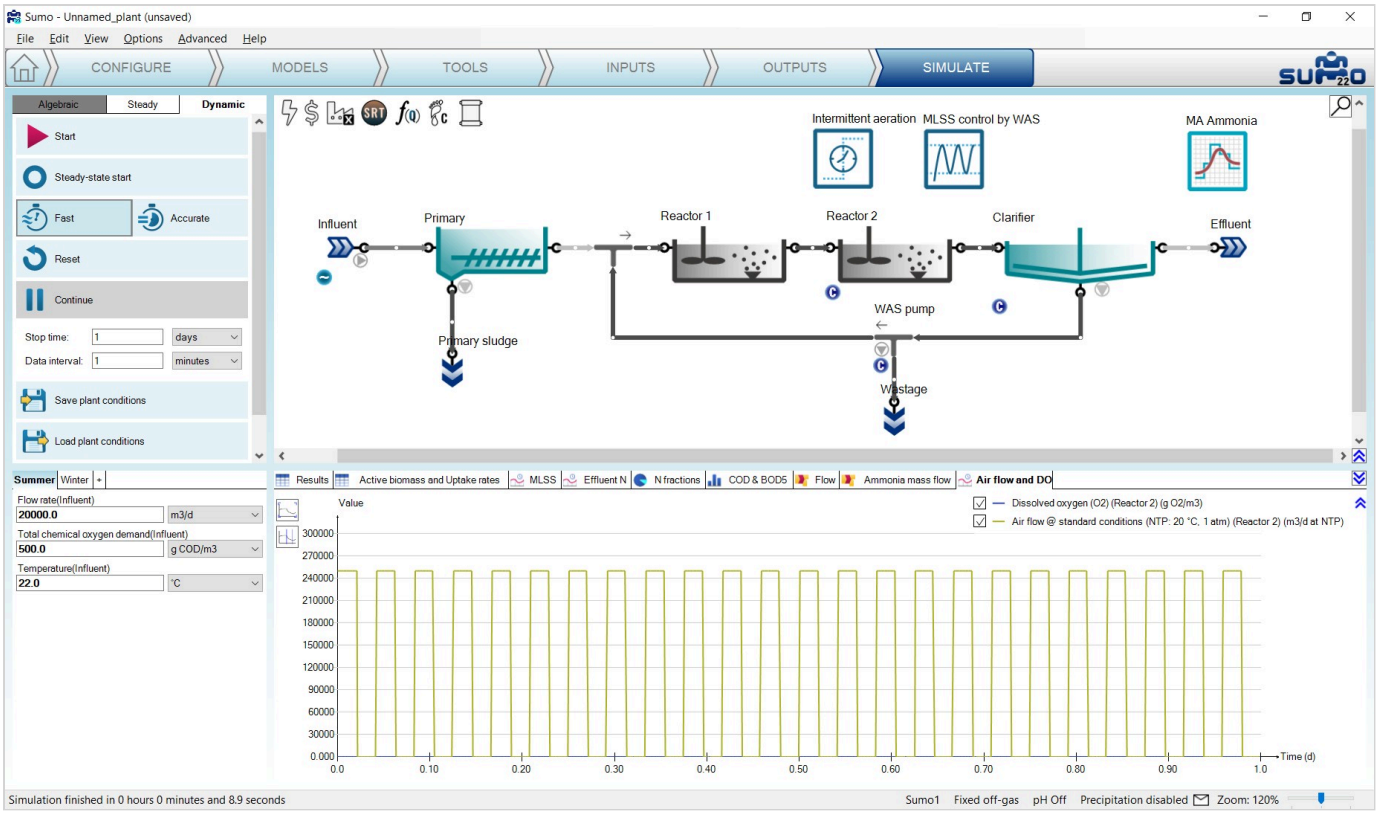


Figure 4.24 - Change of Input air flow set by Time based on-off controller

Unchecking the curve for the *Air flow*,in the legend, the resulting periodic changes in the dissolved oxygen can be seen in details. (Figure 4.25). The effect of the diurnal flow pattern can also be observed.

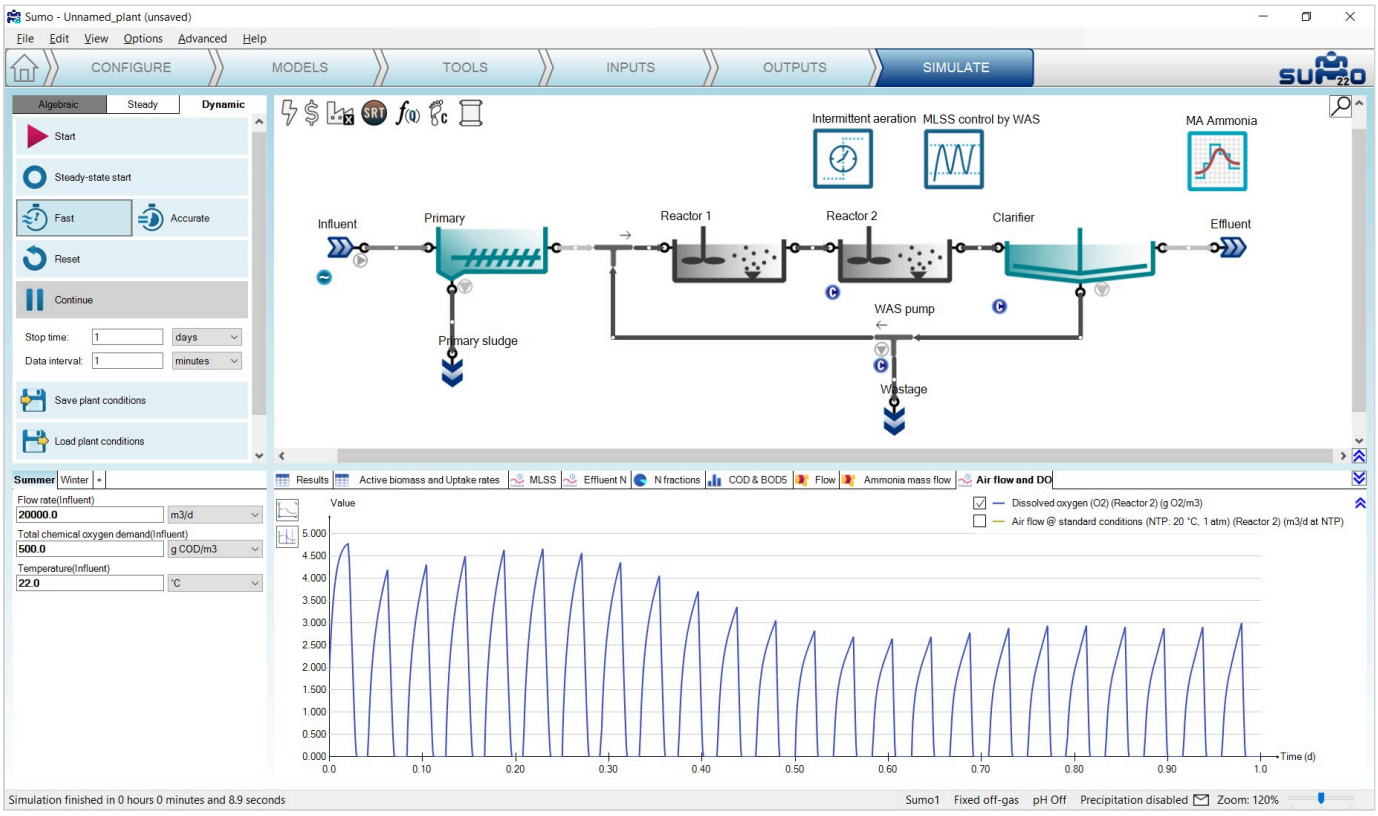


Figure 4.25 - Changes in DO resulting from the Time based on-off controller and the diurnal flow pattern

Switch controller

The Switch controller is a controller that sets the input parameter (manipulated variable) of the desired process unit between two defined values (using an S-shaped function), depending on whether the control variable is above or below a defined threshold.

To demonstrate how this controller works, open the example project, add the controller and configure on the *Tools* tab according to the following. First drag and drop the manipulated process unit (Reactor 1) to the left side of the equation in the bottom right screen panel, then drag and drop the control unit (Effluent) to the right side of the equation. On the bottom left screen panel, select ammonia from the *Frequently used variables* as control variable and select air flow (located under *Aeration settings*) as the manipulated parameter. We will use this controller to apply intermittent aeration in the chosen reactor in order to meet the desired effluent ammonia concentration. Rename the controller (using F2 or right click) to “ABAC” (Figure 4.26). This will rename the tab as well.

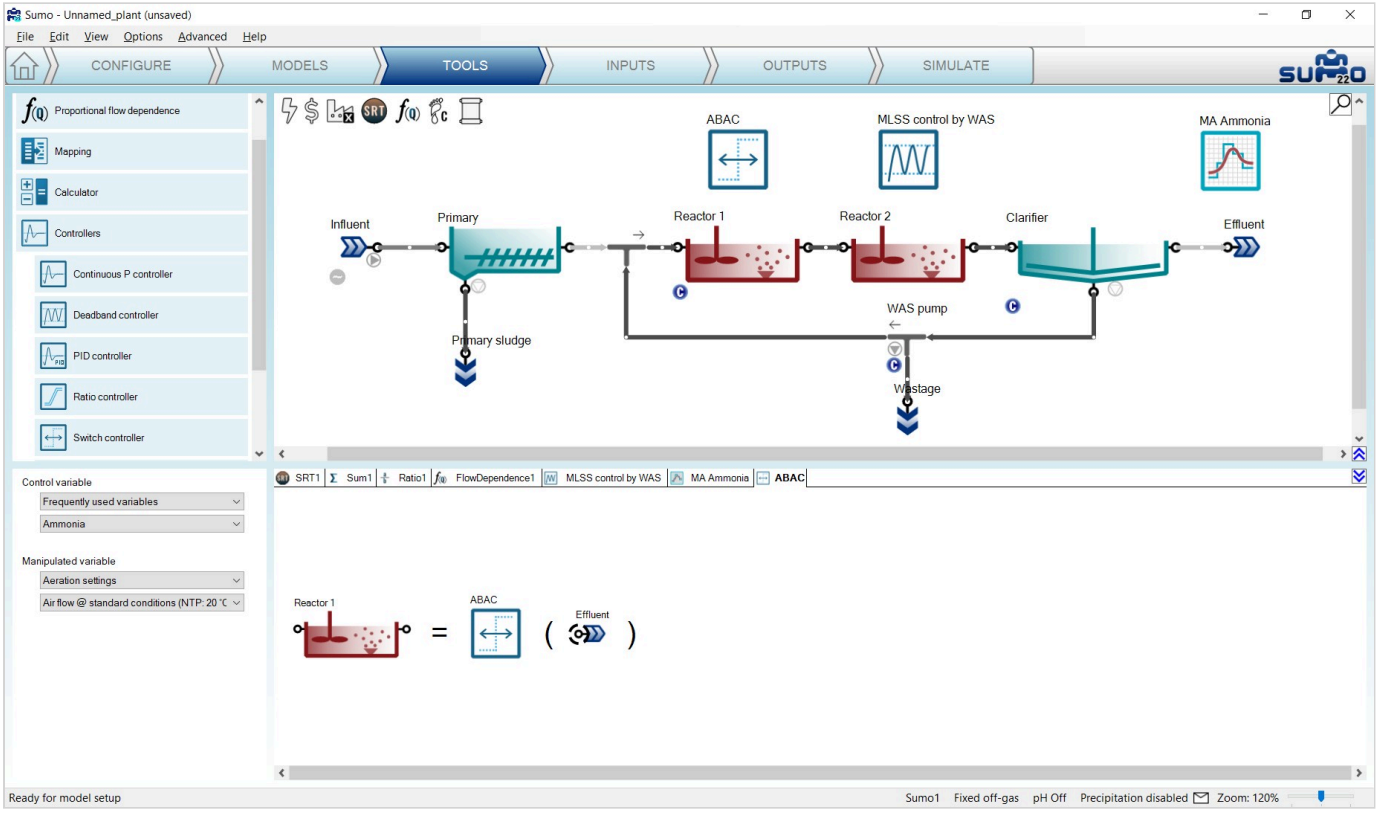


Figure 4.26 - Adding a Switch controller for ammonia-based aeration control

On the *Inputs* tab, select the new *ABAC* controller and review the *controller parameters* table. Set the *Controlled variable threshold* to 0.25 g N/m^3 (this is a somewhat lower value than what the example layout could achieve for effluent ammonia), the *Value of manipulated variable above threshold* parameter to 35000 m^3/d. By clicking on the *Show all* button in the bottom left panel, reveal *Numerical parameters* table and set the *Slope of switch function* to 0.0001 (this parameter sets the slope of the S-shaped function that is used by the controller). Leave all other parameters at default (Figure 4.27).

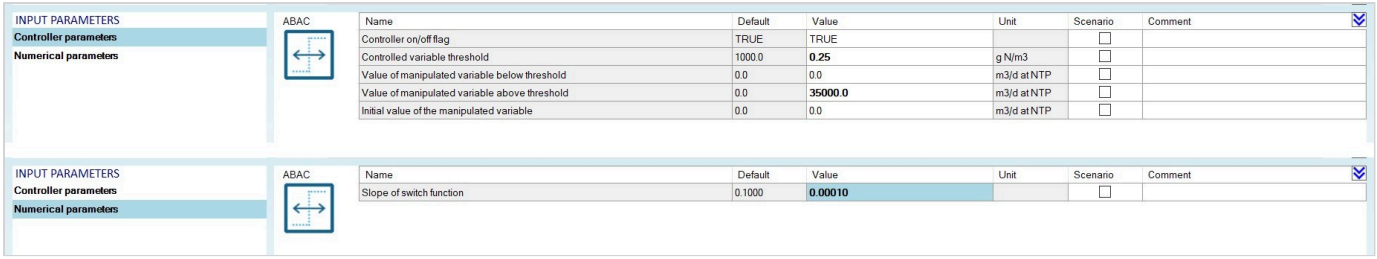


Figure 4.27 - Setup Switch controller parameters

For this exercise, leave the diurnal flow dynamic input table for the influent turned off.

To follow the changes in the aeration of Reactor 1 and its effect on the effluent ammonia, add a timechart on the *Outputs* tab and rename it to “ABAC”. Select Reactor 1 and drop *Dissolved oxygen* and *Air flow @ standard conditions* from the *Operational* menu (same method as described in the PID controller chapter, see Figure 4.11). Then select the *Effluent* process unit and add *Total ammonia* from the *Nitrogen components* menu.

Now go to the *Simulate* tab, set the stop time to 1 day with 1 minute data interval and run a dynamic simulation. During the calculation, you can follow the periodic changes in the air flow on the timechart (Figure 4.28).

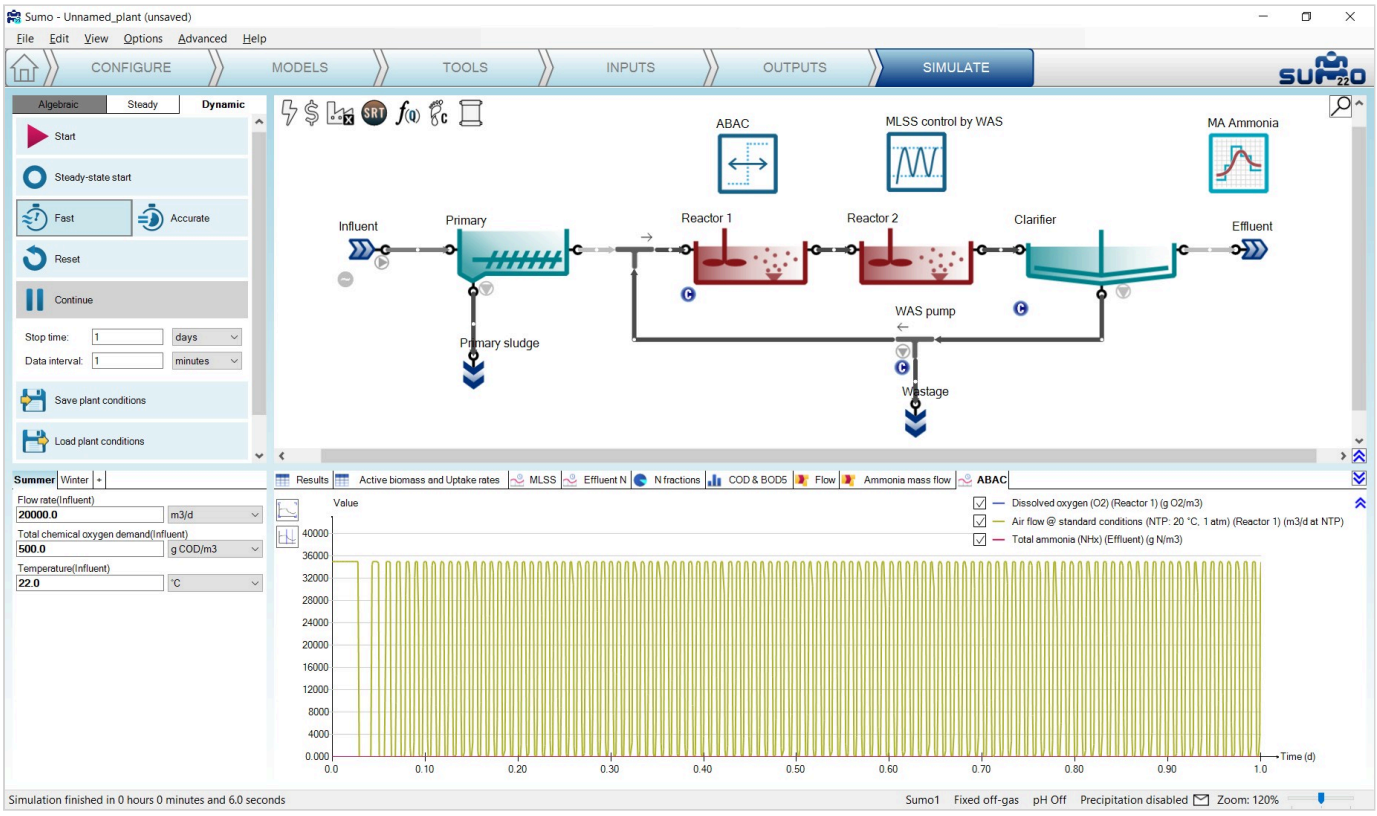


Figure 4.28 - Change of Input air flow set by Switch controller

Unchecking the curve for the *Air flow* in the legend, the resulting periodic changes in the reactor dissolved oxygen and the effluent ammonia can be seen in details. (Figure 4.29).

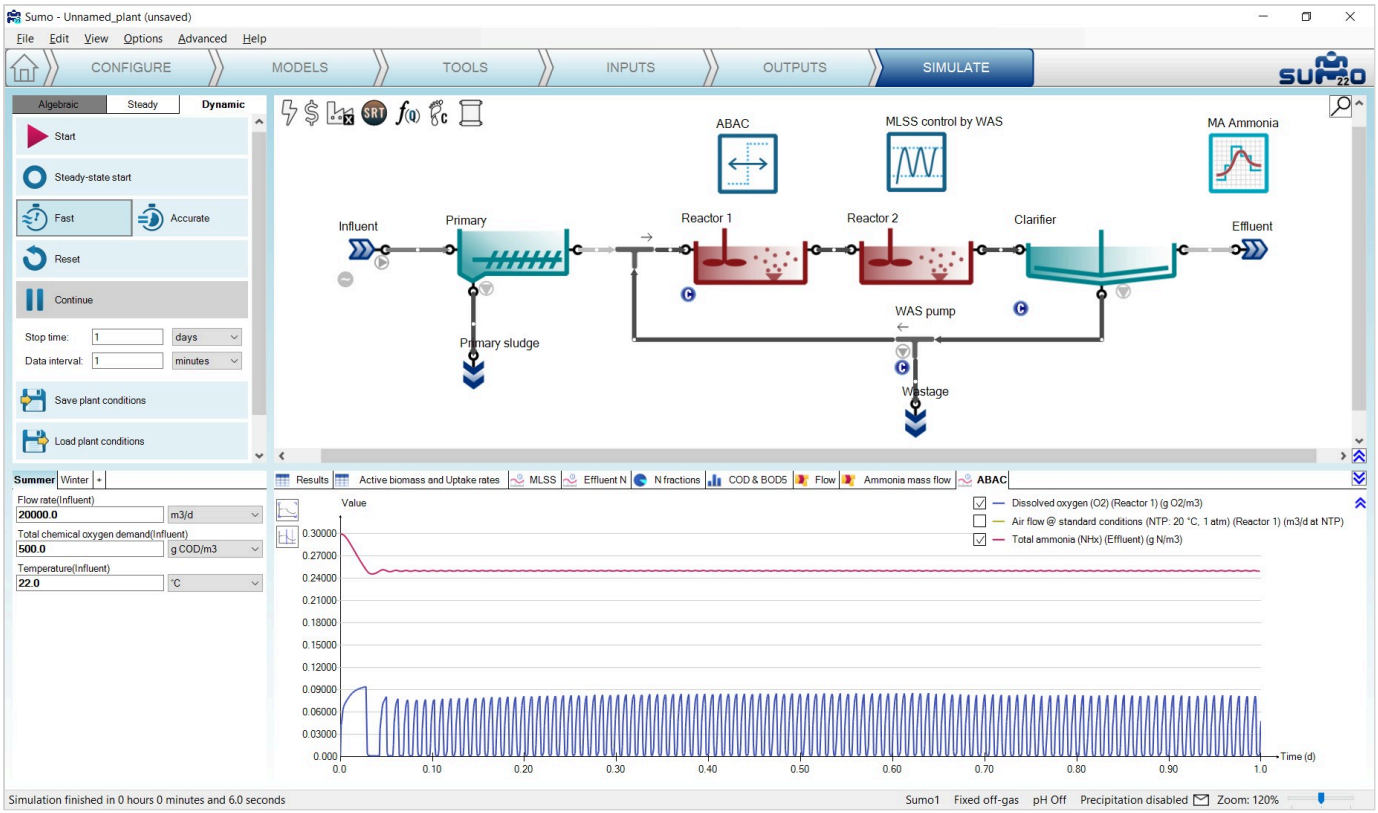


Figure 4.29 - Changes in reactor DO and effluent ammonia resulting from the Switch controller without diurnal flow

Now turn on the dynamic input table for the influent on the *Inputs/Dynamics* tab, increase the *Value of manipulated variable above threshold* of the ABAC controller to 70000 m^3/d on the *Inputs/Constants* tab and run a new simulation from steady state. On the same timechart, you can follow how the controller adjusts the aeration in order to maintain the effluent ammonia concentration around the desired value despite of the diurnal flow pattern (Figure 4.30). As an exercise, you can investigate how the controller would work with the previous *Value of manipulated variable above threshold* setting and what effect would that have on the effluent ammonia.

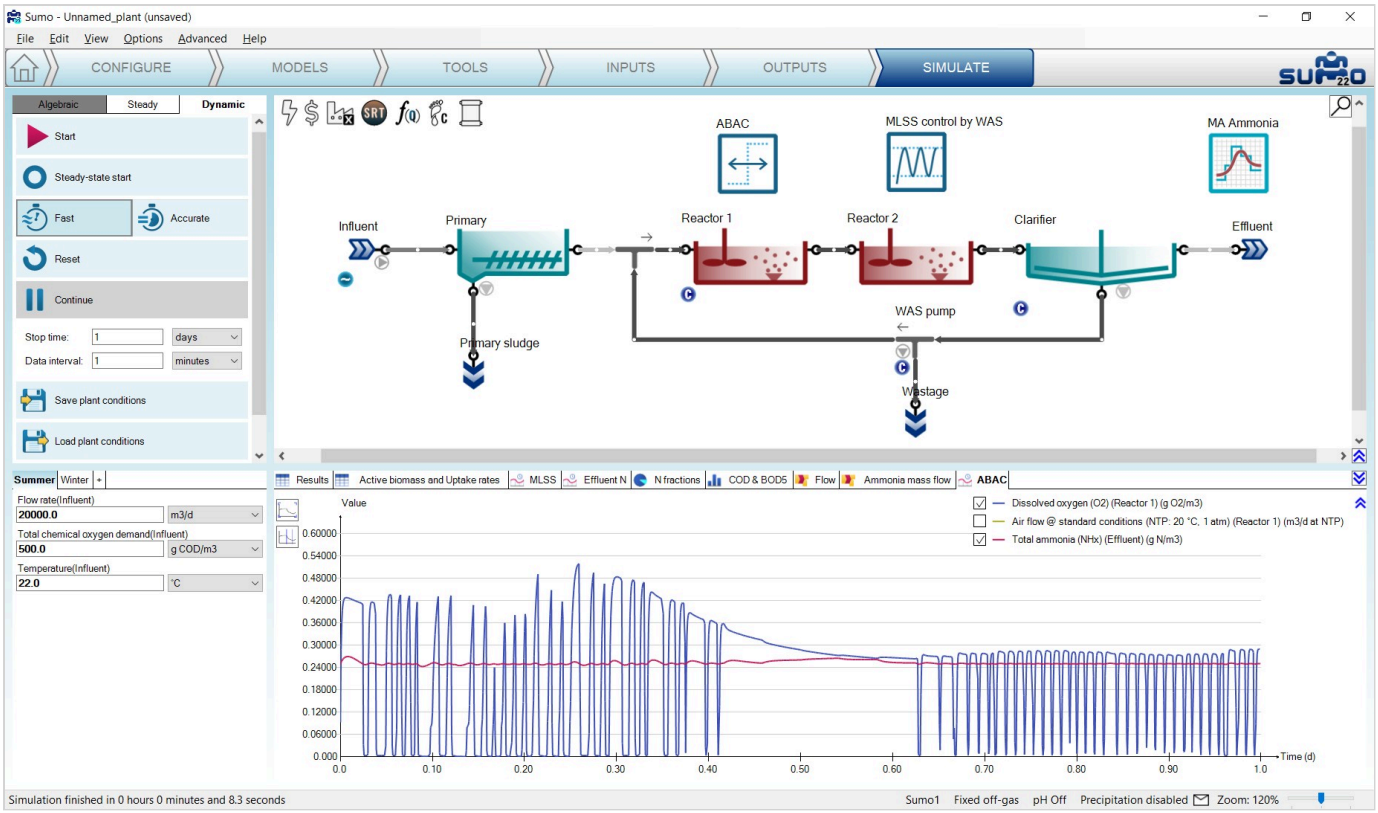


Figure 4.30 - Changes in reactor DO and effluent ammonia resulting from the modified Switch controller with diurnal flow

Cascade controller

Cascade controllers can as well be set up in Sumo22, using the methods described above. To set up a cascade controller example, a PID and a Time-based on-off controller will be used in conjunction. Based on the time-based controller example it can be easily shown how the DO calculation effects the process in the reactors. To see the effect of calculated DO, the example prepared with the PID controller will be continued. In that example, the DO is calculated in Reactor 2 (Figure 4.31).

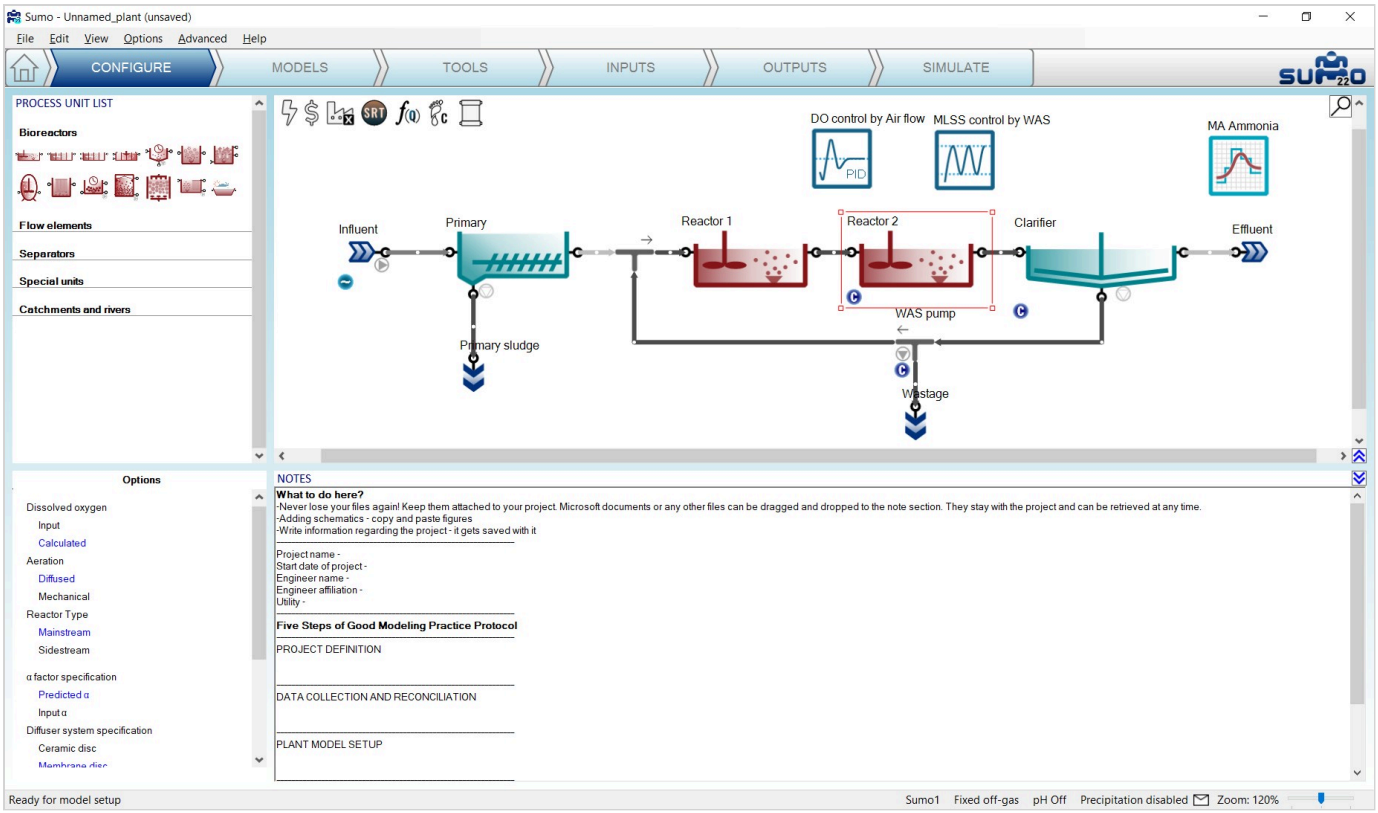


Figure 4.31 - Reactor 2 with Calculated DO and PID controller set up in a previous example

Go to the *Tools* tab and add a Time based on-off controller. In this example, we will generate a high-low setpoint, time-based aeration, by changing the DO setpoint, which is controller setpoint of the PID controller. To set up the Time based on-off controller, drag and drop the *DO Control by Air flow* controller icon from the drawing board to the left side of the equation in the bottom right panel and select *Controlled variable setpoint* from the *Controller parameters* menu in the bottom left panel. Rename the unit (using F2 or right click) – along with the tab – to “High-low setpoint aeration”. (Figure 4.32)

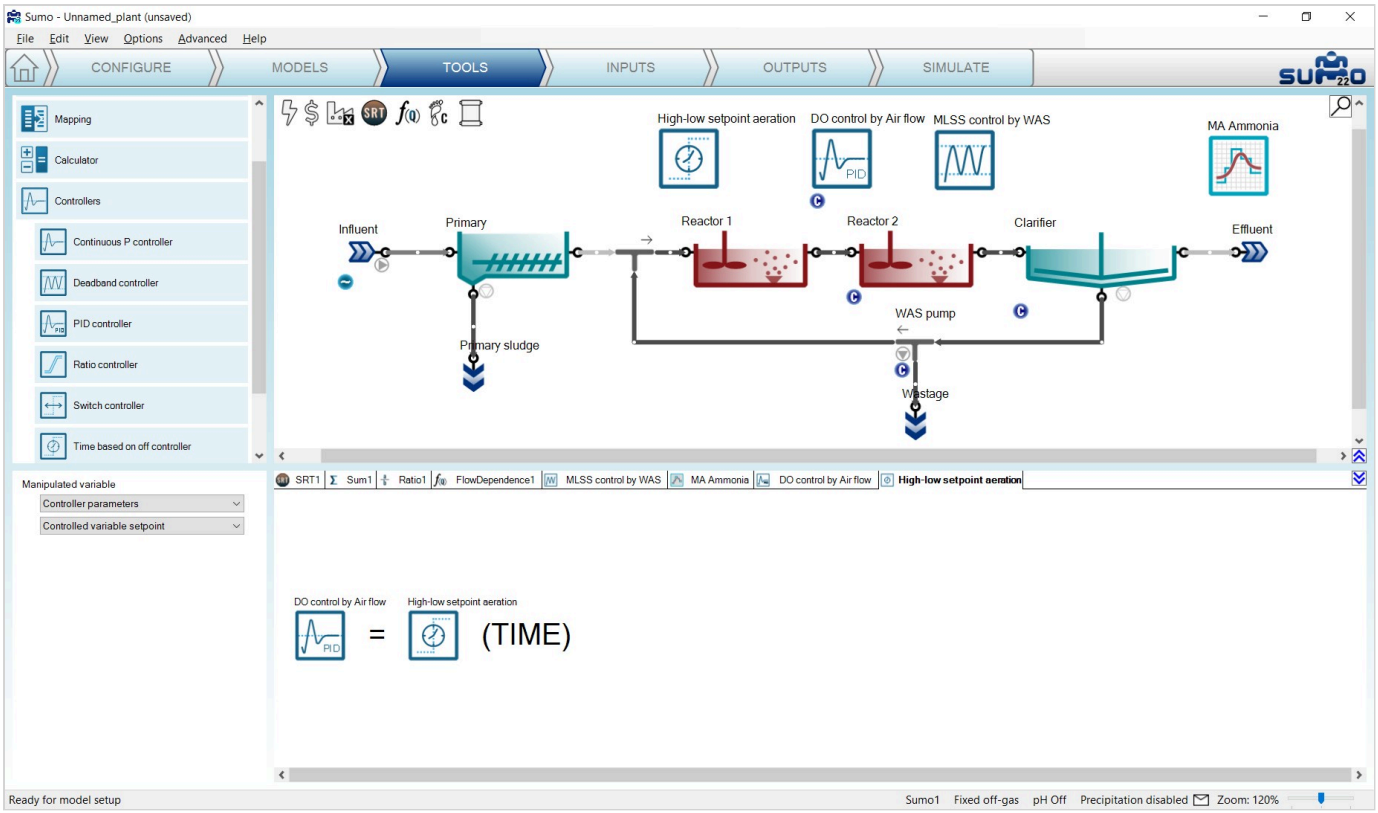


Figure 4.32 - Time based on-off controller setup

On the *Inputs* tab, select the new *High-low setpoint aeration* controller and in the *Time based on-off controller parameters* menu set the following (Figure 4.33):

- the *Cycle length* to 2 h (this is the default value),
- the *Duration while the manipulated variable is set to high* to 1 h (higher setpoint will be in effect for 1 h),
- *Low value of the manipulated variable* to 50% (or 0.5 without unit, depending on the *Unit system* settings), this equals 0.5 g O_2/m^3 as dissolved oxygen setpoint, and leave the other parameters as default.

Now select the *DO control by Airflow* controller and in the *Controller parameters* menu, set the *Controller time step* to 1 min (Figure 4.33).

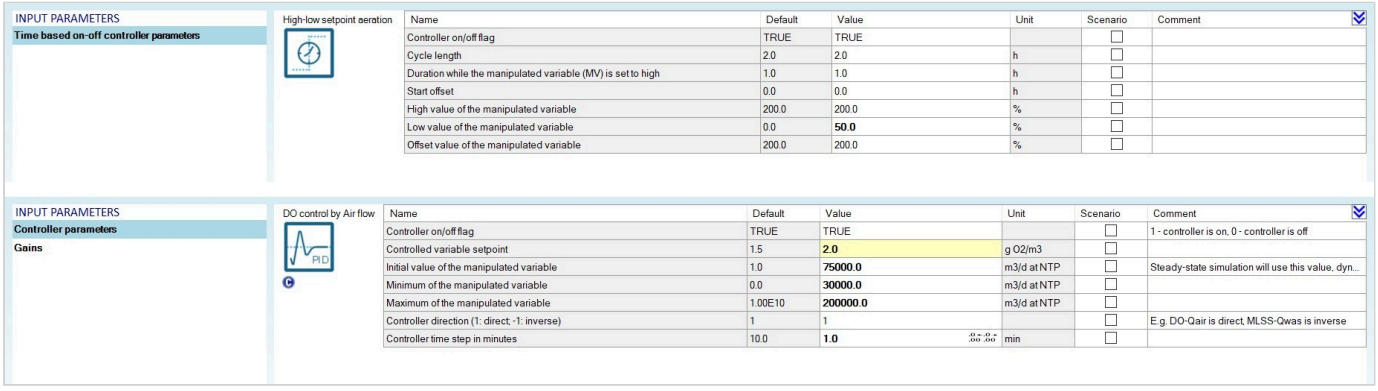


Figure 4.33 - Cascade controller setup for intermittent aeration

Go to the *Simulate* tab, set the stop time to 1 d and the data interval to 1 minute and start simulation. Select the “Air flow and DO” timechart. The change of DO follows the aeration change controlled by the PID controller (Figure 4.34). Compare the new results with the results of the simple Time based on-off controller exercise on Figure 4.25.

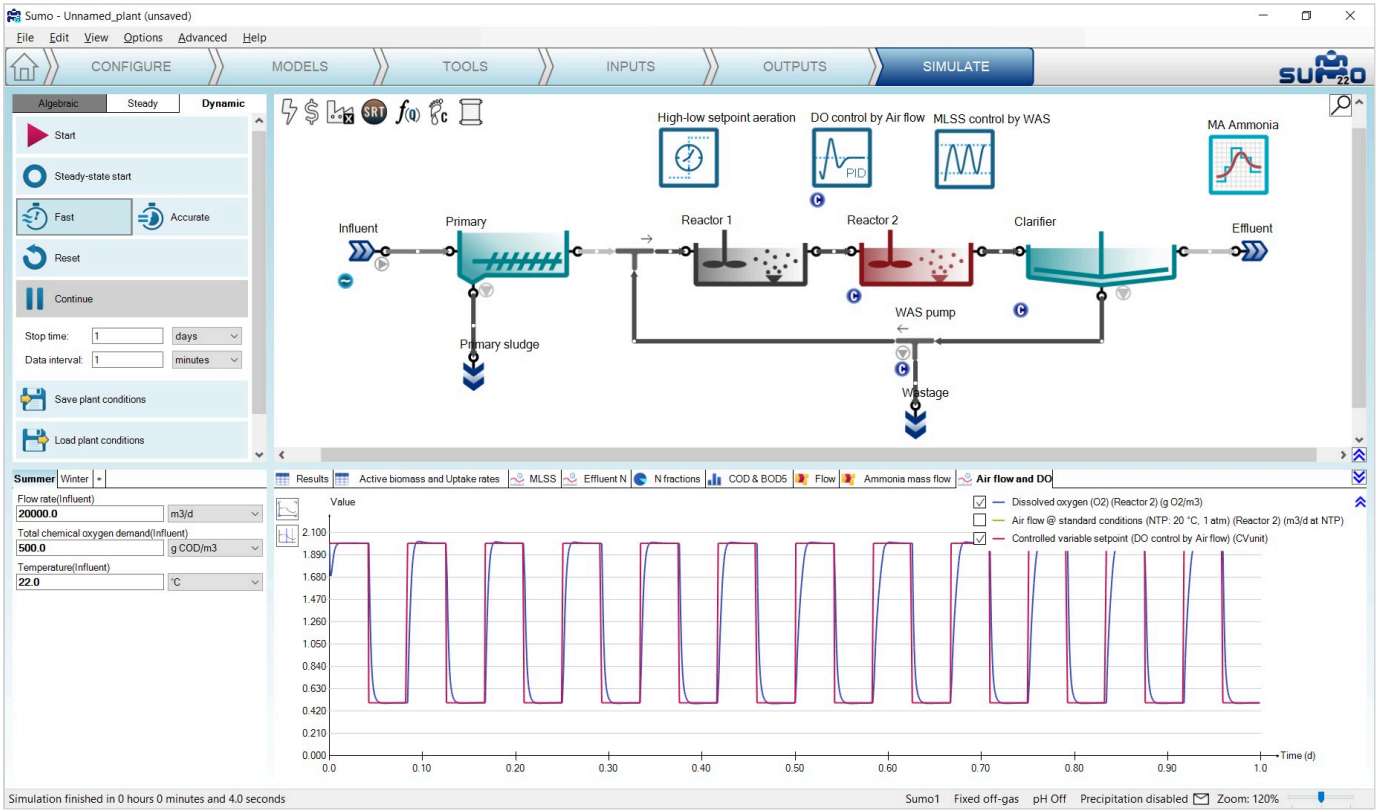


Figure 4.34 - The change of DO at Reactor 2 with PID aeration control of intermittent aeration

The change of Input air flow (Figure 4.35) shows a really different profile compared with the simple Time based on-off controller exercise (Figure 4.24).

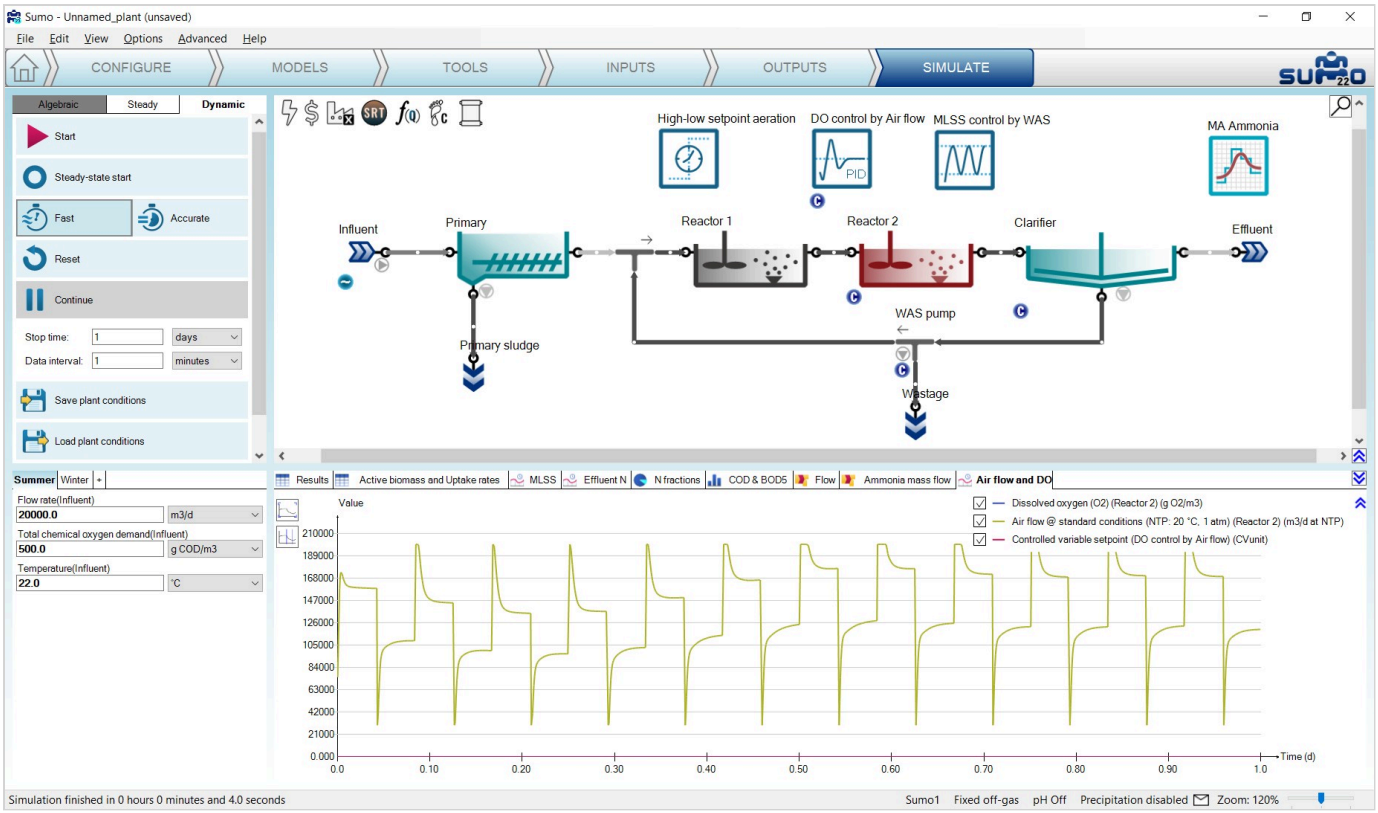


Figure 4.35 - Input air flow dynamics of Reactor 2 with PID aeration control of intermittent aeration

Energy and cost calculations

Sumo features additional layers of energy and cost calculations, based on the process model. The energy mode can be used to assess the electricity demand of aeration, mixing, pumping and other equipment operation, as well as the available potential to produce electricity from biogas produced in digesters (enabling self-sufficiency assessment and scenario analysis for energy savings). The cost layer can be useful for evaluating and improving plant operation from an economic standpoint, by comparing the various cost items associated with the components of the energy balance and the usage of chemicals. In this chapter, an overview of the possibilities will be presented, based on the example project built in the How to use Sumo for simulations chapter.

The status of the energy and cost layers is indicated by the first two icons in the top left corner of the plant layout screen panel (Figure 5.1). By default, the energy mode is inactive and cost calculations are limited to basic inputs. While the energy mode is inactive, the cost center can be supplied with input data by selecting the **$** icon in the *Inputs* tab. At this level, simple specific prices can be defined for electricity, water and polymer usage, as well as disposal fees and product sales (Figure 5.2).

Figure 5.1 - The ‘Energy center’ and ‘Cost center’ icons precede the ‘Plantwide’ icon

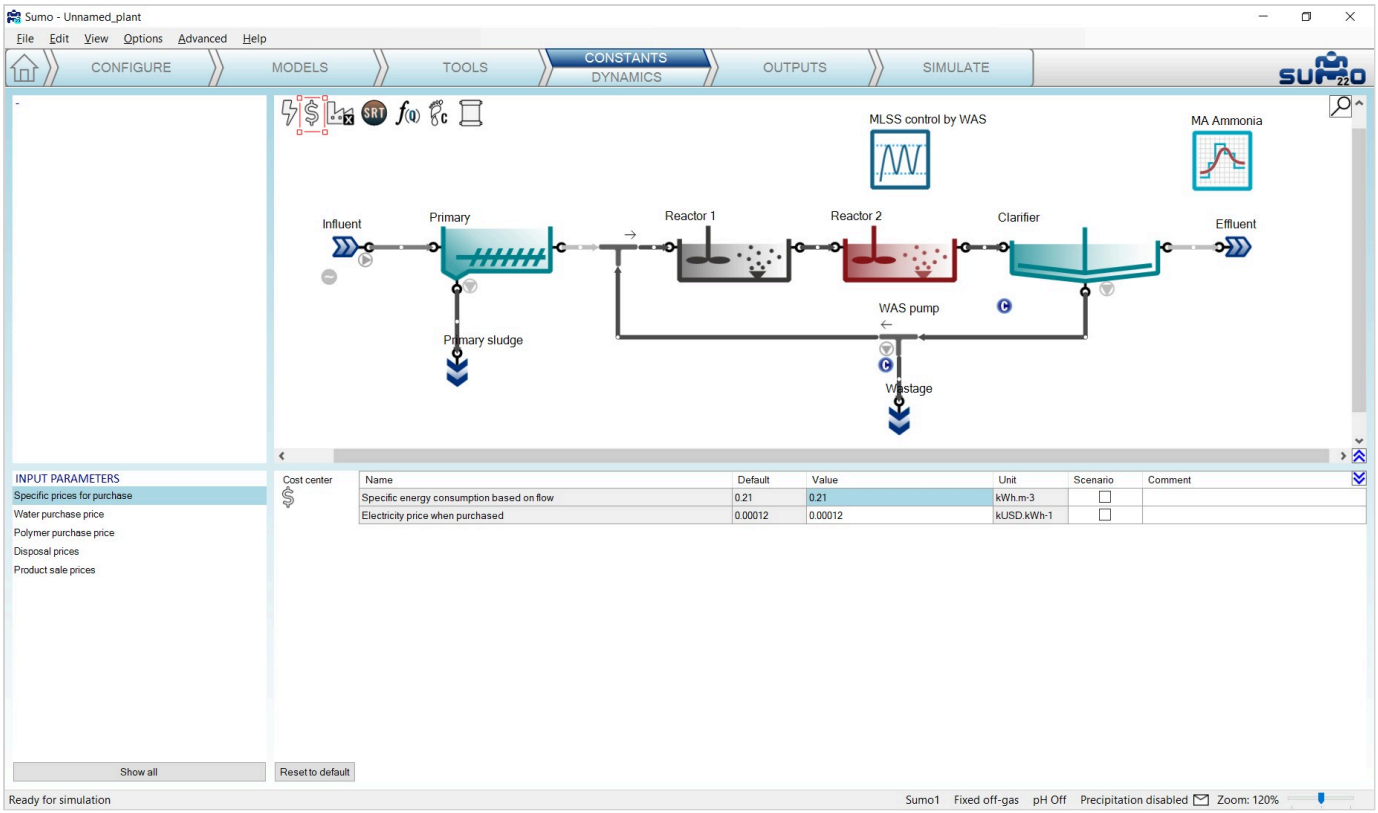


Figure 5.2 – Basic settings available for the ‘Cost center’ on the Inputs tab

In order to fully exploit the capabilities of cost calculation, the energy mode shall be activated. This can be done by double-clicking on the *Energy center* icon (which will turn to yellow) or right-clicking and selecting “Turn Energy On”. Along with this, the *Cost center* icon will turn to black from hollow, and the specific price input options will also adapt to the energy mode (as well as the underlying cost calculations).

The *Energy center* plantwide input parameters are also available on the *Inputs* tab, by selecting the lightning bolt icon (Figure 5.3). Here you can specify general energy consumers that are grouped into periphery consumers (ventilation, water supply and miscellaneous), other variable and fixed consumers, as well as different on-site electricity producers and power storage options (depending on the settings of the *Configure* tab, see below).

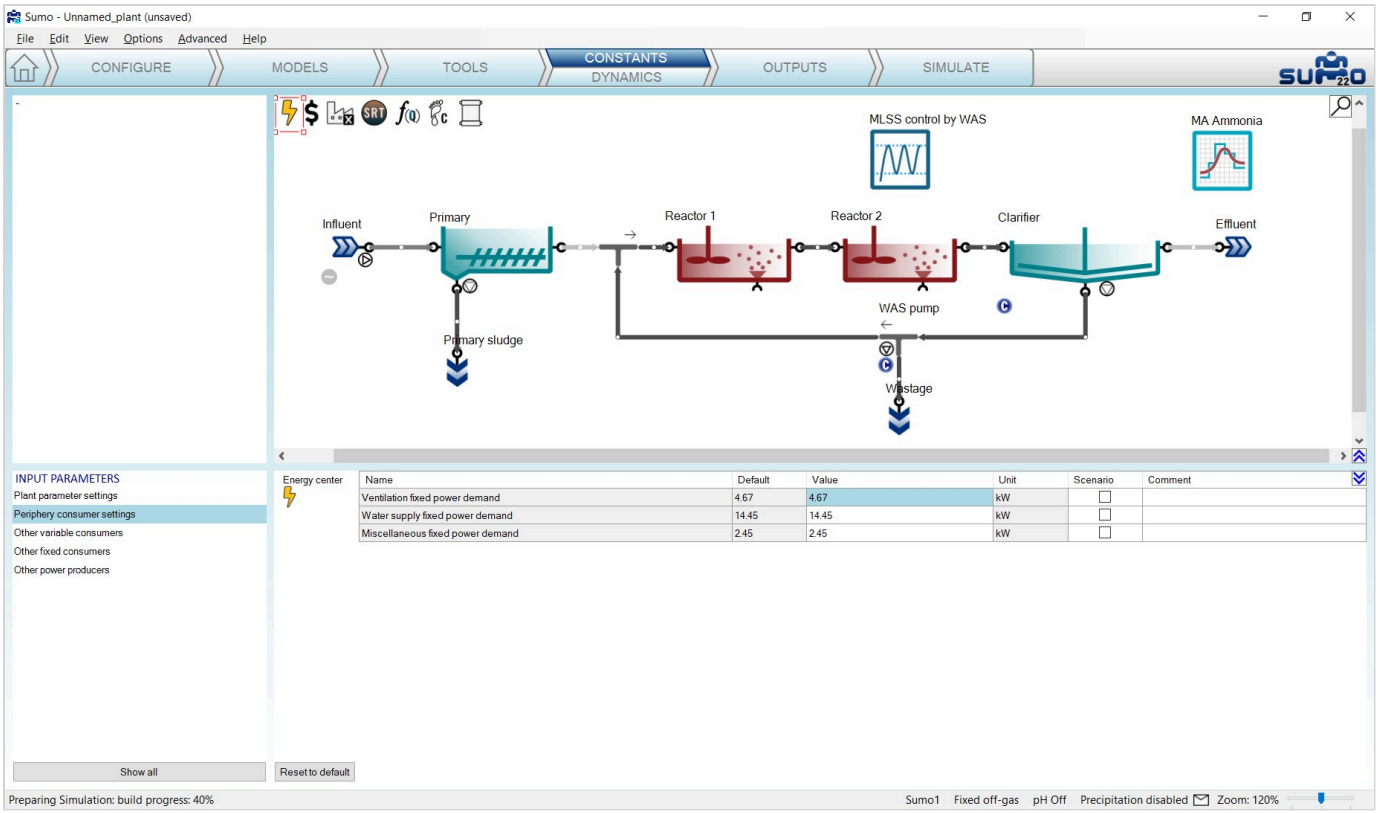


Figure 5.3 – Basic settings available for the 'Energy center' on the Inputs tab

Apart from the plantwide inputs, the *Energy center* has a lot more to offer. Moving over to the *Configure* tab, you will see that the process unit library got extended with three new categories: *Aeration units* (blowers), *Production units* (biogas tank, CHP unit and flare) and *Connectors* (for gaseous phase flows – air and biogas). It is also on this page (in the bottom left screen panel), where you can specify whether the periphery power demands should be calculated based on PE (Population Equivalent) load, flow or entered directly in kW; as well as indicate whether the plant has PV units or batteries installed as on-site electricity production and storage options. (Figure 5.4).

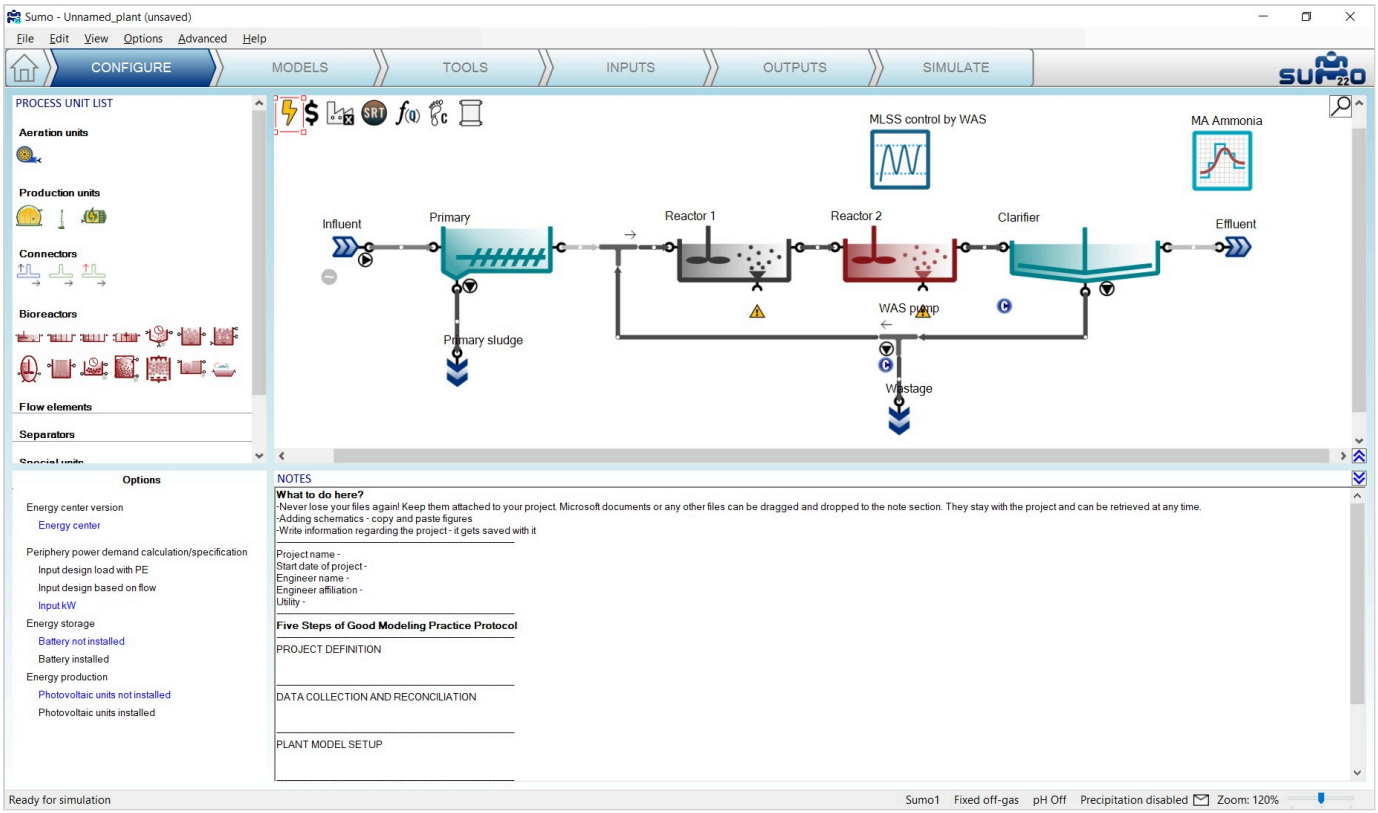


Figure 5.4 – Energy related process units and energy center specification on the Configure tab

While on the *Configure* tab, let us extend the plant layout by adding a blower unit to the second reactor, connecting it to the air input port that appeared at the bottom of the reactor (Figure 5.5). Technically, we could attach another blower unit to the first reactor as well (or use an air connector unit to split the air flow from one blower to the two tanks), however, since it is not aerated, the air flow demand would be zero, thus there is no need for a blower there.

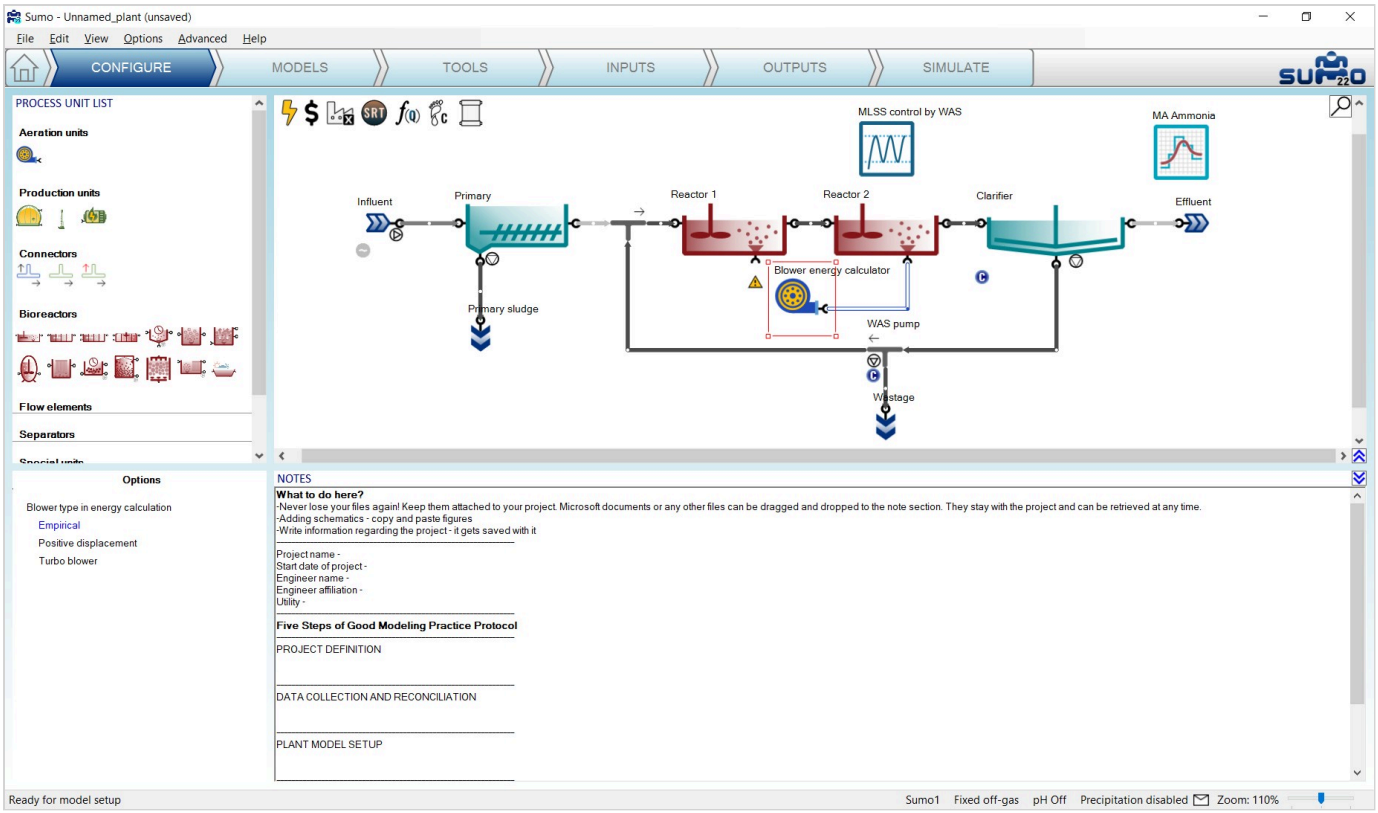


Figure 5.5 – Connecting a blower unit to a reactor

In the process unit options, you can specify between simple empirical (default), positive displacement and turbo blowers. The latter two come with delicate calibration tools that are available from the *Inputs* tab (just like the *Influent tool*), which offer full customization capabilities, based on blower manufacturer data. These tools are described in more detail in the Technical Reference. For our example, we will stick with the empirical blower.

You may also have noticed that the appearance of the pump icons by the influent, the clarifier and the flow splitter process units has slightly changed. When the energy mode is active, you can specify different pumping options for these process units in the bottom left screen panel; including gravitational flow (no pumping), empirical pump model (default), as well as more detailed centrifugal, displacement and screw pump models (Figure 5.6). The latter ones feature elaborate tools that are available from the *Inputs* tab, offering detailed pump customization based on manufacturer data. To learn more about these tools, the reader is referred to the Technical Reference. For this simple example, we will keep all pumps with the simple empirical model. It is also possible to assign pumps to the individual pipes by selecting them and specifying the pump type (there will be no visual notation of these pumps on the drawing board, but they will be included in the energy and cost calculations).

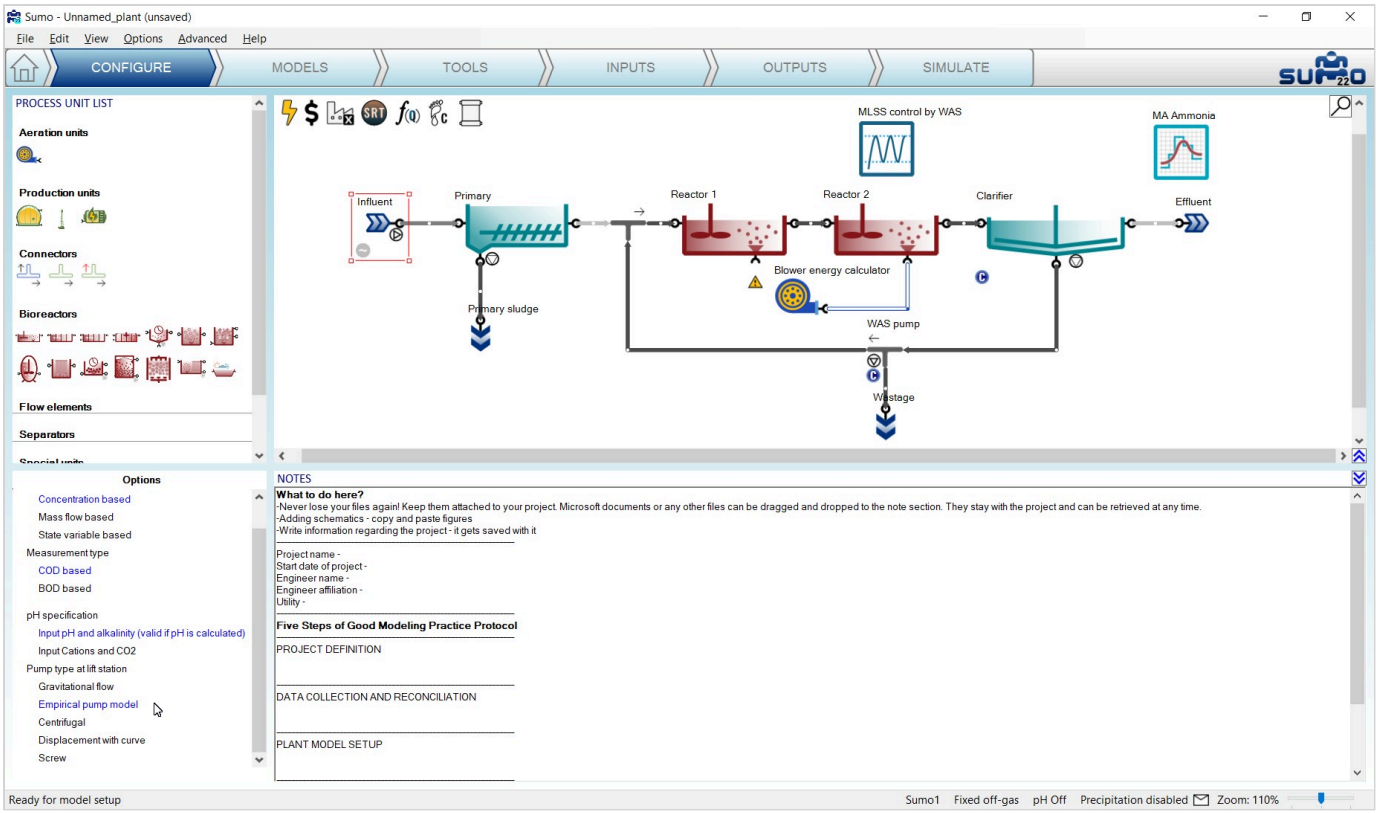


Figure 5.6 – Pump type specification for the influent in the process unit options

Moving over to the *Inputs* tab, the plant model will start to be recompiled (which is necessary for adding the extended features of the energy mode). The appearance of the pump icons will change from ‘not in operation’ to ‘in operation’ and the pump settings (in our example the efficiency) can be specified in the input parameters of the respective process units, one by one (as demonstrated for the influent on Figure 5.7). When using one of the detailed pump models, an extensive set of parameters will be available, to be used in conjunction of the respective pump tool.

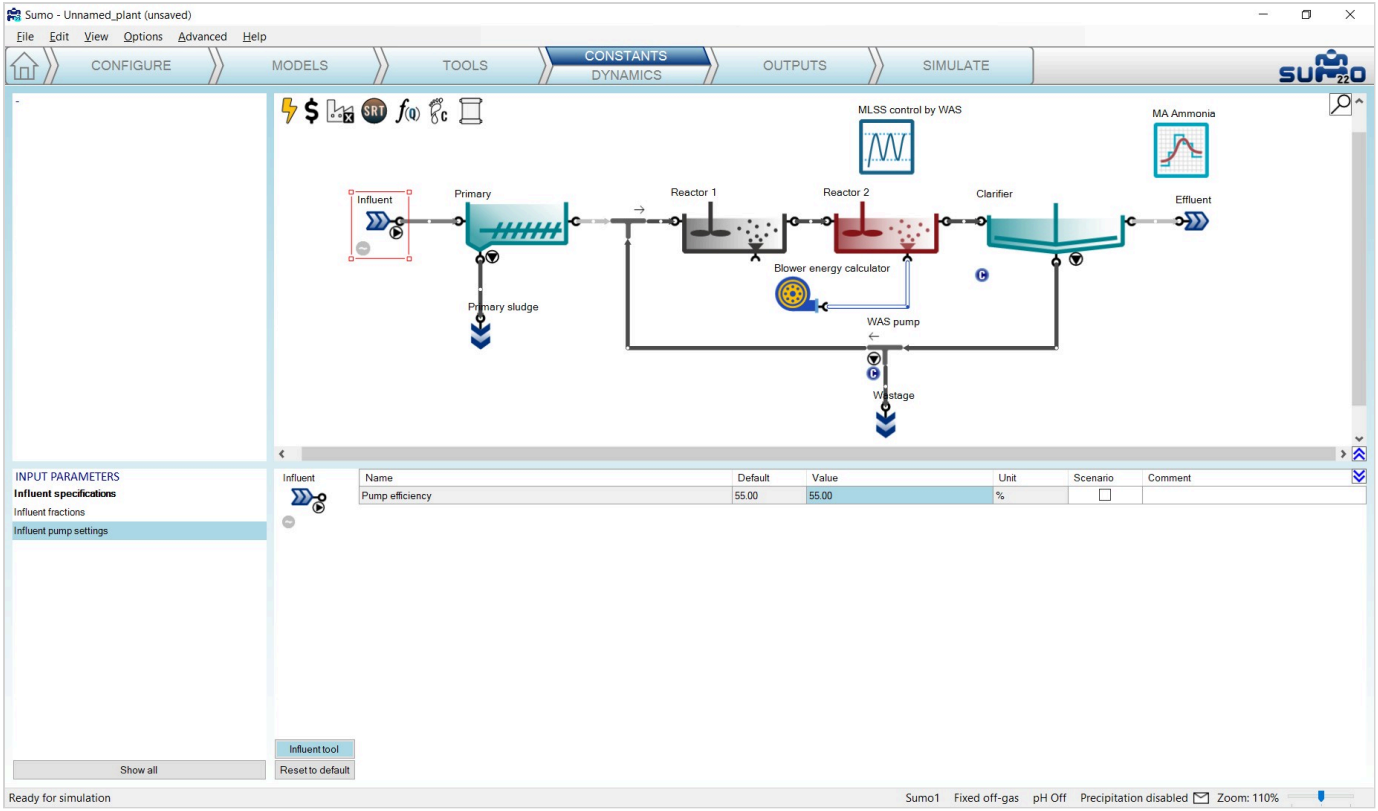


Figure 5.7 – Empirical pump settings for the influent on the Inputs tab

Similarly, the main input parameter for the blower in our example will be the efficiency, while selecting one of the more detailed blower models will require a range of additional parameters, whose proper calibration shall be performed using the respective blower tool.

Moving over to the *Outputs* tab, we can add various energy and cost related output information; such as a blower variables table by selecting the blower unit, adding a table and dragging over the variable group (Figure 5.8); an overview table of plant operation costs for the given simulation period by selecting the *Cost center* icon, adding a table and pulling the relevant variable group over on it (Figure 5.9); or piecharts showing the share of different energy consumer groups and categories in the plant by selecting the *Energy center* icon, adding piecharts and dragging over the respective variable groups to the charts.

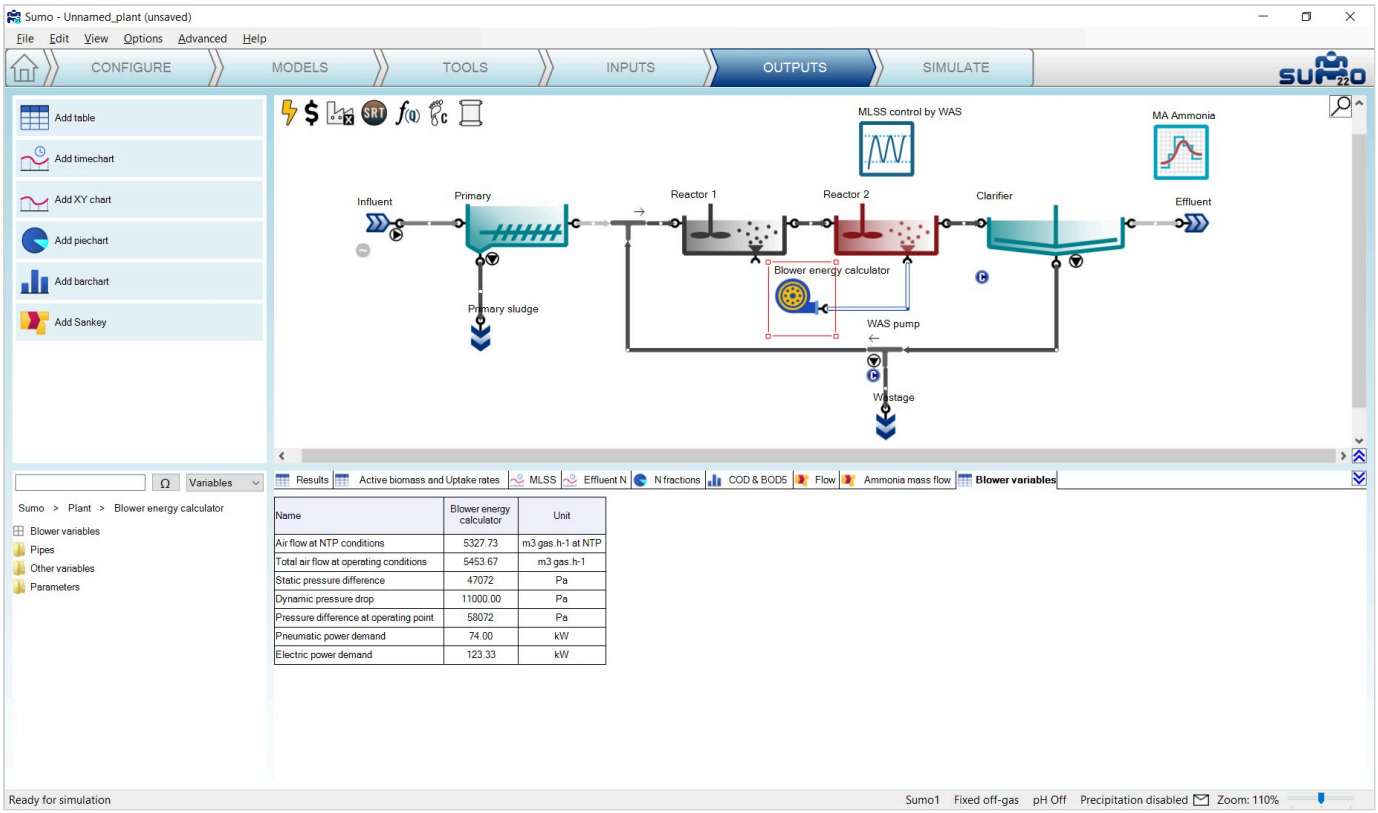


Figure 5.8 – Adding blower variables table on the Outputs tab

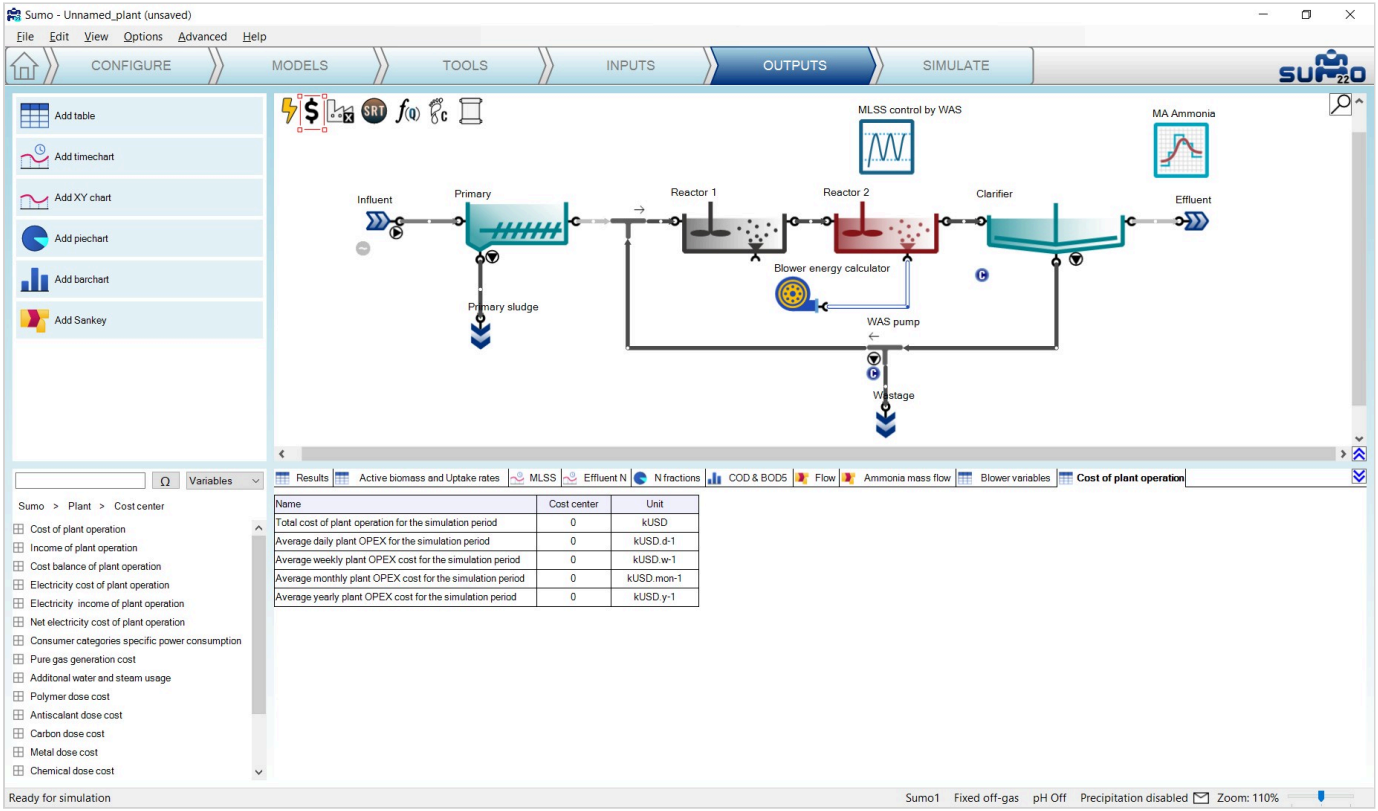


Figure 5.9 – Adding plant operation cost table on the Outputs tab

On the *Simulate* tab, after running a 30-day simulation from steady-state, you can review the energy and cost related information calculated by the model for this period. For example, it can be seen that most of the energy demand in this simple tutorial example comes from the electricity consumption of the biological treatment (Figure 5.10); basically aeration and mixing (Figure 5.11).

You can add various other energy and cost related outputs to analyze the performance of the plant in more detail, as well as extend the blower/pump models by specifying and calibrating the more detailed model options.

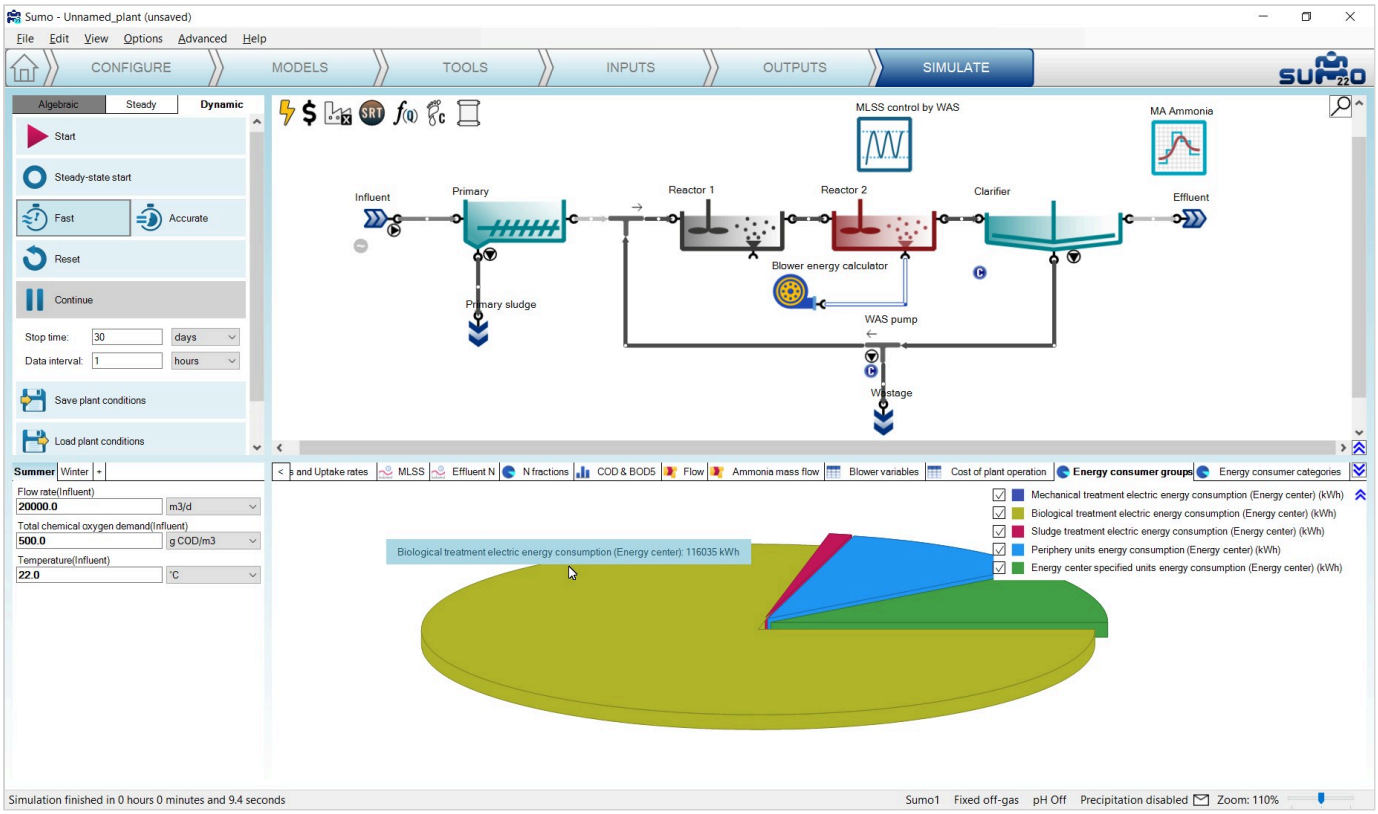


Figure 5.10 – Simulation results regarding the relative share of energy consumer groups

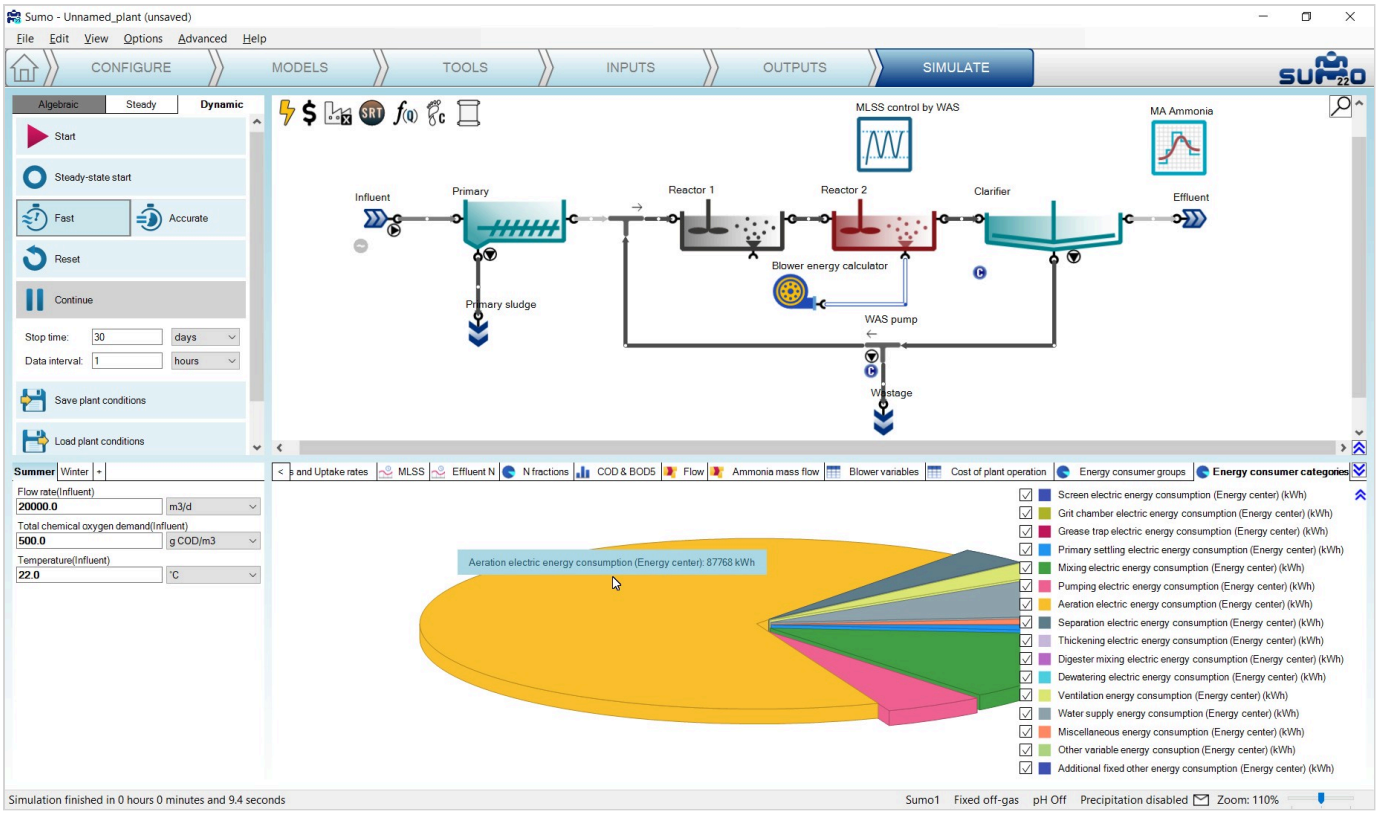


Figure 5.11 – Simulation results regarding the relative share of energy consumer categories

The usage of energy units associated with sidestream treatment (biogas tank, CHP unit, flare) is demonstrated by three of the factory examples: Tutorial Plant 2 with energy, AB plant with energy, UASB plant with energy.

Carbon footprint calculations

This chapter will explain a new plantwide feature introduced in Sumo22. Using this feature enables the carbon footprint (CFP) assessment of plant operation for a given period, based on the process model and optionally, the energy calculations.

Methodology

CFP assessment takes account of greenhouse gas (GHG) emissions related to the investigated activity. In the case of the wastewater industry the associated GHGs are CO_2, CH_4 and N_2O (in general, there are number of other GHGs, however those are not characteristic of wastewater treatment processes). The assessment can address three levels, referred to as Scope 1, 2 and 3 (Table 6.1). Scope 1 covers direct GHG emissions originating from the processes, while Scope 2 and 3 deal with indirect emissions (the former is dedicated to GHG emissions pertaining to the supply of energy demands, the latter covers all other third-party GHG emissions, such as chemicals production, transportation of materials and personnel to and from the facility, etc.). By its nature, the choice of boundaries for Scope 3 can be very arbitrary, and often some crucial

information elements needed for proper accounting are uncertain or biased. Thus, for comparative studies it is rather advisable to settle with Scope 1 and 2 carbon footprint assessment. The Sumo CFP tool provides these two levels.

Table 6.1 – Scopes of carbon footprint assessment.

SCOPE 1	Direct emissions from the investigated process
SCOPE 2	Indirect emissions from energy consumption (imported power from external sources)
SCOPE 3	Other indirect emissions associated with the process (external, third-party emissions)

The status of the CFP calculation mode is indicated by the footprint icon in the top left corner of the plant layout screen panel (Figure 6.1). By default, CFP is disabled. To enable it, double-click on the CFP icon (whose image will change, depending on further conditions, see Table 6.2) or right-click and select "*Turn carbon footprint calculations on*".

Figure 6.1 - The 'CFP' icon is the second from the right

For carbon footprint assessment heavily relies on the proper estimation of off-gas mass flows, it is a requirement to have "*Calculate gas phase conc*entrations" selected in the *Gas phase* category of *Model options* on the *Models* tab. As long as the "*Input gas phase concentrations*" option is selected, the CFP icon will be hollow red when turned on, indicating that an additional model option choice must be made before CFP calculations become active. With calculated off-gas, the icon will change from hollow to black fill and the letter '**C**' on its right side will change to '**S1**' (referring to Scope 1) or '**S2**' (referring to Scope 2), depending on whether the Energy mode is switched off or on, respectively. Without energy calculations, the CFP calculations obviously lack the information needed for Scope 2 coverage, hence the two distinguished signals. Nevertheless, both levels of assessment will be valid for comparison with other assessments that were made on the same level.

Table 6.2 – CFP icon images shown under various conditions.

CFP OFF	**CFP ON**		
	fixed off-gas	calculated off-gas	
		Energy OFF	Energy ON

When enabled, CFP will automatically gather the following information from the various process units that are part of the plant layout:

- Stripping rates of GHGs from bioreactors and other process units with reactive volume
- Fugitive biogas mass flows from digesters and dewatering units
- Biosolids handling (assuming on-site incineration or transportation for off-site treatment)
- Incomplete biogas combustion (when the Energy mode is enabled)
- Energy consumption and production (when the Energy mode is enabled)

Regarding the process emissions, carbon dioxide and methane are always calculated based on the process model: stripped gas mass flows are fetched from liquid stream bioreactors, while fugitive gas mass flows are collected from solid stream bioreactors (digester, UASB) and dewatering units. In the case of nitrous oxide, the methodology depends on the process model used for the simulation. If the model includes N_2O as a state variable (for an explanation of what is a state variable, please see the Technical Reference), then its emissions are calculated according to the process model, just like for the other two GHGs (Tier 1 method). Otherwise, N_2O emissions will only be estimated based on the influent TKN via a plantwide emission factor (Tier 2 method), which, depending on the configuration, can be highly variable (0.01% - 1.8%, for details see Ahn et al, 2010). It is important to highlight that the choice between the two approaches is made automatically by Sumo, using a check in the actual process model. Therefore, it is generally advised to use a process model that has N_2O as a state variable (e.g. **Sumo4N**, which can be found under *Focus models* on the *Models* tab) in order to avoid high uncertainty in estimating nitrous oxide emissions.

In the case of process-derived carbon dioxide, an important requirement is that a CFP assessment should only take into account the fraction of emissions that originates from the breakdown of materials containing fossil carbon (e.g. cleaning products, pharmaceuticals, and other petroleum-based products present in the wastewater). The CO_2 produced by natural processes (originating from biogenic carbon) must be excluded. Therefore, estimating the share of fossil carbon is important in the various material streams of the plant. This can vary considerably, depending on the composition of the raw wastewater. Sumo considers default values for mainstream, side stream, biogas and biosolids based on literature. These can be adjusted/tuned by the user (e.g. for sensitivity analysis or for special applications).

In the final step of a CFP assessment, the emissions of GHGs are converted to CO_2-equivalent units using a conversion factor called Global Warming Potential (GWP), which is provided by the periodically published official reports of the *Intergovernmental Panel on Climate Change* (IPCC). GWP values differ from one GHG to another (by definition, the GWP of CO_2 is always 1, the values for all other gases are relative to this reference) and also vary depending on the reference time horizon chosen for benchmarking (100 years is the most often used period). GWP values based on the 100 and 20 years time horizons are presented by Table 6.3 to demonstrate the considerable differences between the three GHGs under investigation and also, to support the recommendation for using process model based N_2O emission estimations (in a CFP assessment, 1 kg of N_2O will be equivalent to about 265 kg of CO_2 emitted).

Table 6.3 – GWP values (*source: IPCC*)

GWP	Reference time horizon	
	20 years	**100 years**
CH_4	84	28
N_2O	264	265

Regarding the CFP of energy consumption, the assessment must consider the specific CFP of the utilized power generation approach (which is most often a mixture). Various technologies have quite different associated CFP per unit of power produced (see Table 6.4). Thus, the energy mix in general, and sometimes its temporal variation as well, is an important factor to take into account. Sumo offers a tool that serves as a database for properly setting up Scope 2 CFP calculations.

Table 6.4 – Typical specific CFP values for various power producing technologies

Technology	Specific CFP [g CO_2-eq/kWh]
Hydro	24
Solar	45
Natural gas	490
Wind	11
Nuclear	12
Coal	820

Usage

For the demonstration purpose we will use the "*A2O with P recovery and energy plus CFP*" example project, which is available on the welcome screen or from the *Help* menu.

After opening the example project, while on the *Configure* tab, select the *Carbon footprint* icon (located in the top left part of the layout panel) in order to look at the *Process unit options*. As CFP calculations are already turned on in this project, the process unit options are visible in the bottom left window panel. This is the place where the handling method of biosolids and the time horizon for GWP estimation base can be specified (Figure 6.2).

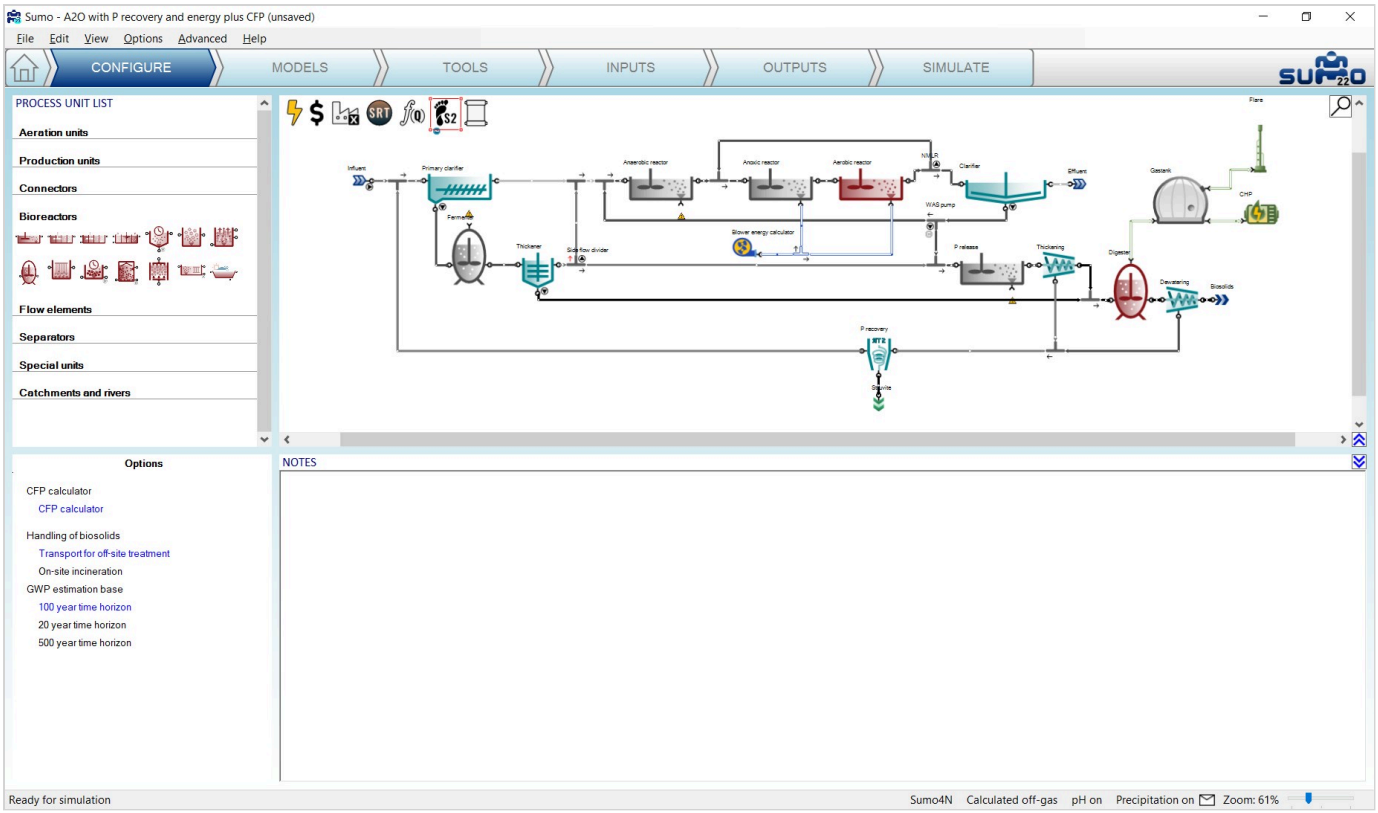


Figure 6.2 - CFP unit general options

Moving over to the *Inputs* tab, the general input CFP parameters will appear. In the first table the *Fossil carbon fractions* can be specified (Figure 6.3). The second table contains the *Sludge handling parameters* (these depend on the previous choice of sludge handling method, see Figure 6.4). The third table contains the set of *Electricity CFP parameters*, which are used in conjunction with the Energy mode settings, enabling on-site and off-site power production methods (Figure 6.5). The latter table becomes active only when the Energy mode is turned on (enabling Scope 2 CFP calculations, like in this example project).

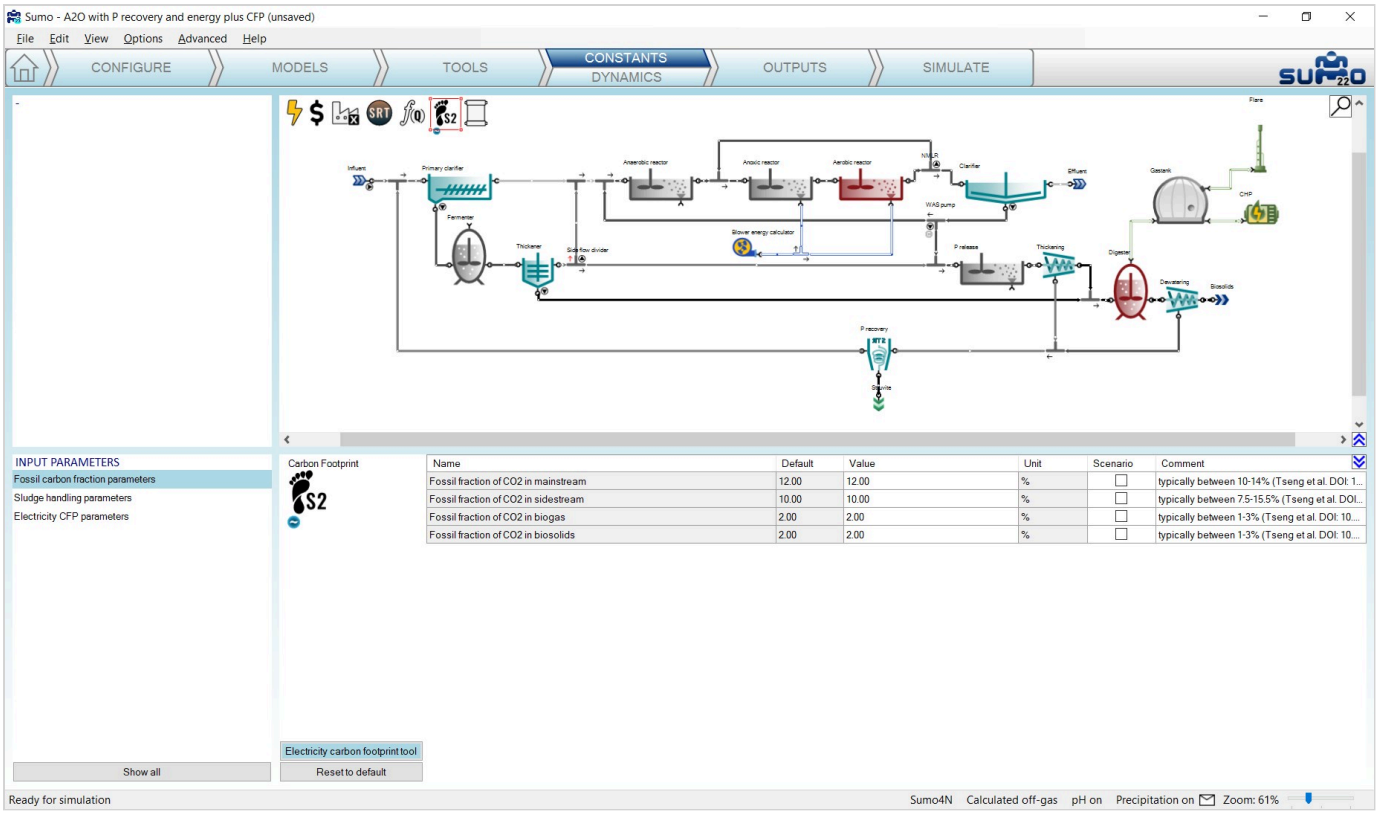


Figure 6.3 - CFP unit fossil carbon fraction input parameters

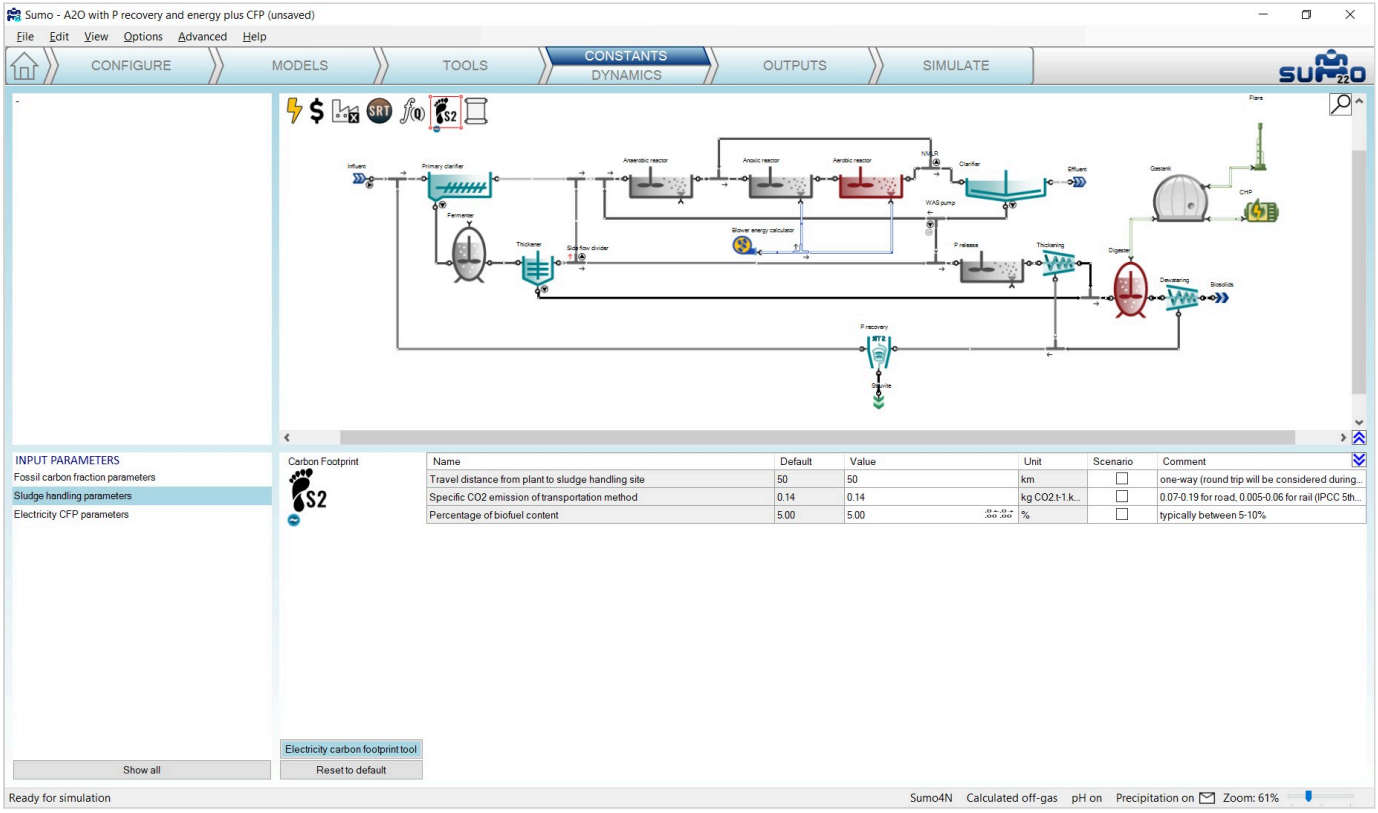


Figure 6.4 - CFP unit sludge handling input parameters

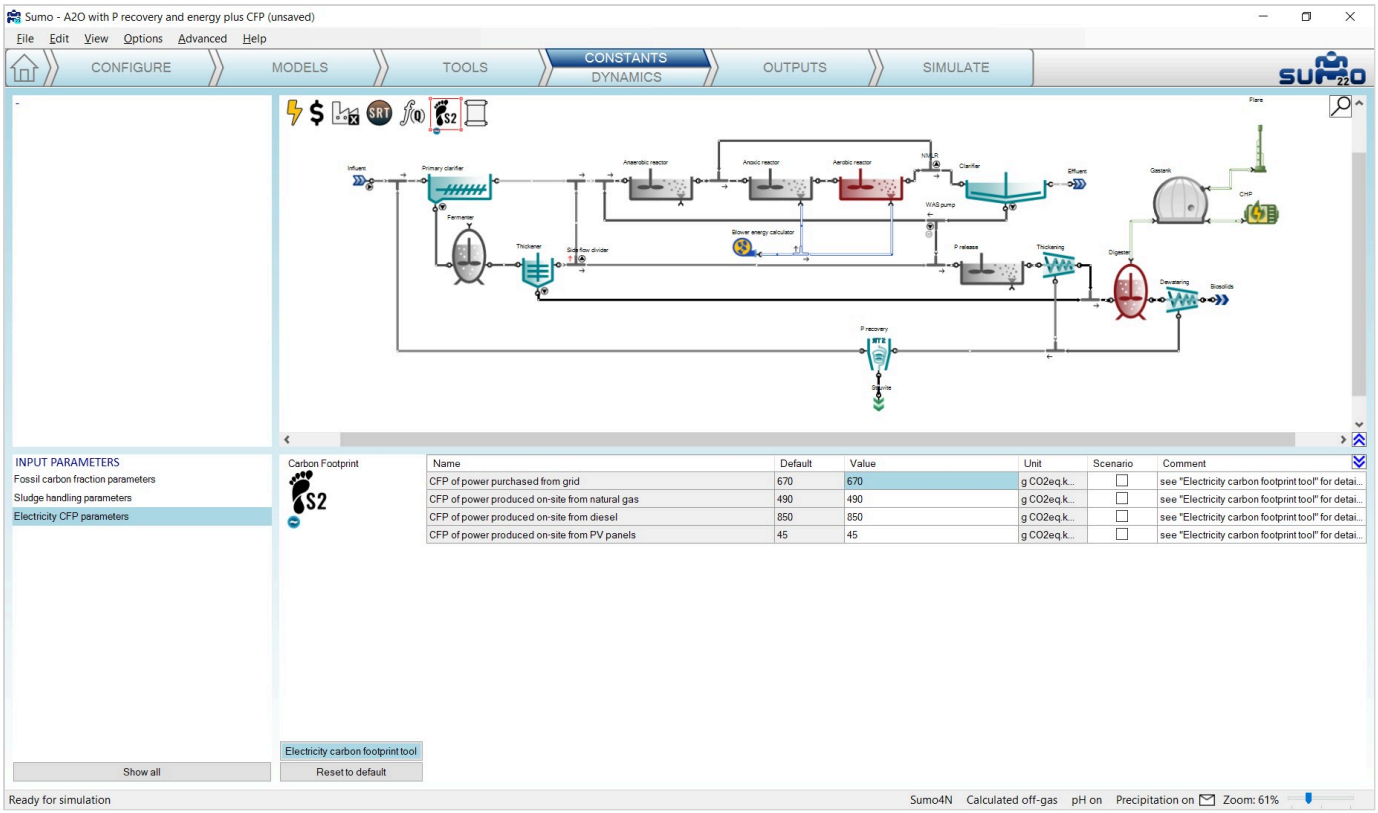


Figure 6.5 - CFP unit electricity CFP input parameters

Below the parameter tables you can find a button for opening the '*Electricity carbon footprint tool*', the database that is aimed to help determining correct grid and off-grid power CFP values, based on available regional and technology specific data. The example project uses one of the diurnal grid power CFP patterns from this tool (you can check it out by clicking on the *Constants/Dynamics* tab, see Figure 6.6).

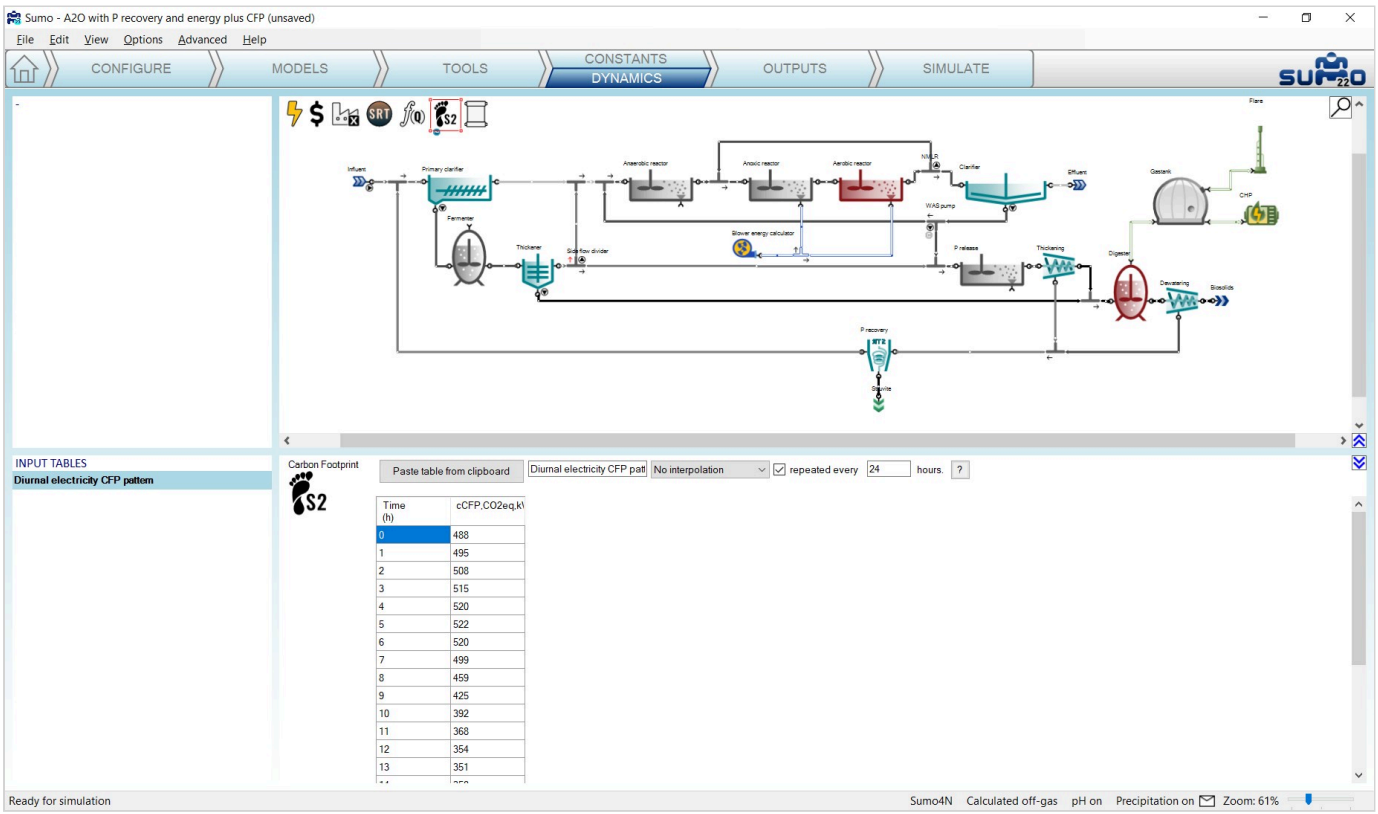


Figure 6.6 - Dynamic input table for electricity CFP parameter

In order to assess all process-related CFP, new parameters have been added to the *Digester* and *Dewatering* process units. While on the *Inputs/Constants* tab, select the *Digester* on the drawing board and click the *Show all* button in the bottom left panel, then select the *Gas phase settings* table. You will find here the *Fraction of fugitive biogas* parameter, which has been modified in the example project from the default 0 to 1% (Figure 6.7). Similarly, when selecting the *Dewatering* unit, in the *Settings* table you will find parameters to adjust the fugitive mass flow fractions of methane and carbon dioxide (Figure 6.8).

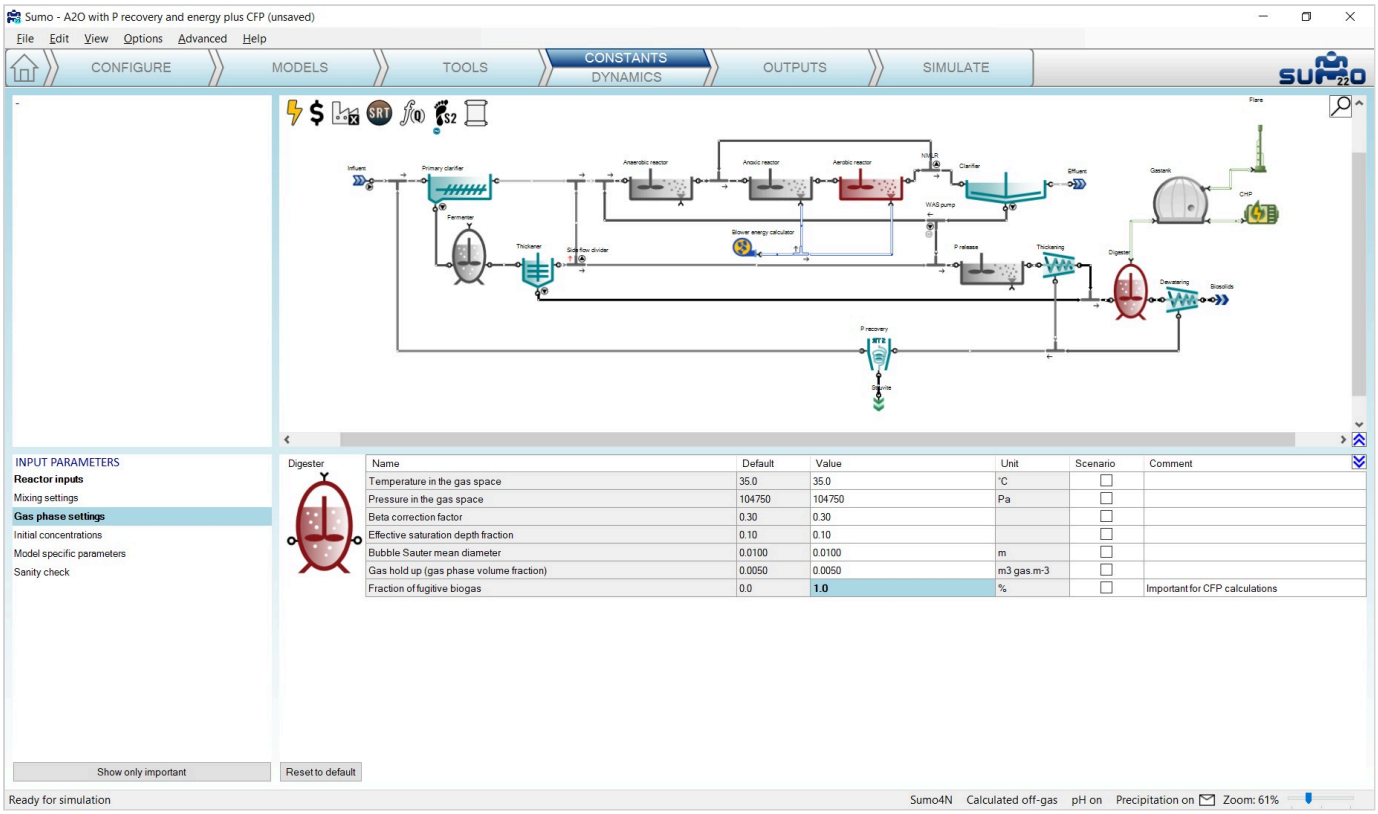


Figure 6.7 - Fugitive biogas fraction input parameter for Digester process unit

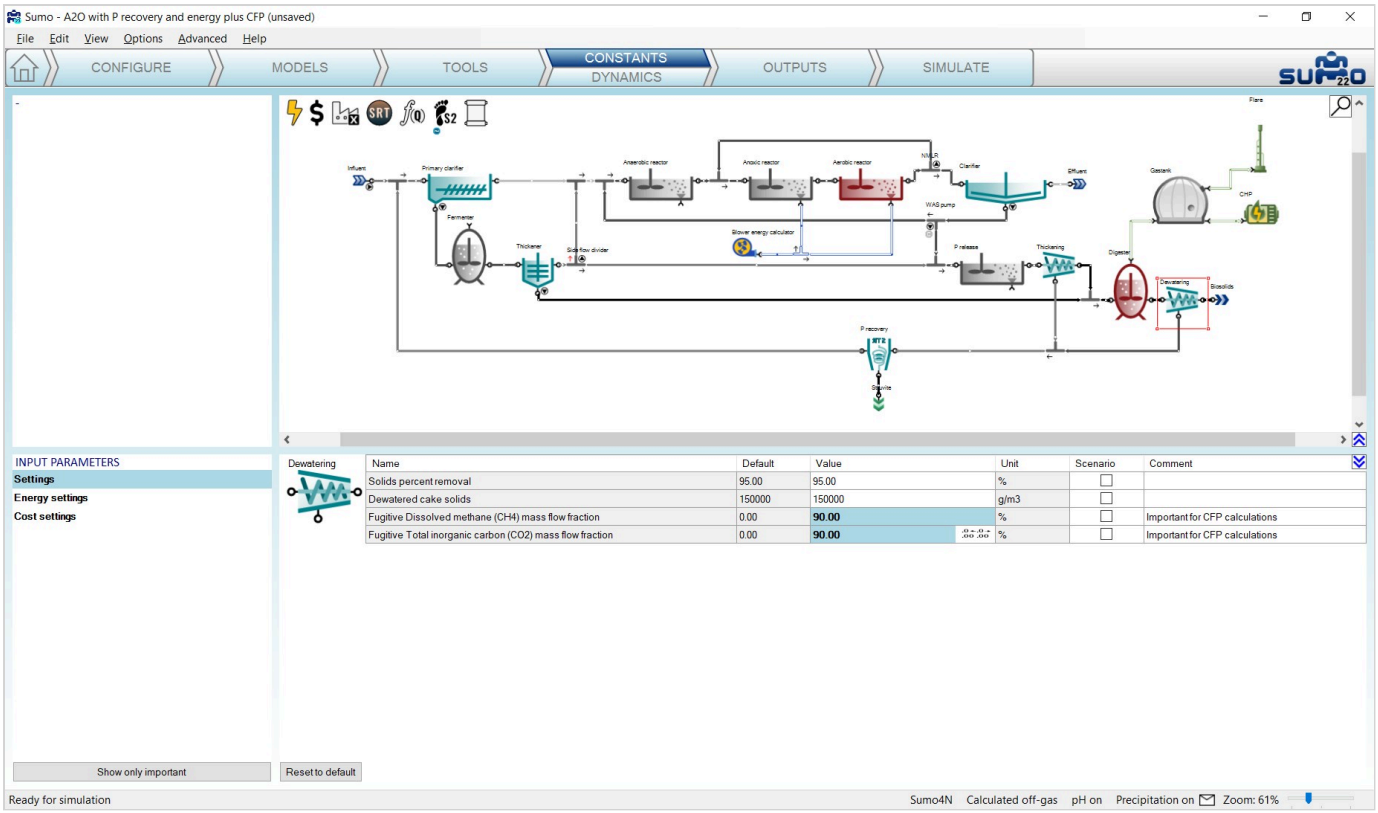


Figure 6.8 - Fugitive mass flow fraction input parameters for Dewatering process unit

When Scope 2 CFP is enabled (Energy mode is active) and biogas processing is considered in the layout, it is also important to set the *Combustion efficiency of methane* parameter (available from the *Combustion settings* parameter table) in both the CHP and Flare process units (Figure 6.9). The value of this parameter is usually somewhere between 99% and 100%, which may seem indifferent, however, even such a little change in GHG emissions originating from incomplete combustion can make up a visible portion of the overall CFP.

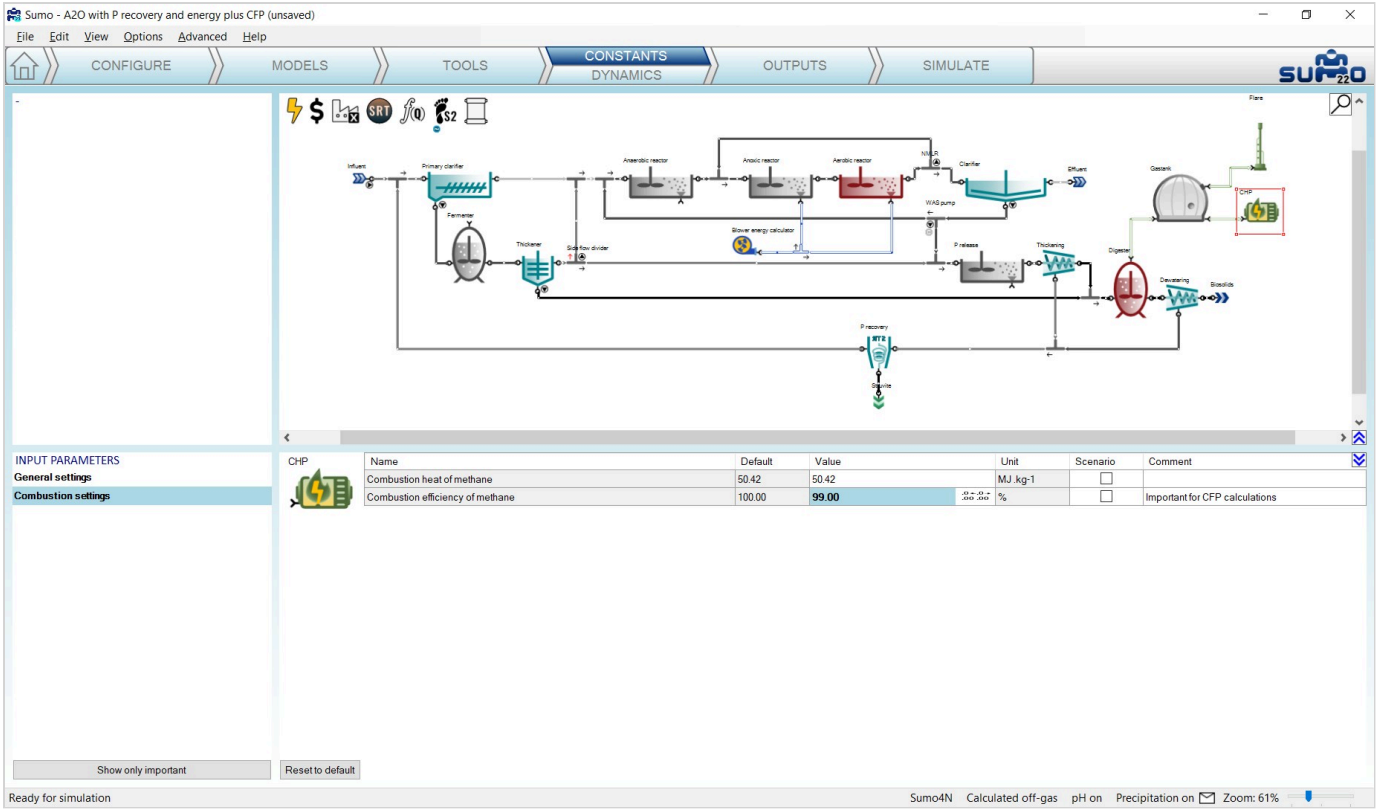


Figure 6.9 - Methane combustion efficiency input parameter for CHP process unit

Results of the CFP assessment can be visualized by selecting the *Carbon footprint* icon on the *Outputs* tab and choosing from the prepared variable groups, such as '*CFP summary*' or more detailed splits of direct and indirect CFP components, as well as CFP component splits focusing on the individual GHGs. Direct and indirect emission rates of GHGs are also available. To get some inspiration on how to use these data, proceed to the *Simulate* tab and launch a 1-day dynamic run from steady state, then review the outputs from the '*CFP summary*' piechart to the '*Electricity CFP*' timechart. From the '*CFP summary*' (Figure 6.10) one can see that about two-thirds of the plant operation CFP for the simulated period comes from power usage, while the rest is about equally distributed between various process-related emissions of the three GHGs. Looking deeper, it turns out that about half of the overall plant operation CFP originates from the activated sludge process, while fugitive losses and incomplete biogas combustion, along with sludge handling (transportation to external handling site in this case) are smaller, yet visible fractions (Figure 6.11). The diurnal variability of electricity CFP is also visible but not outstanding (Figure 6.12).

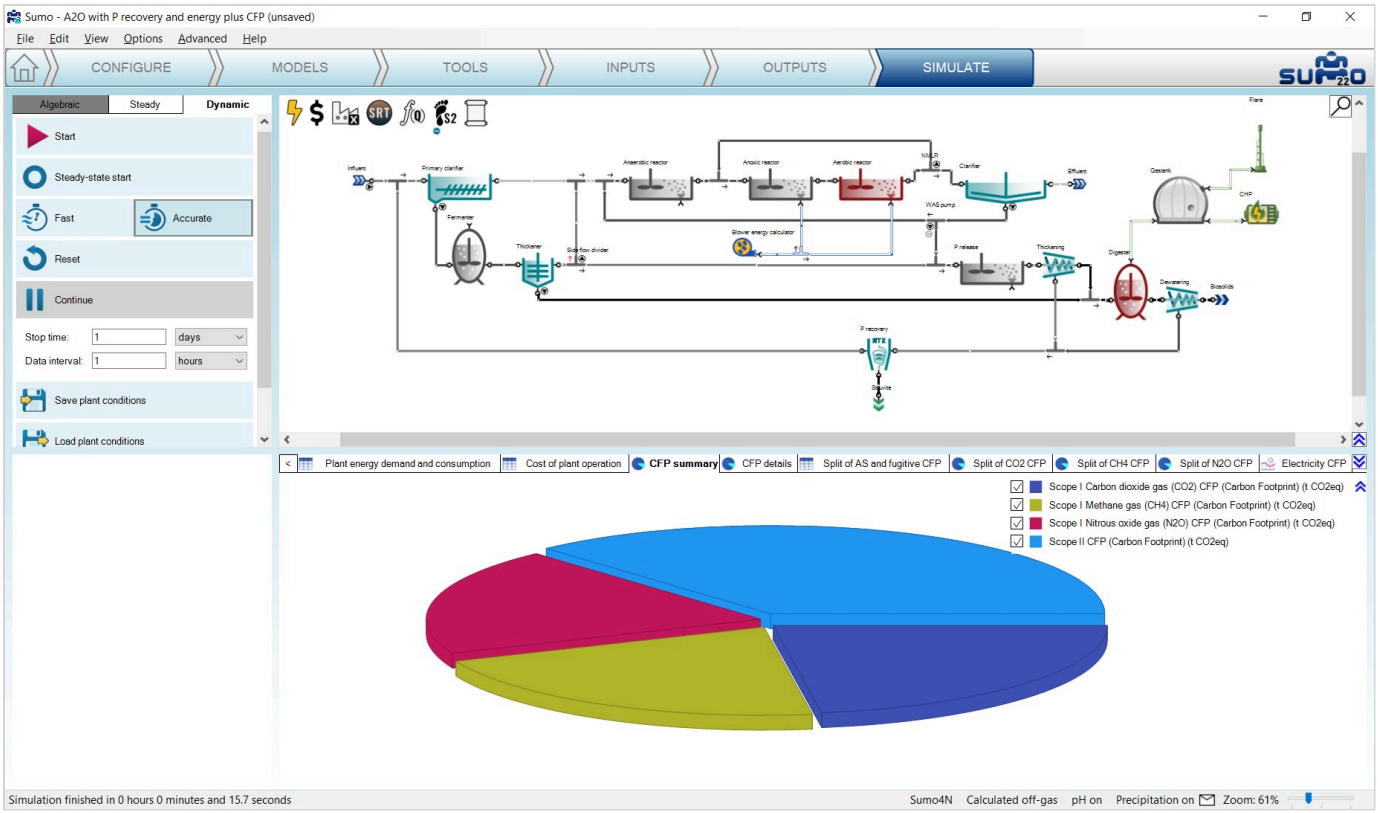


Figure 6.10 - CFP summary piechart

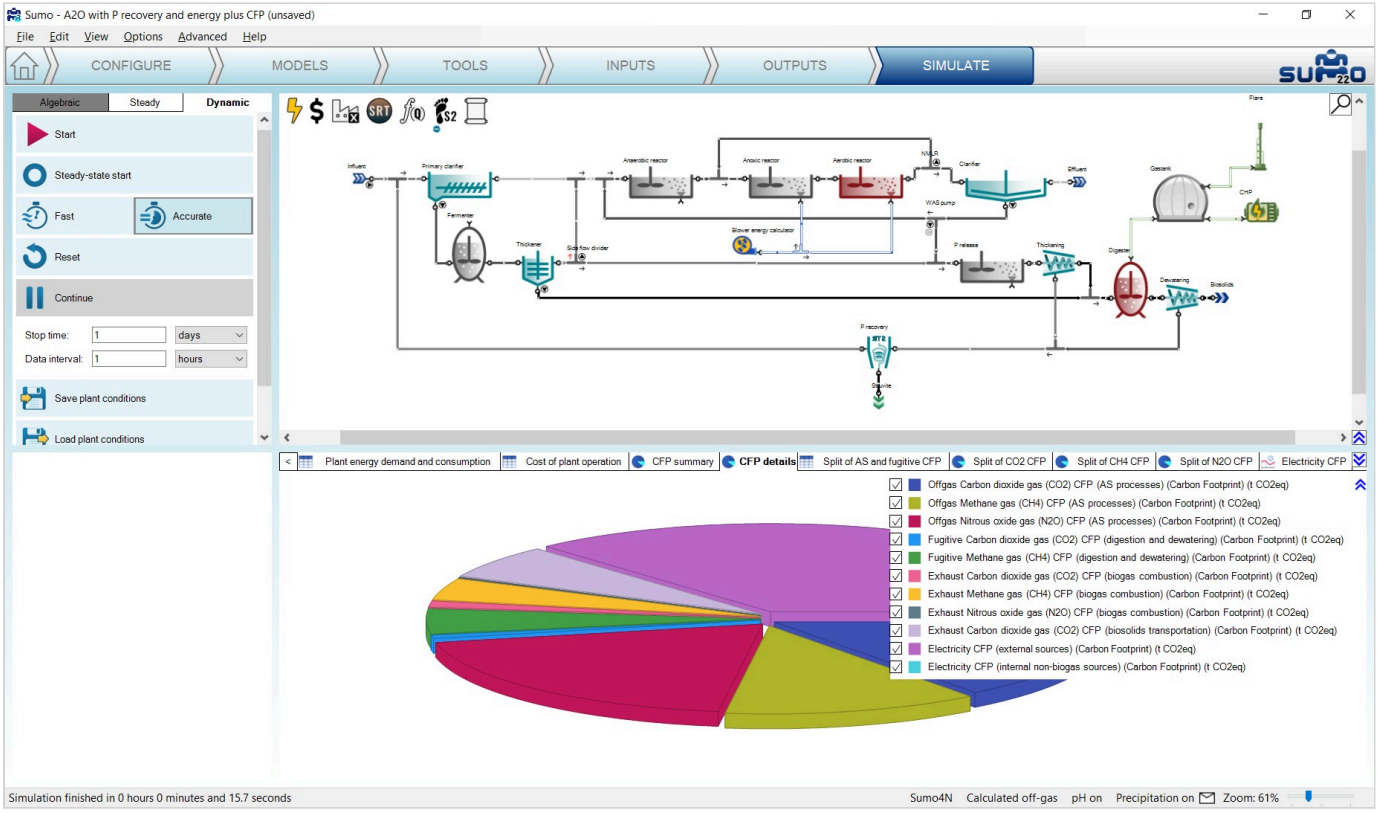


Figure 6.11 - CFP details piechart

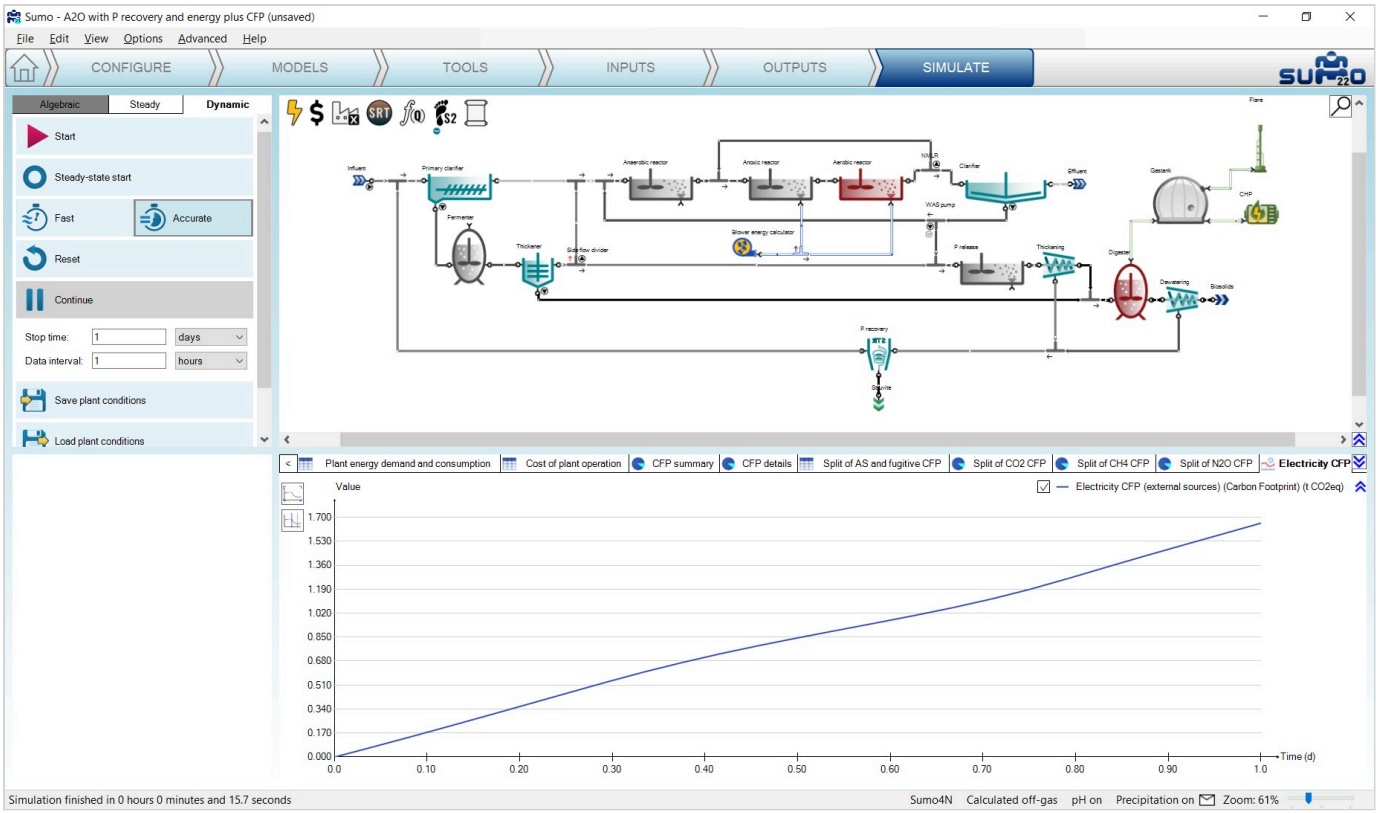


Figure 6.12 - Electricity CFP timechart

Examples

In this chapter, the built-in example configurations are presented covering various process technologies. These examples can be selected from the Welcome Screen, as well as from the *Help* menu. They are located in the install directory.

Tutorial plant

This is the example layout used in this manual.

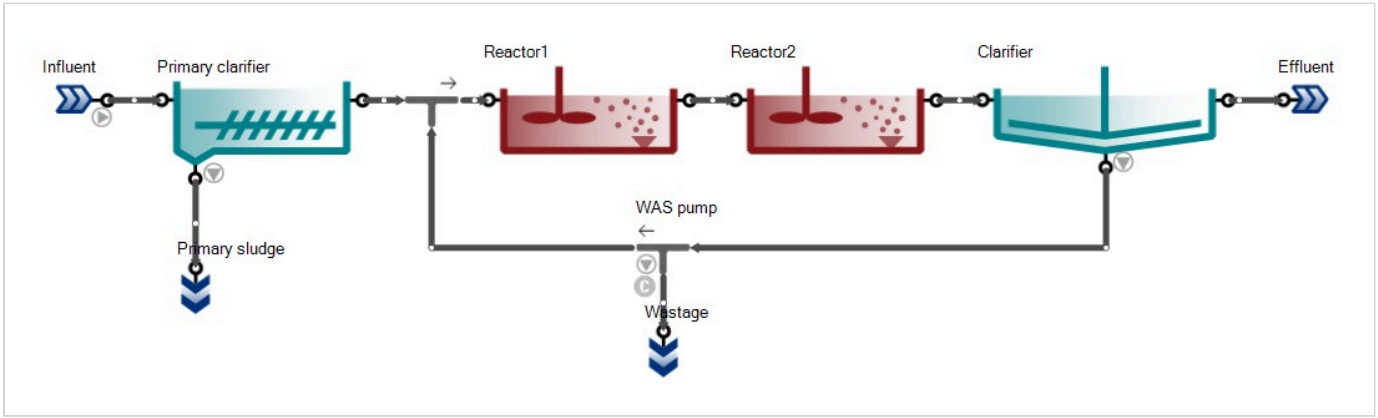


Figure 7.1 - The ‘Tutorial plant’ example layout

Tutorial plant 2

Tutorial Plant 2 is the extended configuration of Tutorial plant, including mesophilic digestion. Off-gas and pH calculations are turned on.

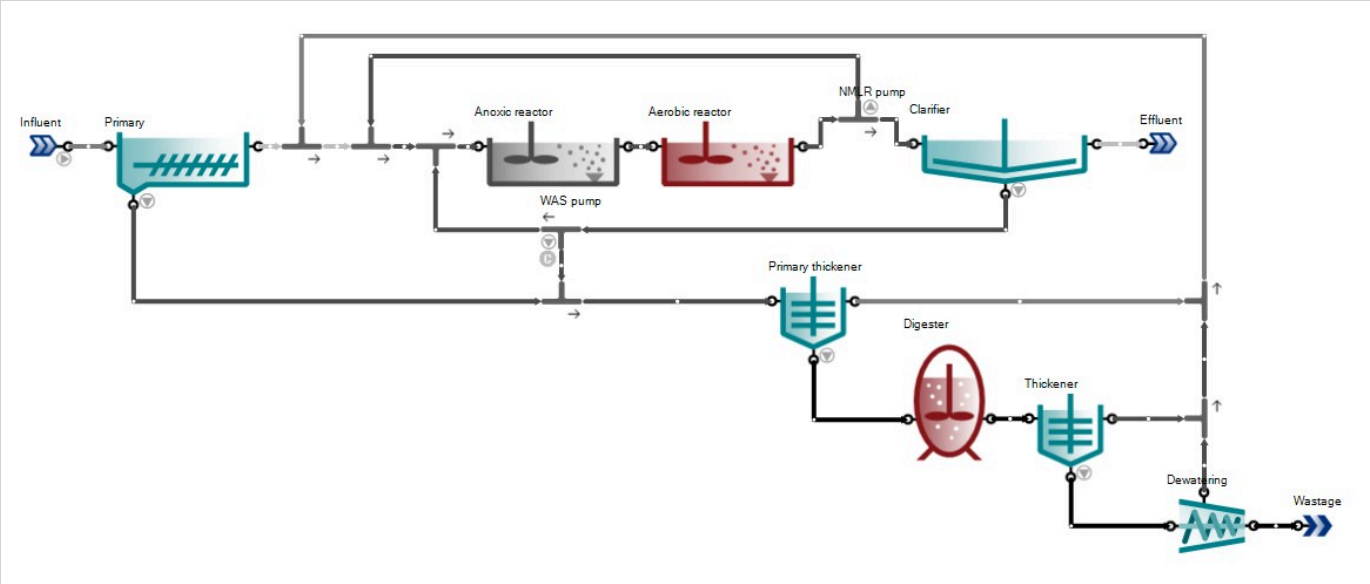


Figure 7.2 - The 'Tutorial Plant 2' configuration

Tutorial plant 2 with energy

Tutorial Plant 2 with energy calculations turned on.

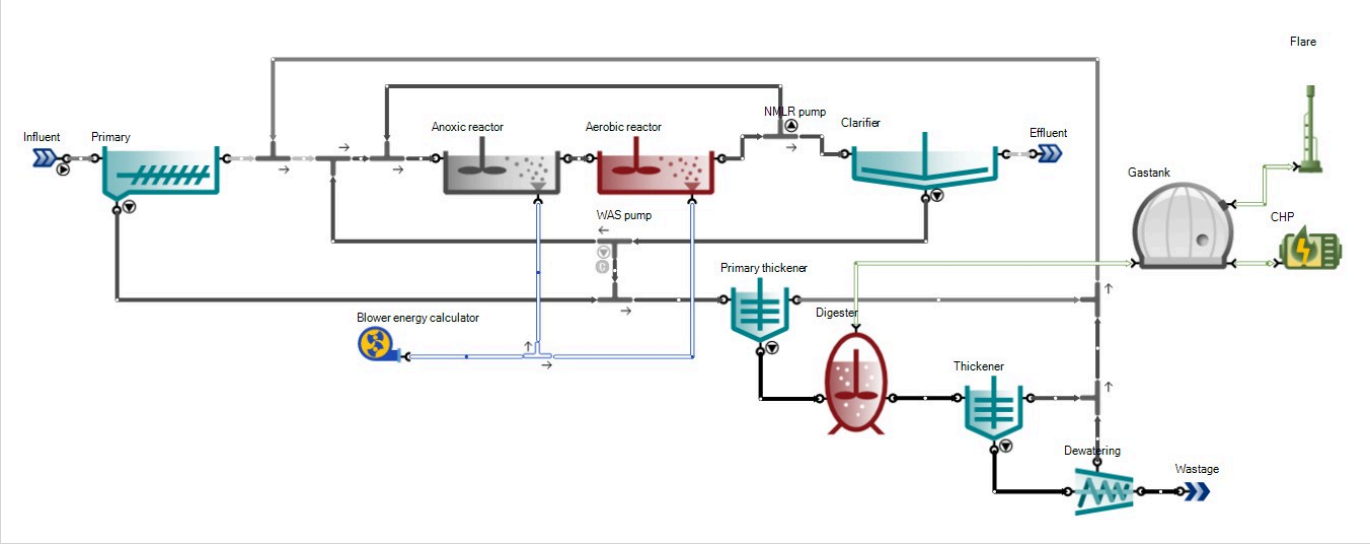


Figure 7.3 - The 'Tutorial Plant 2 with energy' configuration

Tutorial plant 3

Tutorial plant 3 is the extended version of Tutorial plant 2 with sidestream treatment (nitritation and denitritation). This configuration is simulated using the two-step nitrification/denitrification model with Sulfur (Sumo2S). Off-gas, pH and precipitation calculations are turned on.

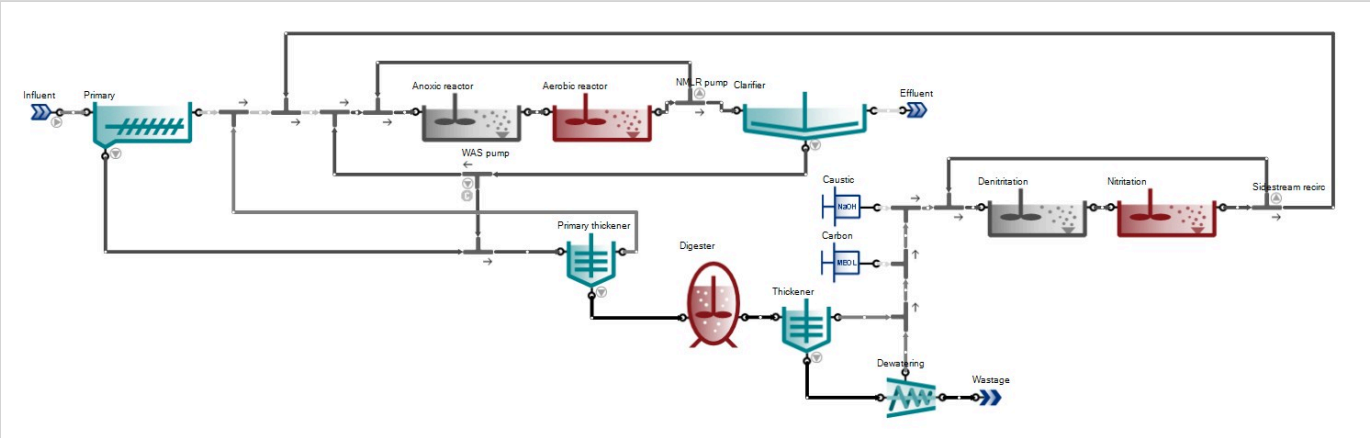


Figure 7.4 - The 'Tutorial plant 3' configuration

Tutorial plant 4

Tutorial plant 4 is the extended version of Tutorial plant 2 with a different sidestream treatment (partial nitritation and anammox). This configuration is simulated using the two-step nitrification/denitrification model. Off-gas, pH and precipitation calculations are turned on.

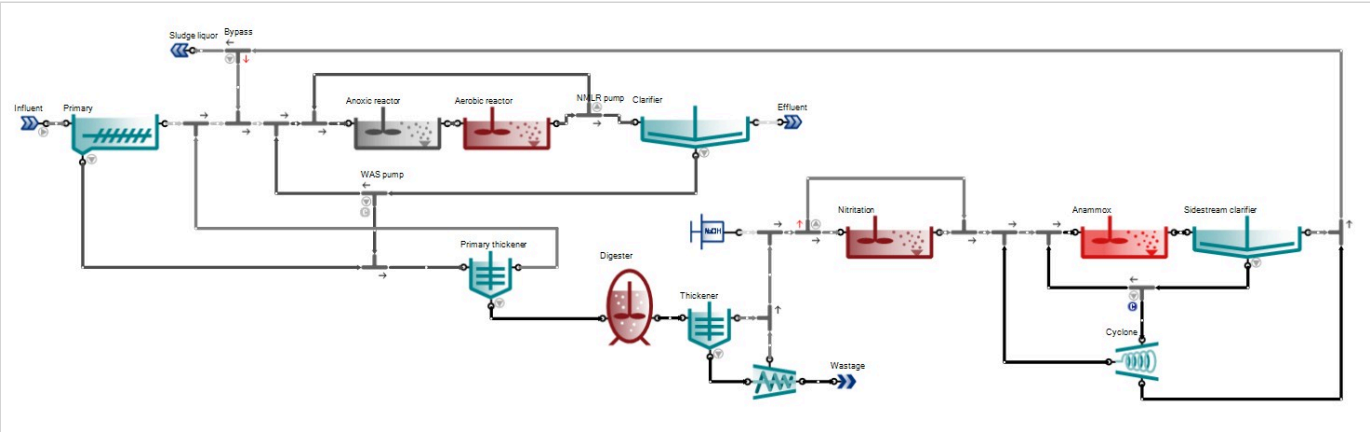


Figure 7.5 - The 'Tutorial plant 4' configuration

A2O plant

A2O configuration with one-step nitrification/denitrification model.

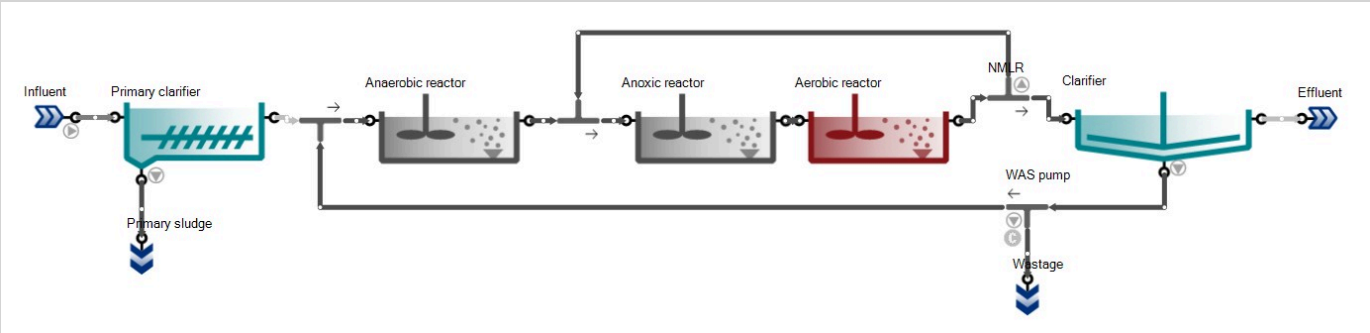


Figure 7.6 - The 'A2O plant' example layout

A2O with P recovery and energy

This layout is the extended version of the A2O configuration with primary sludge fermentation, digestion and P recovery (struvite precipitation). Off-gas, pH and precipitation calculations, as well as energy calculations, are turned on.

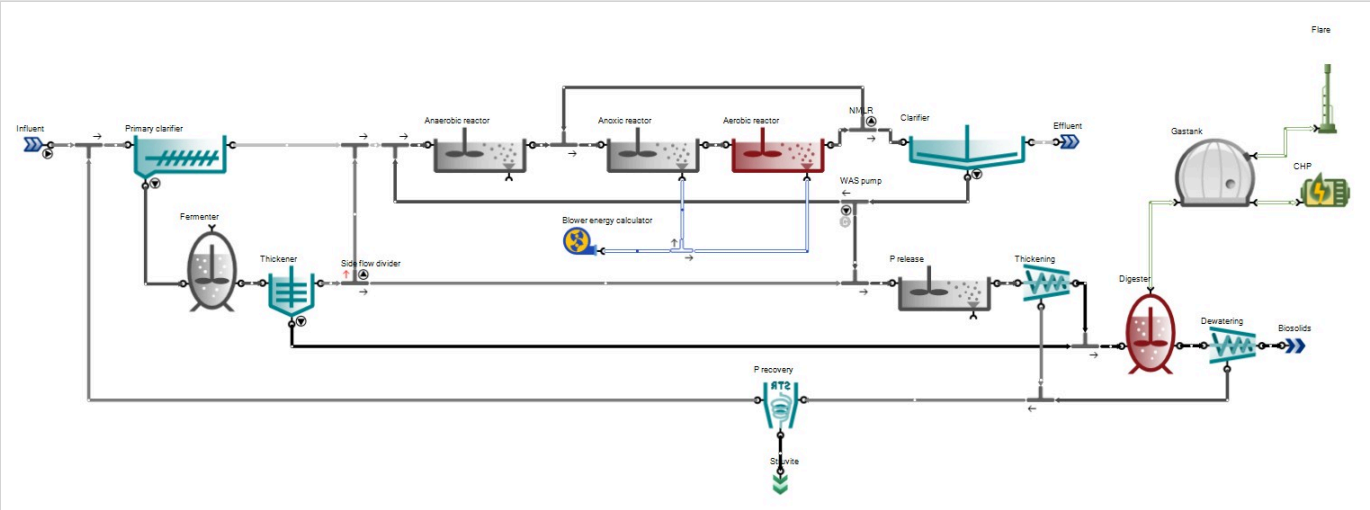


Figure 7.7 – The 'A2O with P recovery and energy' configuration

A2O with P recovery and energy plus CFP

This layout is the same as the previous configuration, extended with carbon footprint (CFP) calculations. For the sake of CFP assessment, the underlying process model is changed to Sumo4N in order to improve accounting for nitrous oxide (a very powerful greenhouse gas) production.

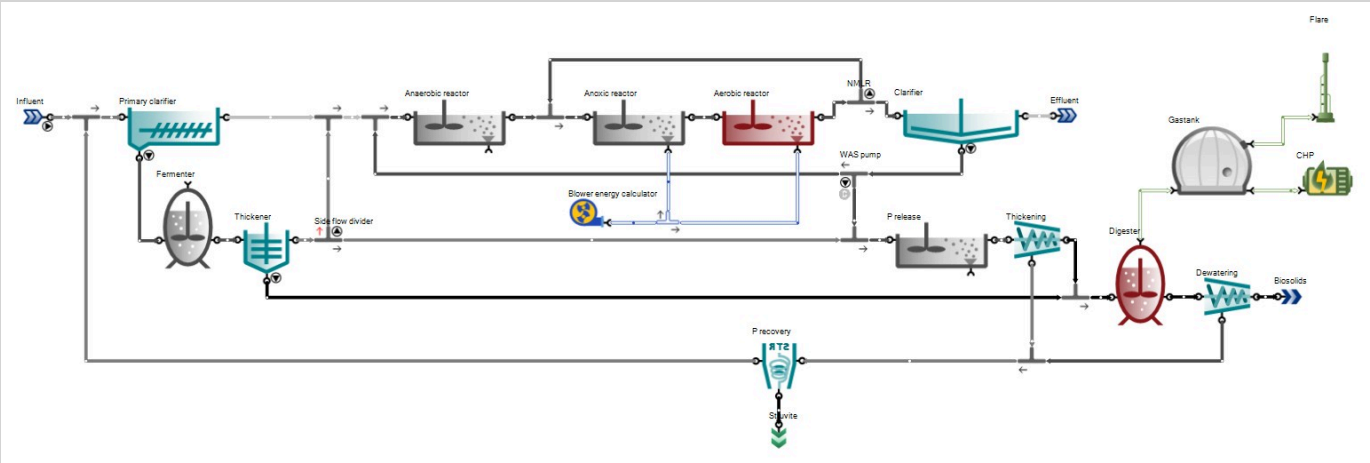


Figure 7.8 – The ‘A2O with P recovery and energy plus CFP’ configuration

AB plant

This layout features an adsorption/bio-oxidation process configuration, known for enhanced carbon capture.

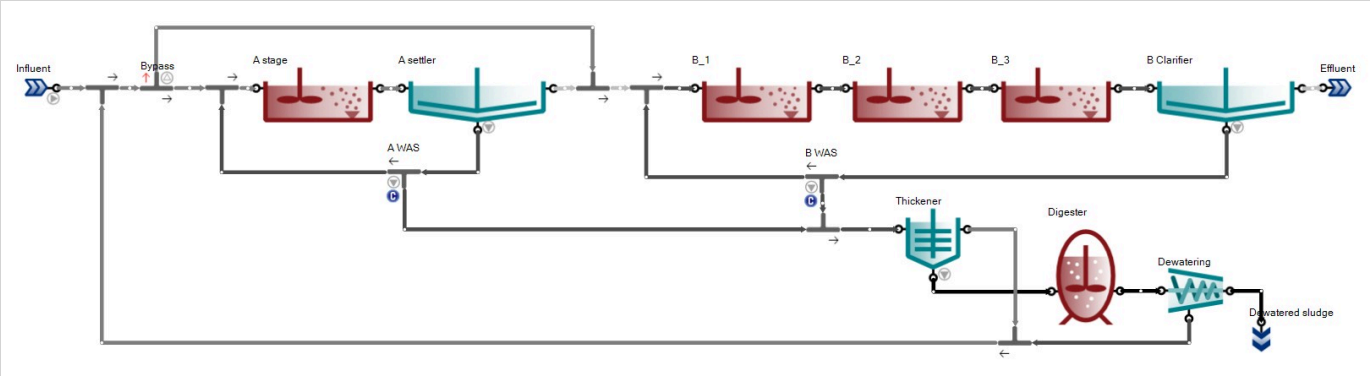


Figure 7.9 - The ‘AB plant’ configuration

AB plant with energy

AB plant with energy calculations turned on.

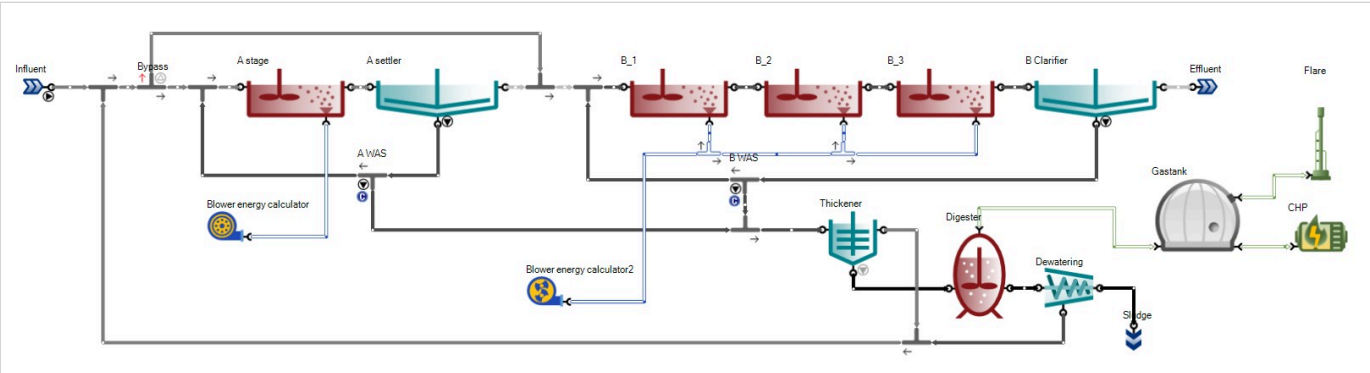


Figure 7.10 - The 'AB plant with energy' configuration

BAF plant

This layout features a treatment plant configuration employing upflow biological aerated filters.

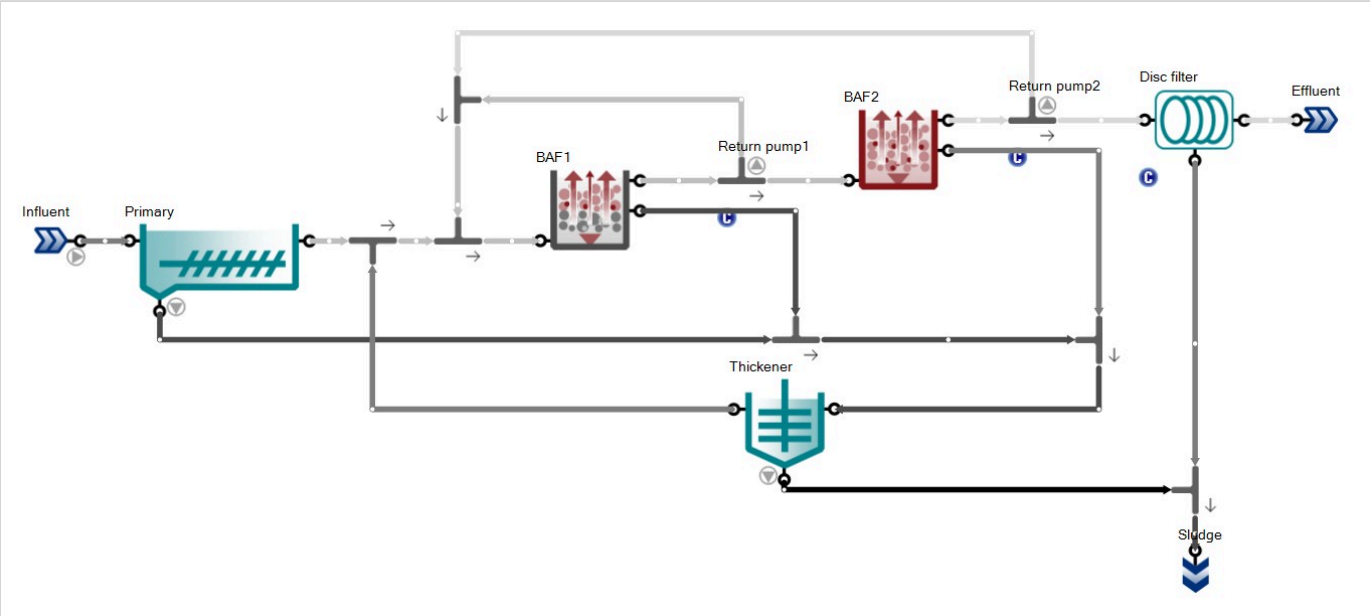


Figure 7.11 - The 'BAF plant' configuration

Bardenpho

Five-stage Bardenpho configuration with one-step nitrification/denitrification model.

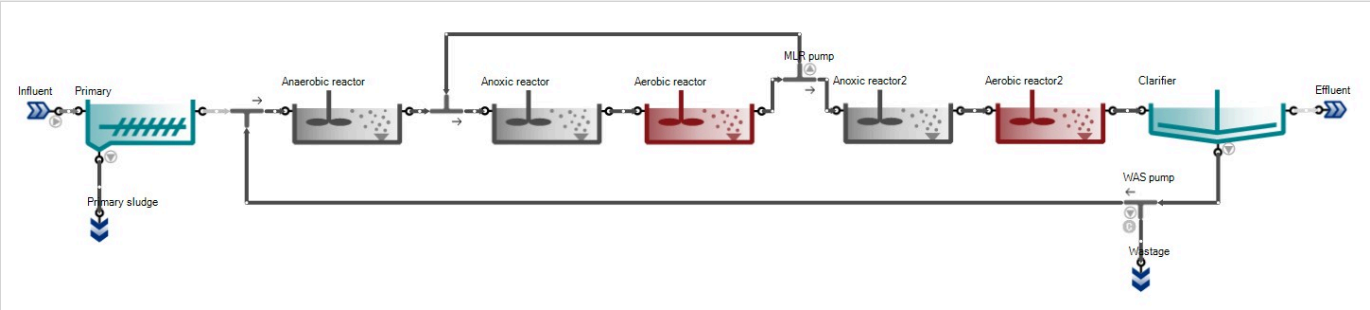


Figure 7.12 – The 'Bardenpho' configuration

HPO configuration

This plant demonstrates the application of high purity oxygen to intensify biological wastewater treatment.

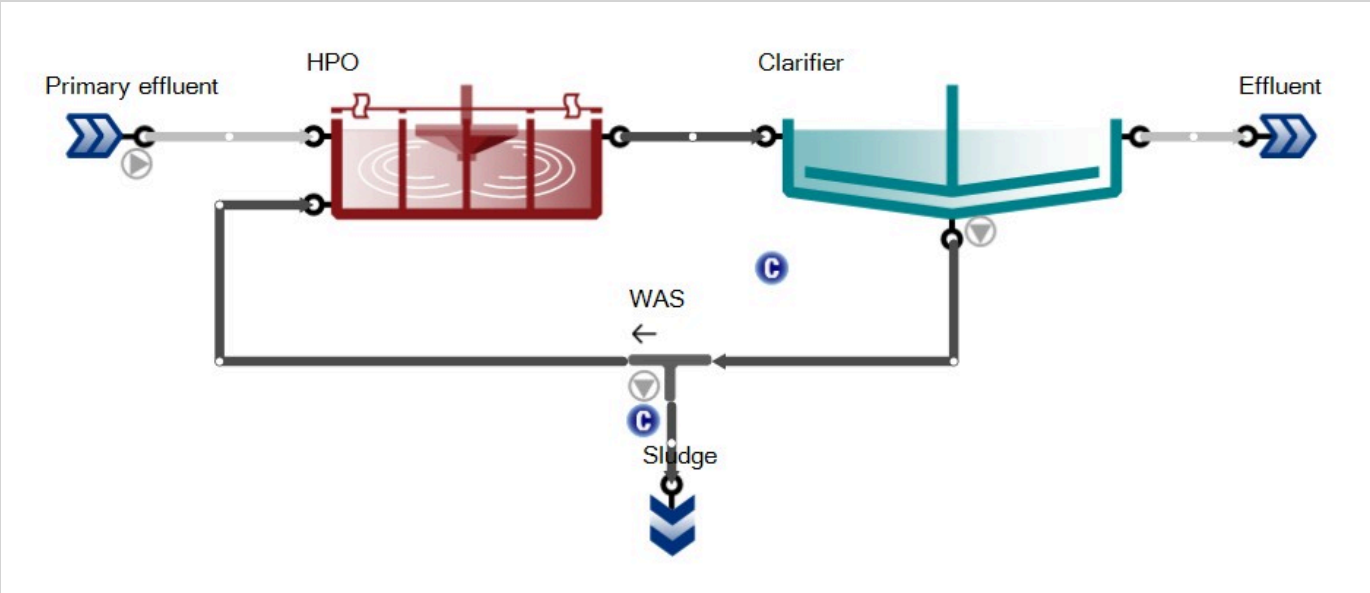


Figure 7.13 - The 'HPO' configuration

Hydraulic SRT

This plant is a demonstration of hydraulic SRT control. The wastage is removed from the reactor itself, and SRT (irrespective of the MLSS content) will be V/Q_{WAS}. Since the reactor volume is 10,000 m^3, 3000 m^3/d wastage will result in 3.3 d of SRT and loss of nitrification at 12°C.

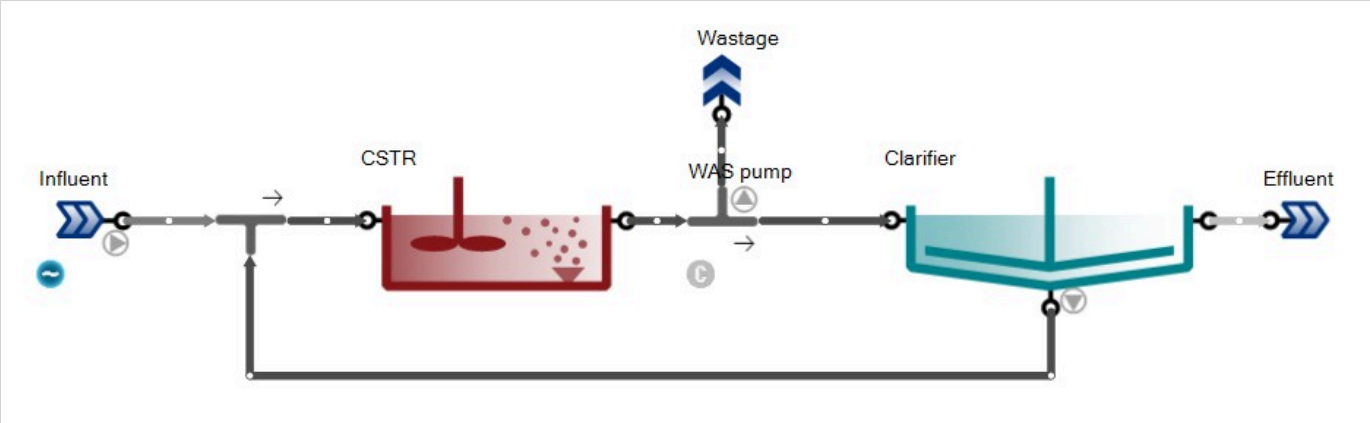


Figure 7.14 - The 'Hydraulic SRT' configuration

MLE configuration

Modified Ludzack-Ettinger configuration with one-step nitrification/denitrification.

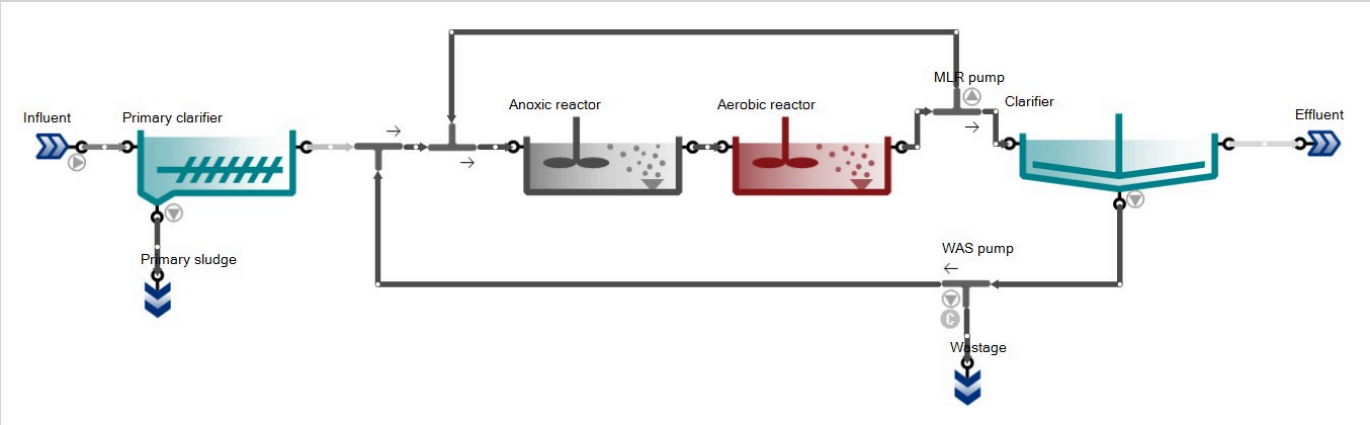


Figure 7.15 – The 'MLE' configuration

MLE with energy

This layout is the MLE configuration extended with energy calculations.

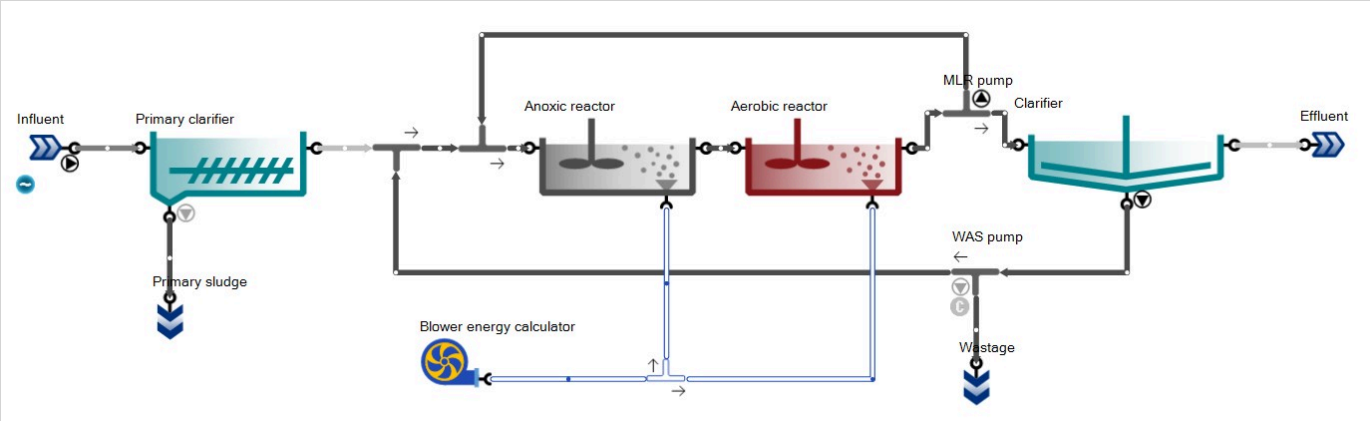


Figure 7.16 – The 'MLE with energy' configuration

MLE with MBR and chemical P removal

This layout is the extended version of the MLE configuration with chemical P removal, using aerated membrane bioreactor as phase separator.

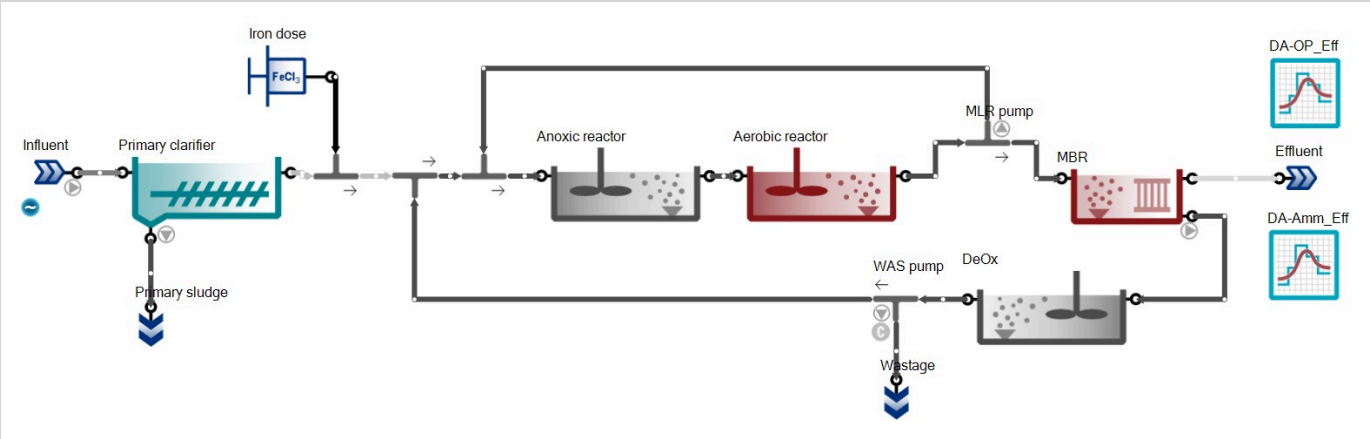


Figure 7.17 – The 'MLE with MBR and chemical P removal' configuration

MLE with MBBR

This layout has two parallel MLE trains with wintertime influent to demonstrate the benefits of upgrading the aerobic reactor with media for enhanced N removal.

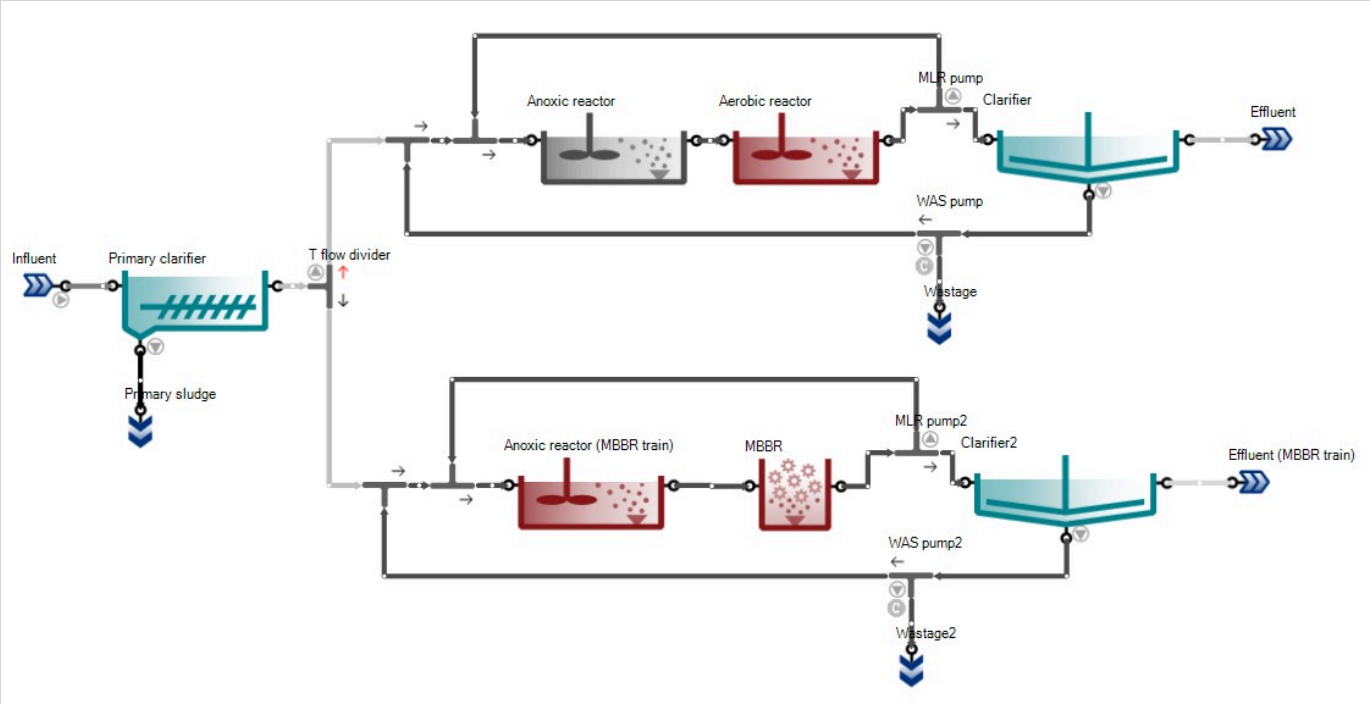


Figure 7.18 – The 'MLE with MBBR' configuration

MLE with urban and river catchment extension

This layout is the extended version of the MLE configuration with an urban catchment and simplified sewer system to generate influent loads and a river catchment with river stretches to model effluent impacts on natural water bodies.

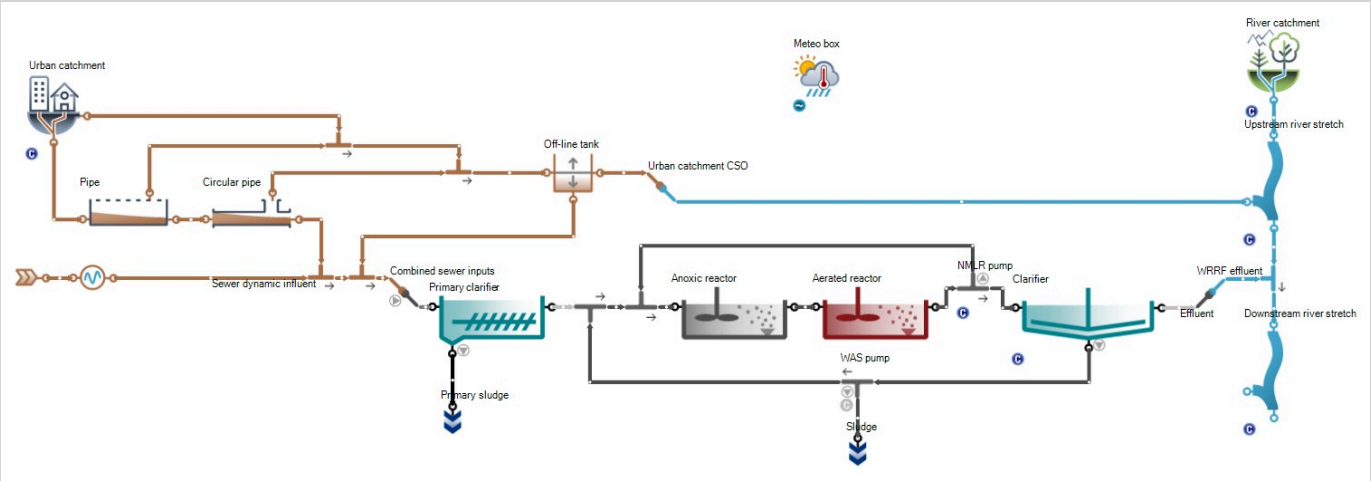


Figure 7.19 – The 'MLE with urban and river catchment extension' configuration

Oxidation ditch

Oxidation ditch example with surface aeration. The ditch is essentially a flow loop and the incoming flow must leave so the outgoing flow must exactly match the influent. The solution to do this in a model is to force the internal flow loop and the rest of the flow overflows to the clarifier. The flow forcing pump does the internal 'recirculation' in the oxidation ditch, while the overflow port automatically equals the input flow rate to the ditch.

To calculate the internal flow (which is usually 50-100 times the influent flow) one needs to multiply the forward linear velocity (usually 0.3-0.6 m/s or 1-2 ft/s) in the ditch with the cross sectional area, which will give a m3/d or MGD flow value. This is the value that should be set in the pump.

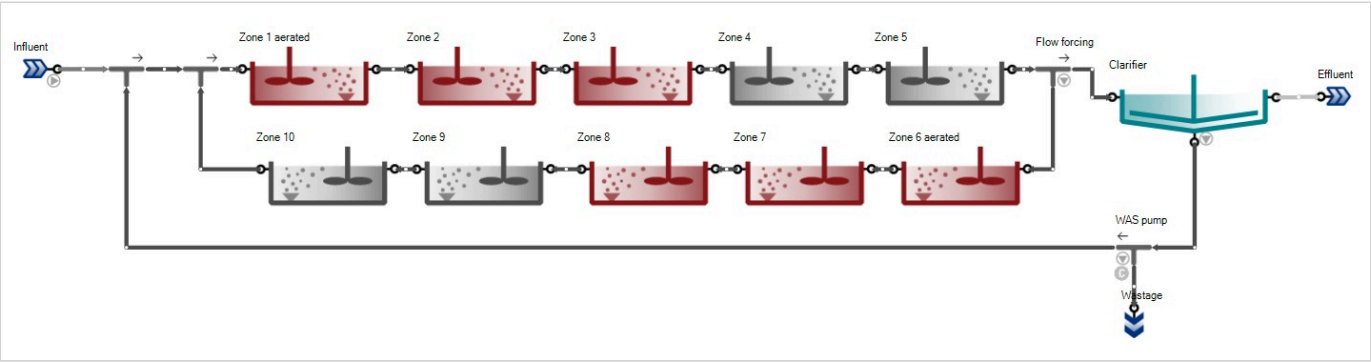


Figure 7.20 – The 'Oxidation ditch' configuration

The Oxidation ditch can be considered ideally mixed as a CSTR for all variables except DO. See the DO profile of the Oxidation ditch on Figure 7.21.

Figure 7.21 – Oxygen profile along the Oxidation ditch

SBR plant

Sequencing batch reactor example with one-step nitrification/denitrification.

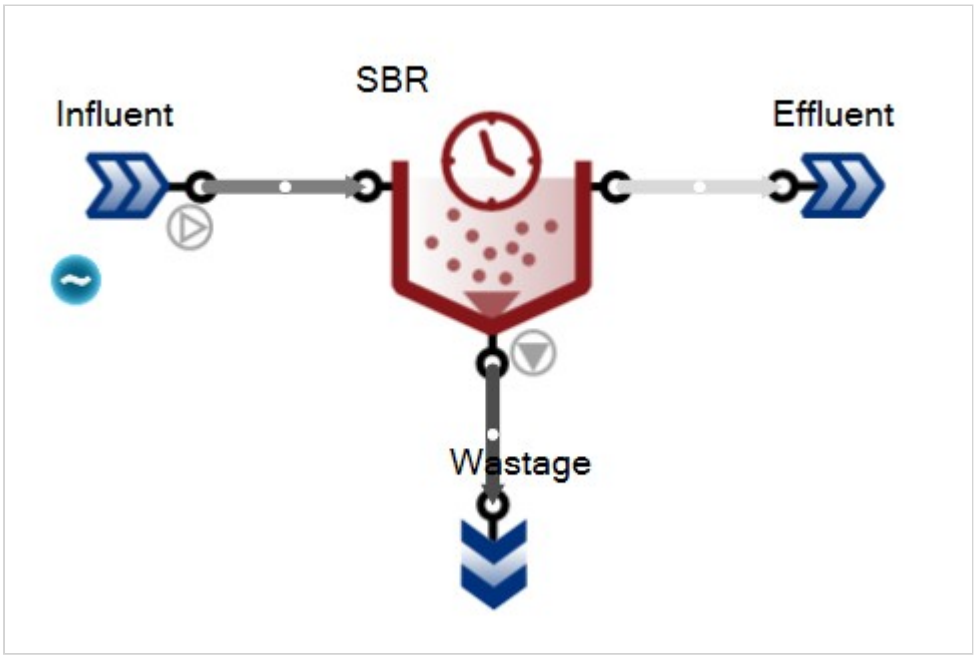


Figure 7.22 - The ‘SBR plant’ example layout

Trickling filter configuration

Simple trickling filter plant example with biofilm model.

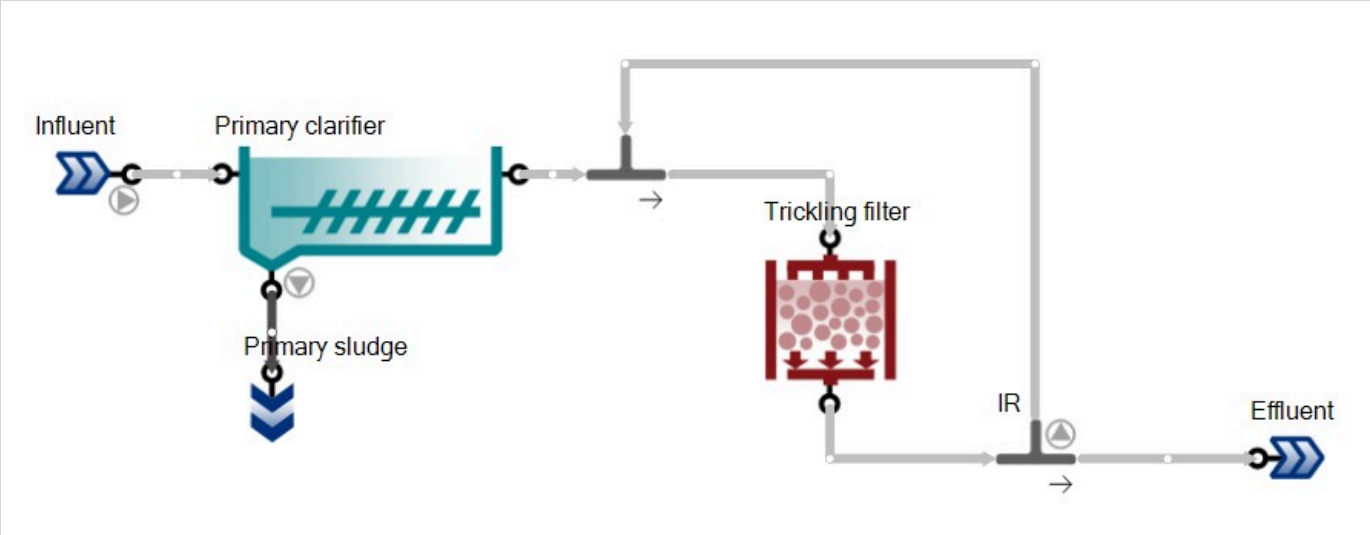


Figure 7.23 - The 'Trickling filter' example layout

THP plant

UCT plant with THP sludge pretreatment stage before digestion. Off-gas and pH calculations are turned on.

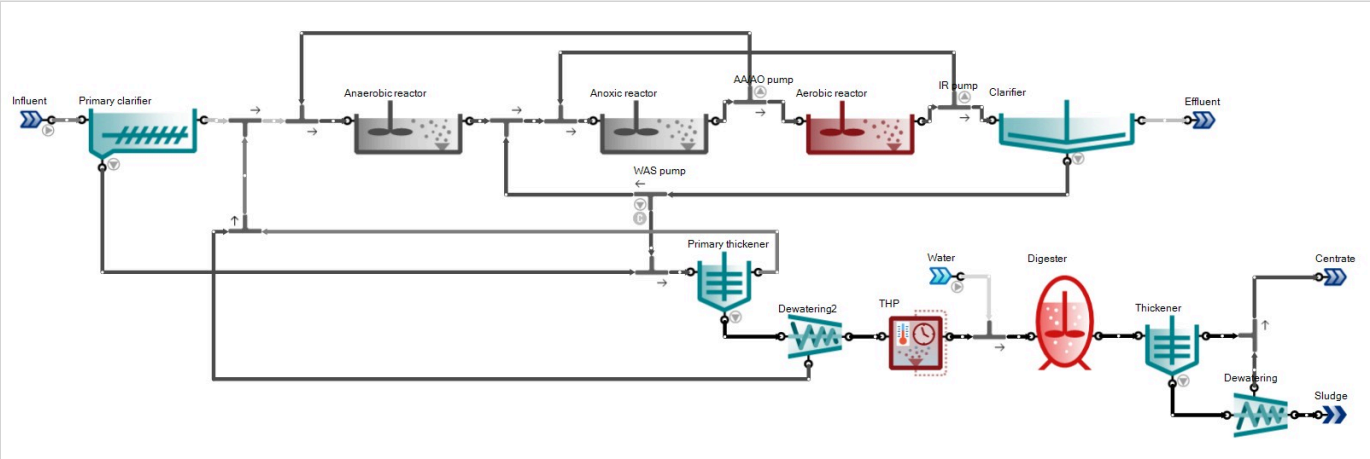


Figure 7.24 – The 'THP plant' configuration

UASB plant with energy

This example layout features a plant with upflow anaerobic sludge blanket reactor with post-aeration and energy calculations turned on.

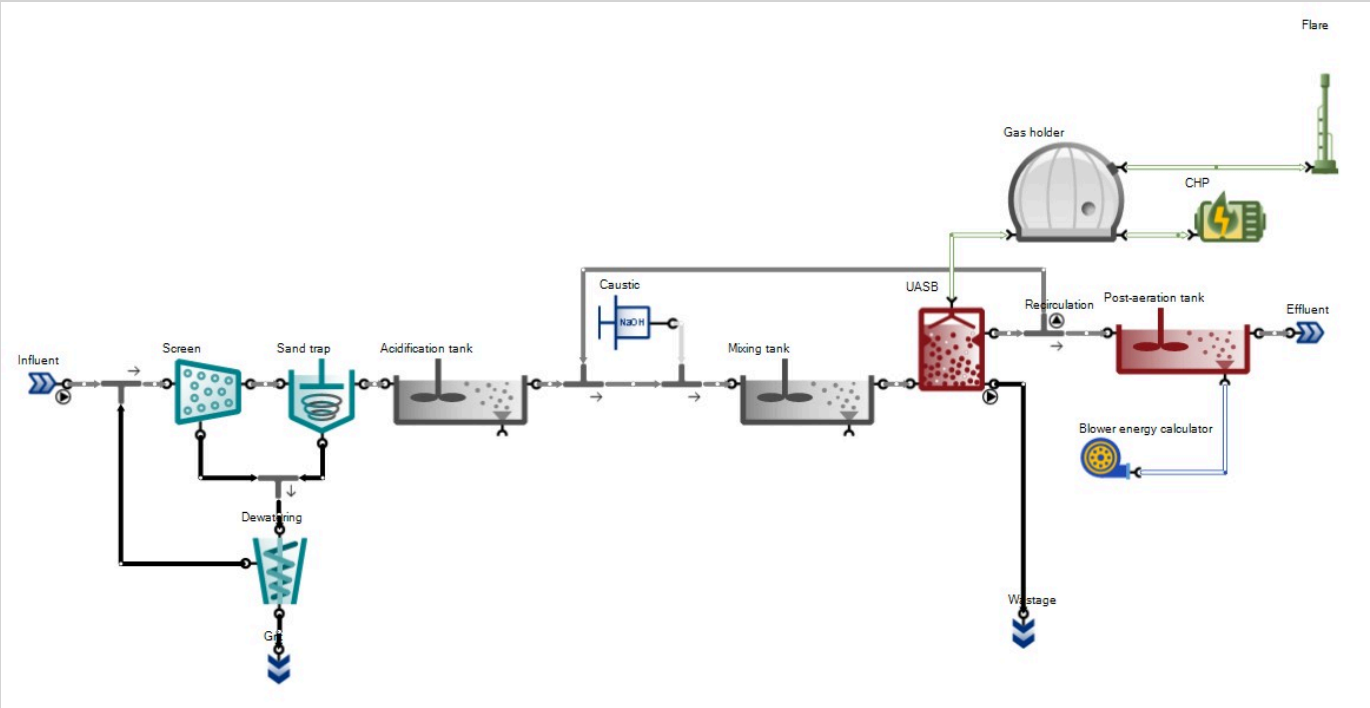


Figure 7.25 – The 'UASB plant with energy' configuration

Three lagoons in series

This example demonstrates the long-term behavior of aerated facultative lagoons.

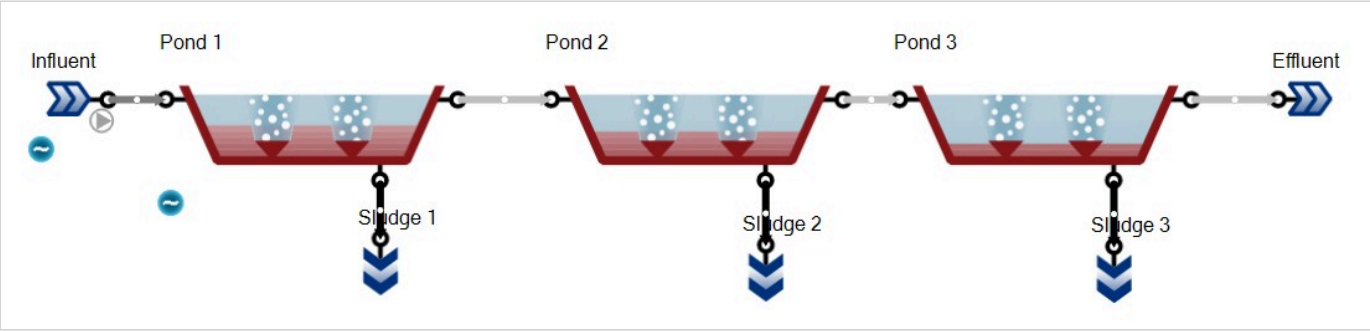


Figure 7.26 – The 'Three lagoons in series' configuration

Two ponds with algae

This example demonstrates the long-term behavior of unaerated ponds relying solely on algae and natural surface aeration.

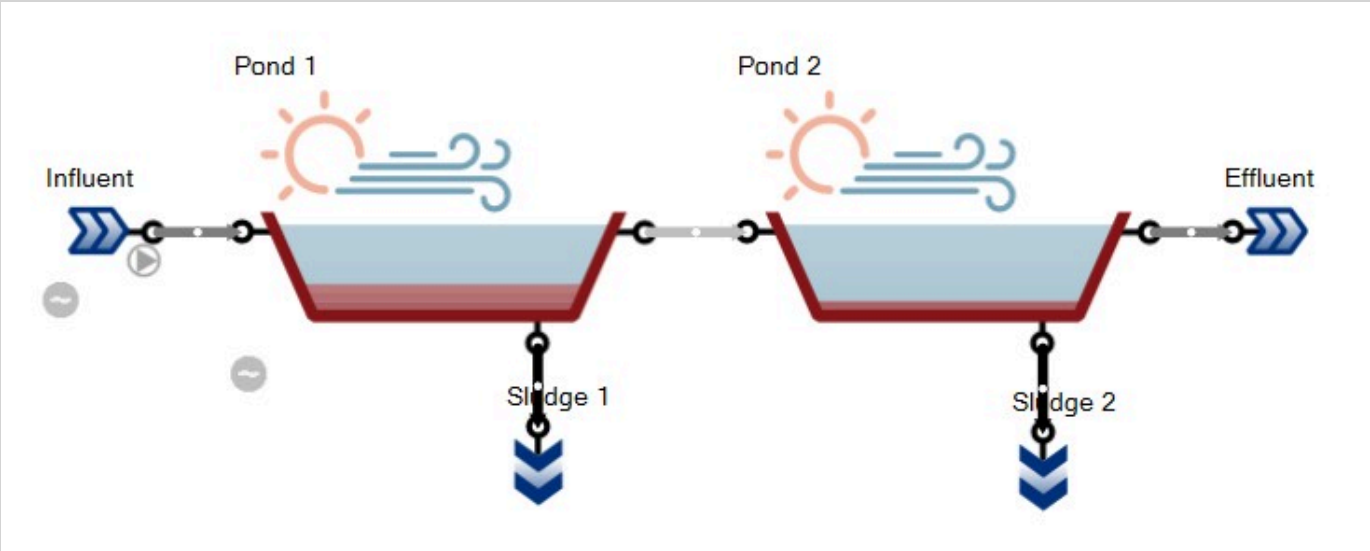


Figure 7.27 – The 'Two ponds with algae' configuration

Titration of ammonia solution

This example demonstrates the ammonium/ammonia relationship depending on pH, using an XY diagram, added from the *Outputs tab* by dropping pH on the X axis and choosing the NH_4^+ and NH_3 in the tank for the Y axis (Figure 7.28).

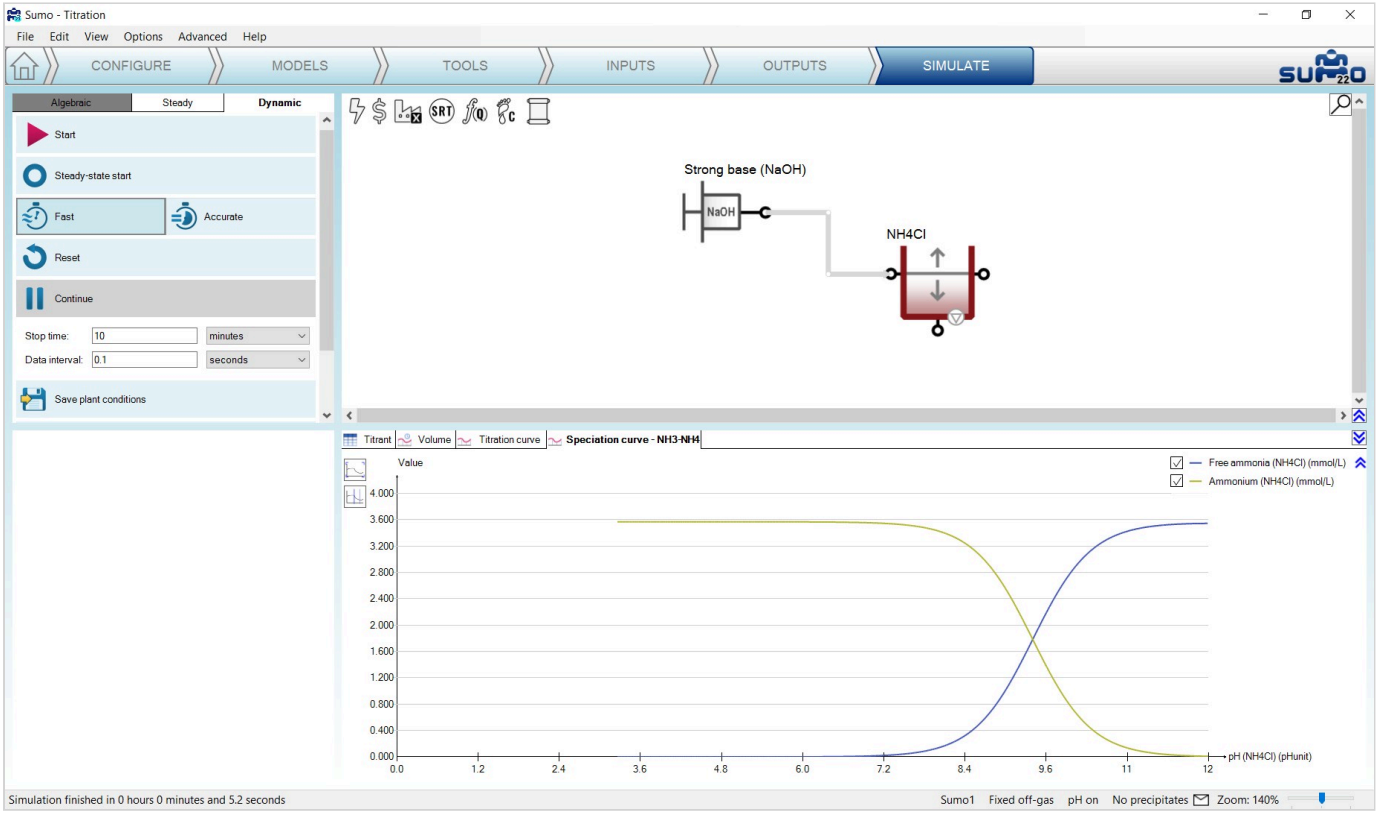


Figure 7.28 – 'Titration example' with simulation

Precipitation

This example demonstrates how the precipitate concentration depends on pH, using the Sumo2S model and an XY diagram, added from the *Outputs tab* by dropping pH on the X axis and choosing the available precipitates (Calcium carbonate as *CaCO3*, Amorphous calcium phosphate as *ACP*, Struvite as *STR*, Vivianite as *Vivi* and Iron sulfide as *FeS*) in the tank for the Y axis (Figure 7.29).

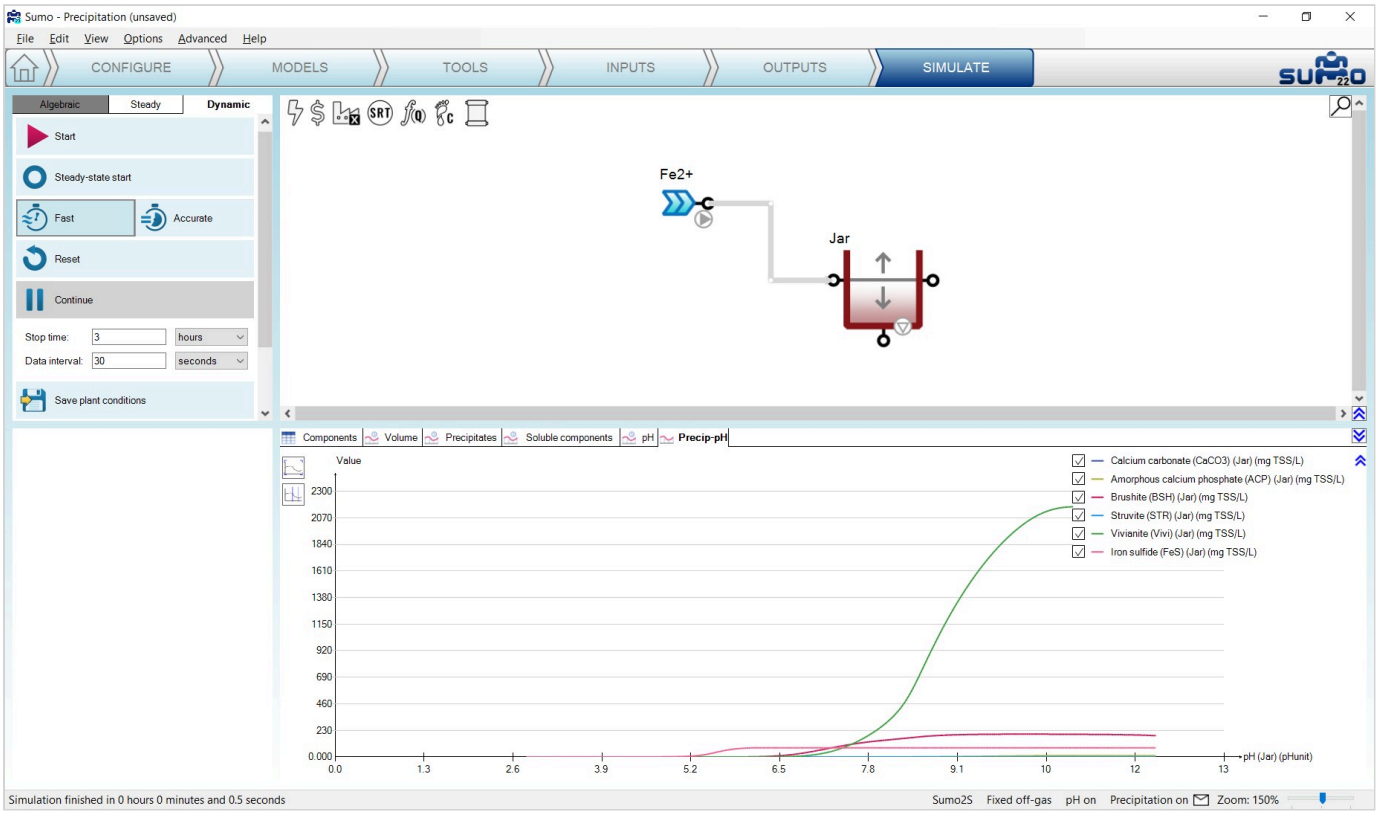


Figure 7.29 – 'Precipitation example' with simulation

Respirometer

This example demonstrates the possibility of simulating a respirometer (Figure 7.30).

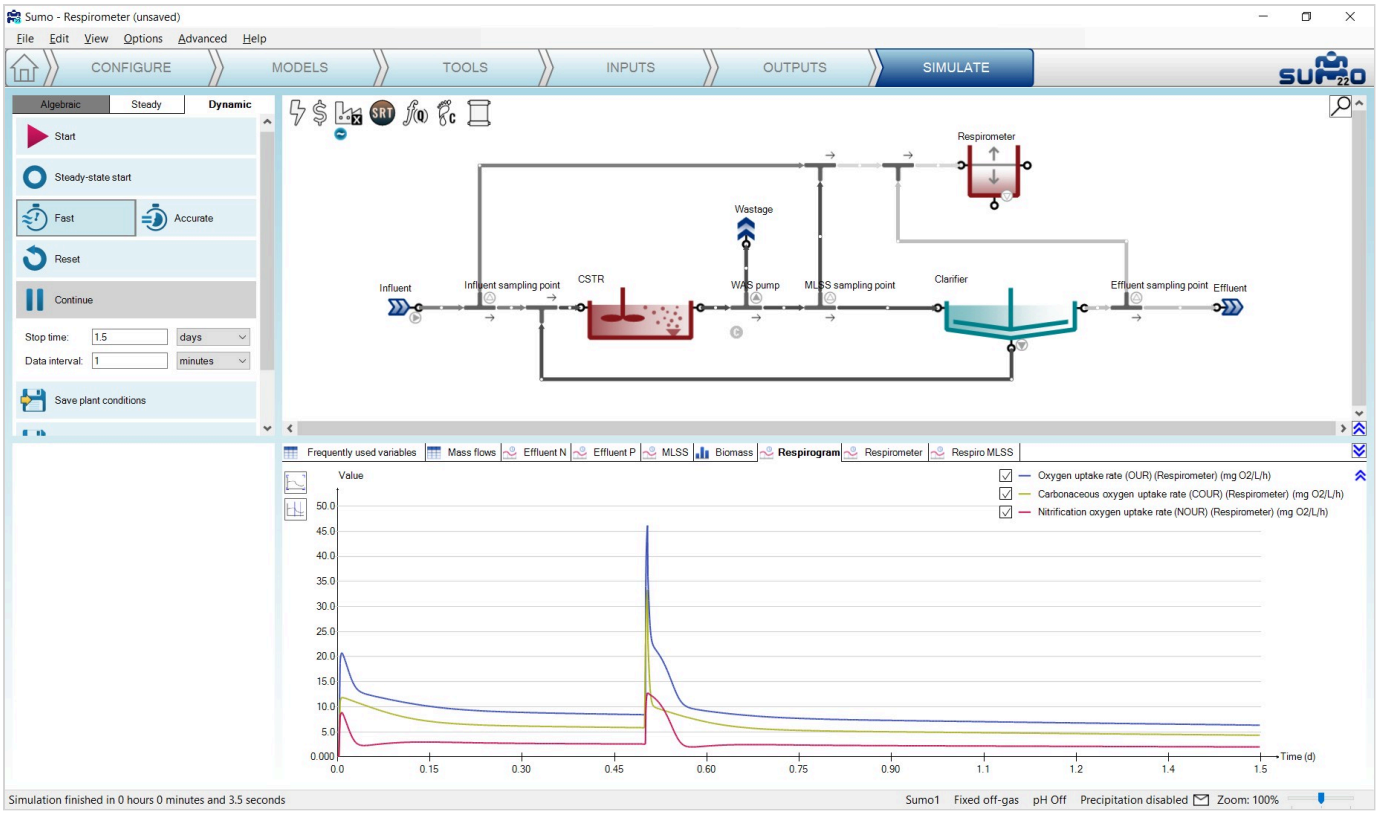


Figure 7.30 – 'Respirometer' example with simulation

P uptake-release test

This example demonstrates the possibility of simulating a P uptake-release jar test using a sample taken from a plant configuration (Figure 7.31).

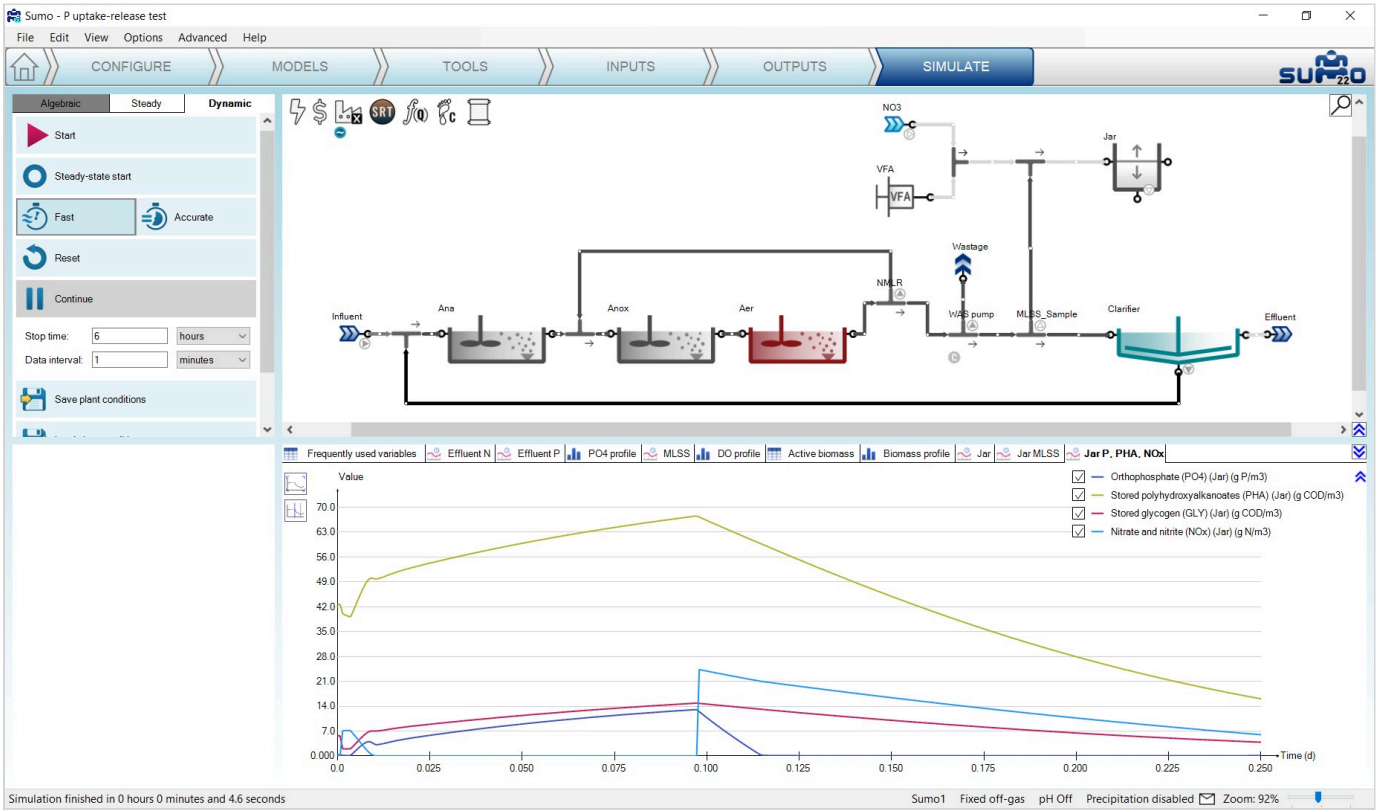


Figure 7.31 – ‘P uptake-release test’ example with simulation

DO and MLSS control

This example demonstrates the implementation of parallel control strategy for MLSS and DO, relying on two PID controllers (Figure 7.32 and Figure 7.33).

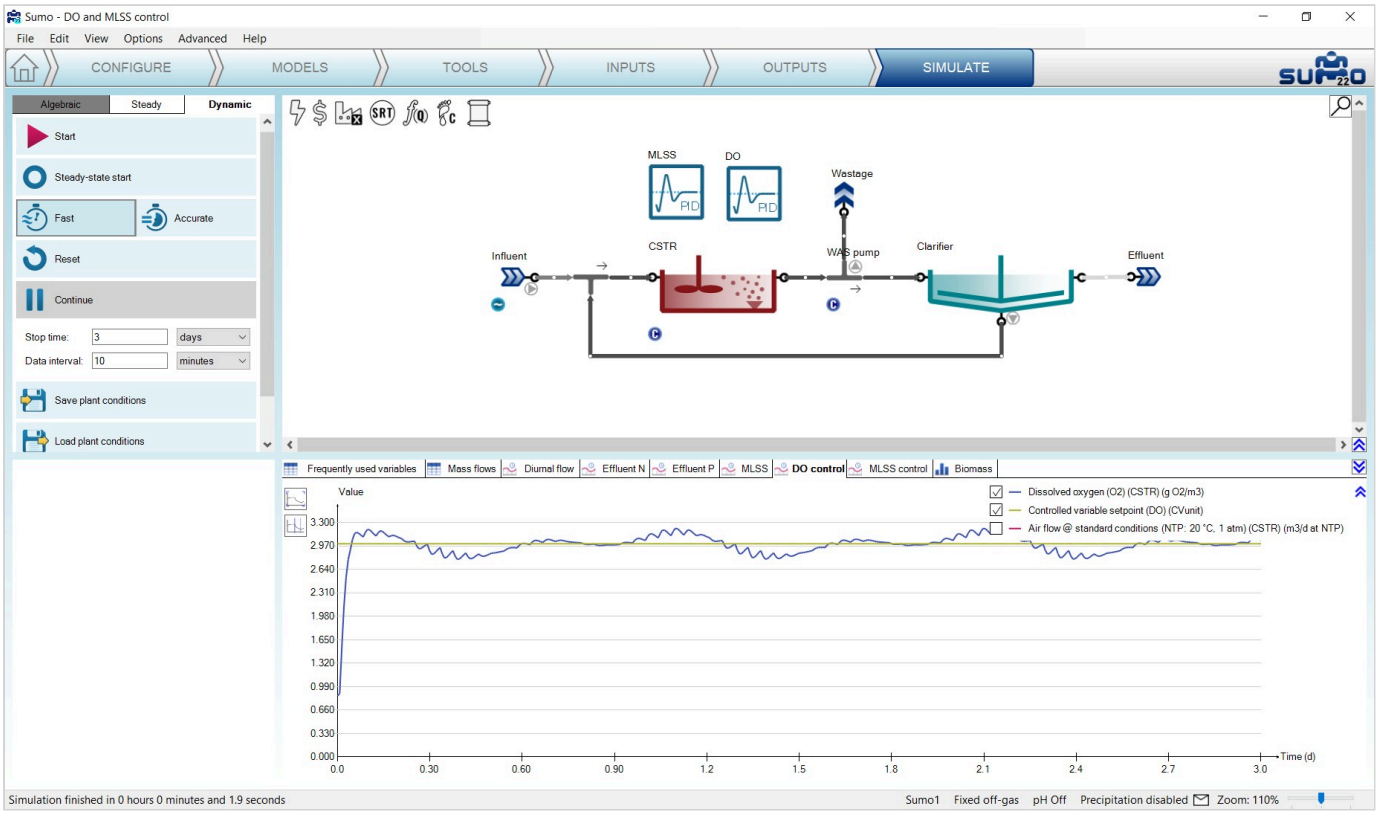


Figure 7.32 – ‘DO and MLSS control’ example with simulation (DO control)

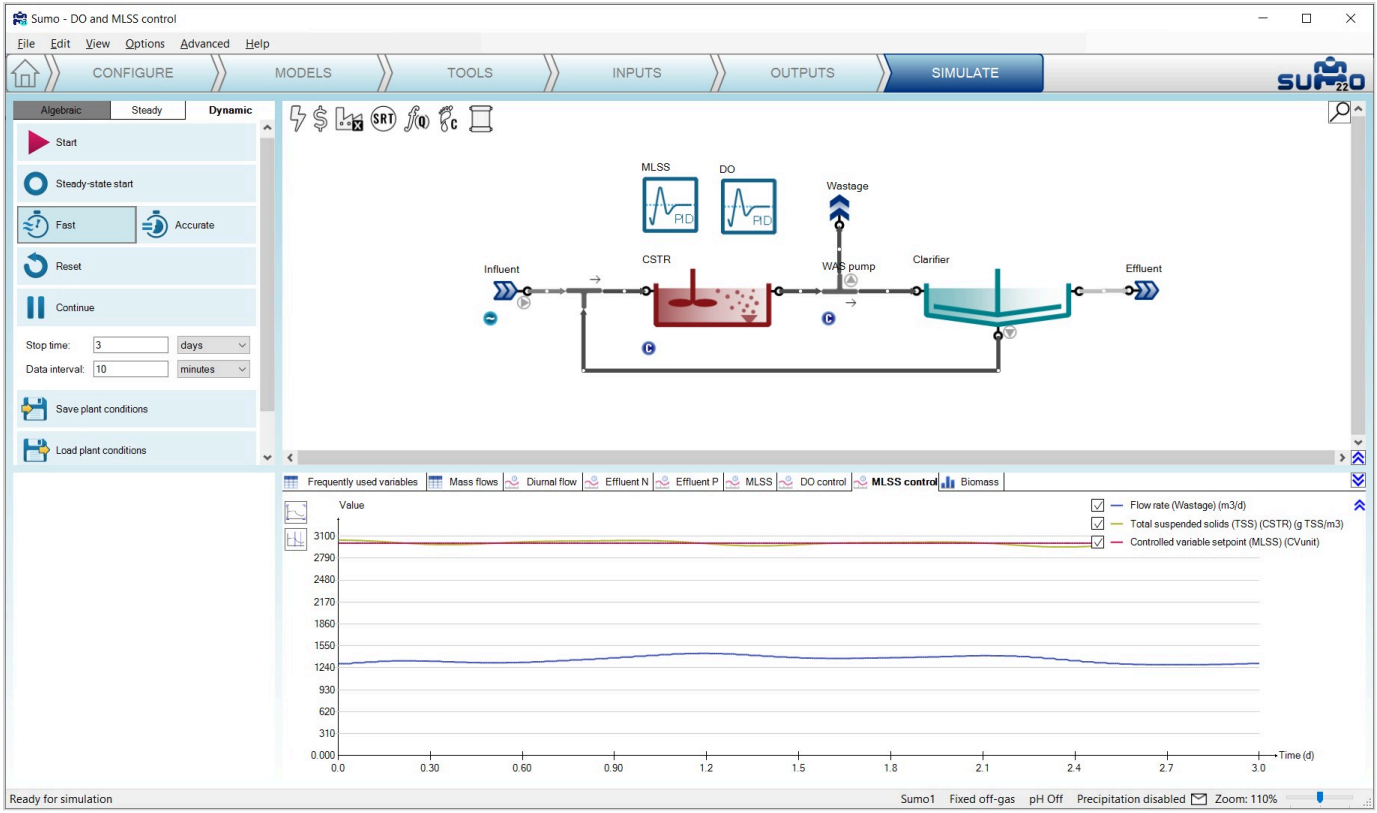


Figure 7.33 – 'DO and MLSS control' example with simulation (MLSS control)

Cascade controller

This example demonstrates the application of the cascade controller strategy for ammonia-based aeration control (ABAC) using two PID controllers (Figure 7.34).

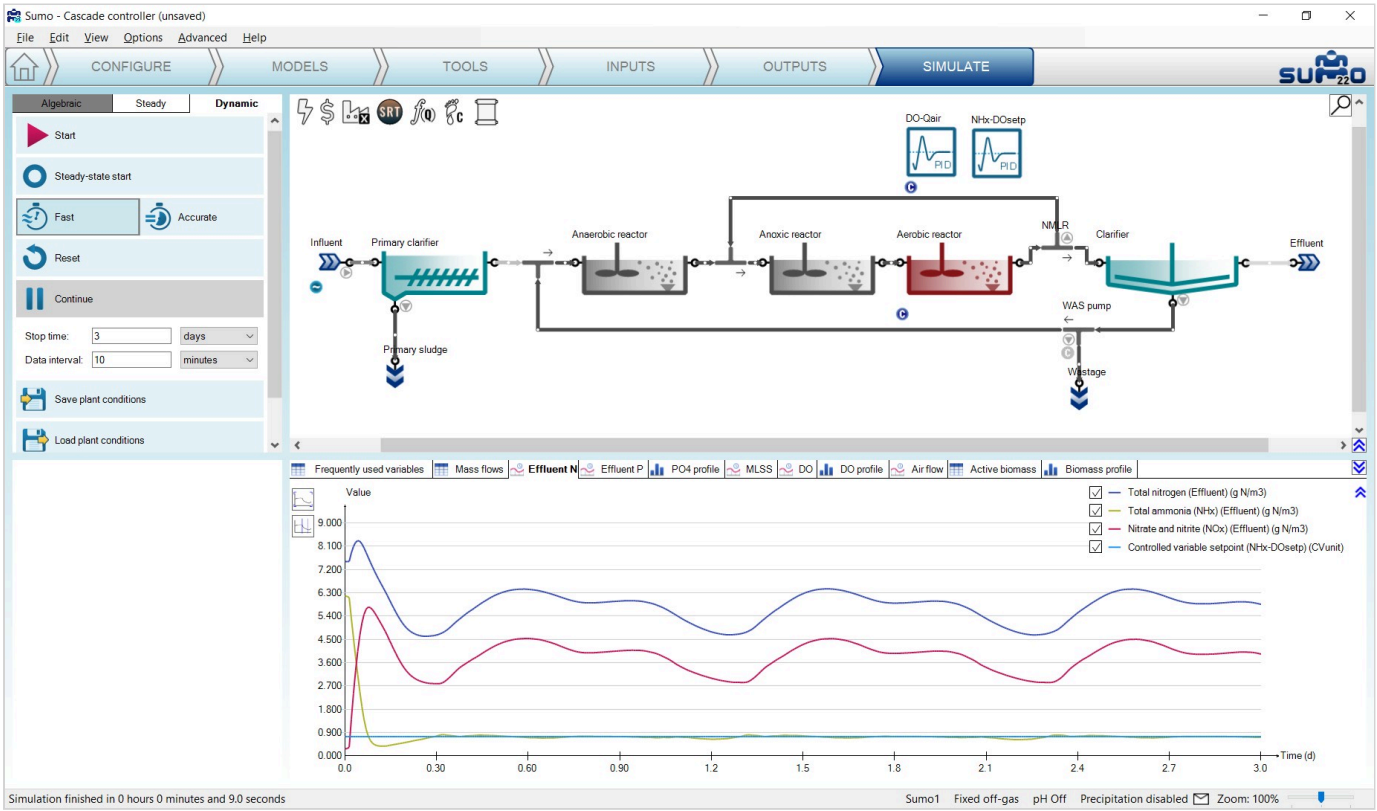


Figure 7.34 – ‘Cascade controller’ example with simulation

Optimal TN control

This example demonstrates the application of the cascade controller strategy to aerate a reactor according to a setpoint of the sum of effluent ammonia and nitrate concentrations, by using a combination of a PID and a time based on/off controller (Figure 7.35).

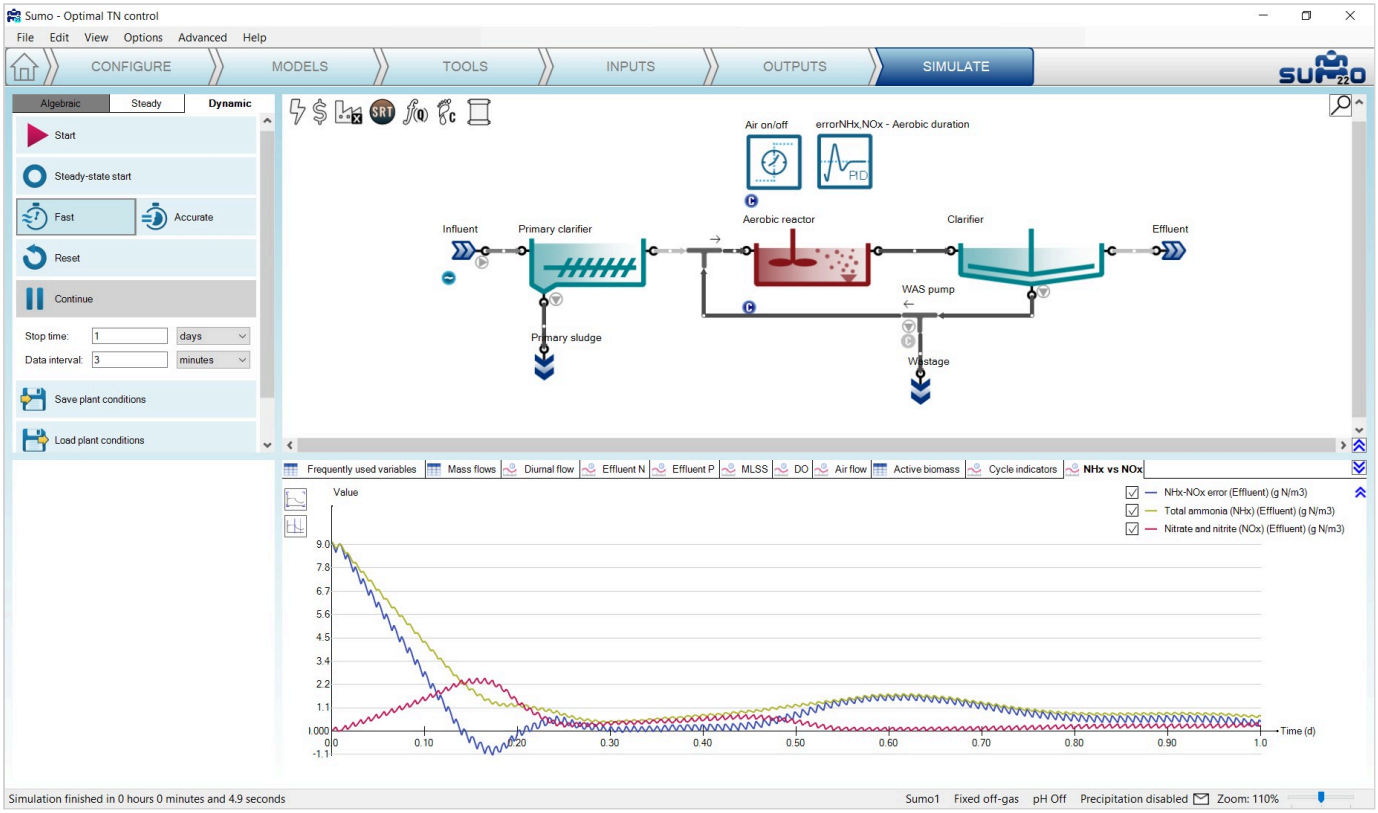


Figure 7.35 – ‘Optimal TN control’ example with simulation

How to use Sumo for plant design

Sumo can be used for plant design as well, based on simple algebraic calculations. This version includes a design tool for AS plants.

AS design calculates the required reactor volume based on design SRT and MLSS.

To set up a plant design example, please follow the steps described below.

Configure

Just like with dynamic configurations, to start the project, the relevant process unit has to be chosen on the *Configure* tab. For the current exercise, this will be the *AS design* from the *Special units* group. This unit is

restricted to be only available for the design model. As the selection of the latter will take place in the model setup, at this point the unit will be indicated as invalid, crossed out with red lines (Figure 8.1).

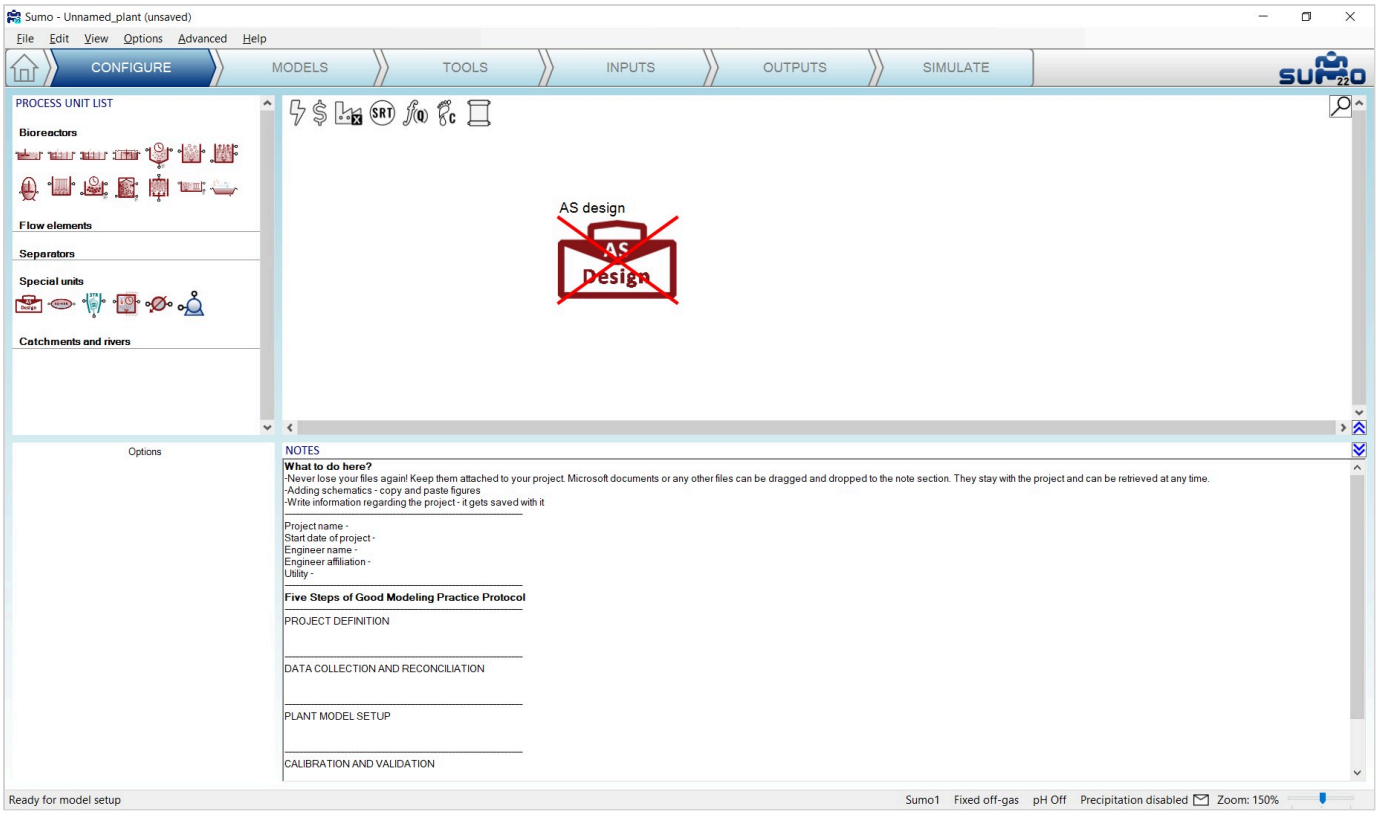


Figure 8.1 - Configuration of AS design

Models

On the *Models* tab, please choose the *Design model* on the top left panel, which is available under *Model selection/Museum, focus and custom models/Other models/Design*. The process unit will become indicated as valid (Figure 8.2).

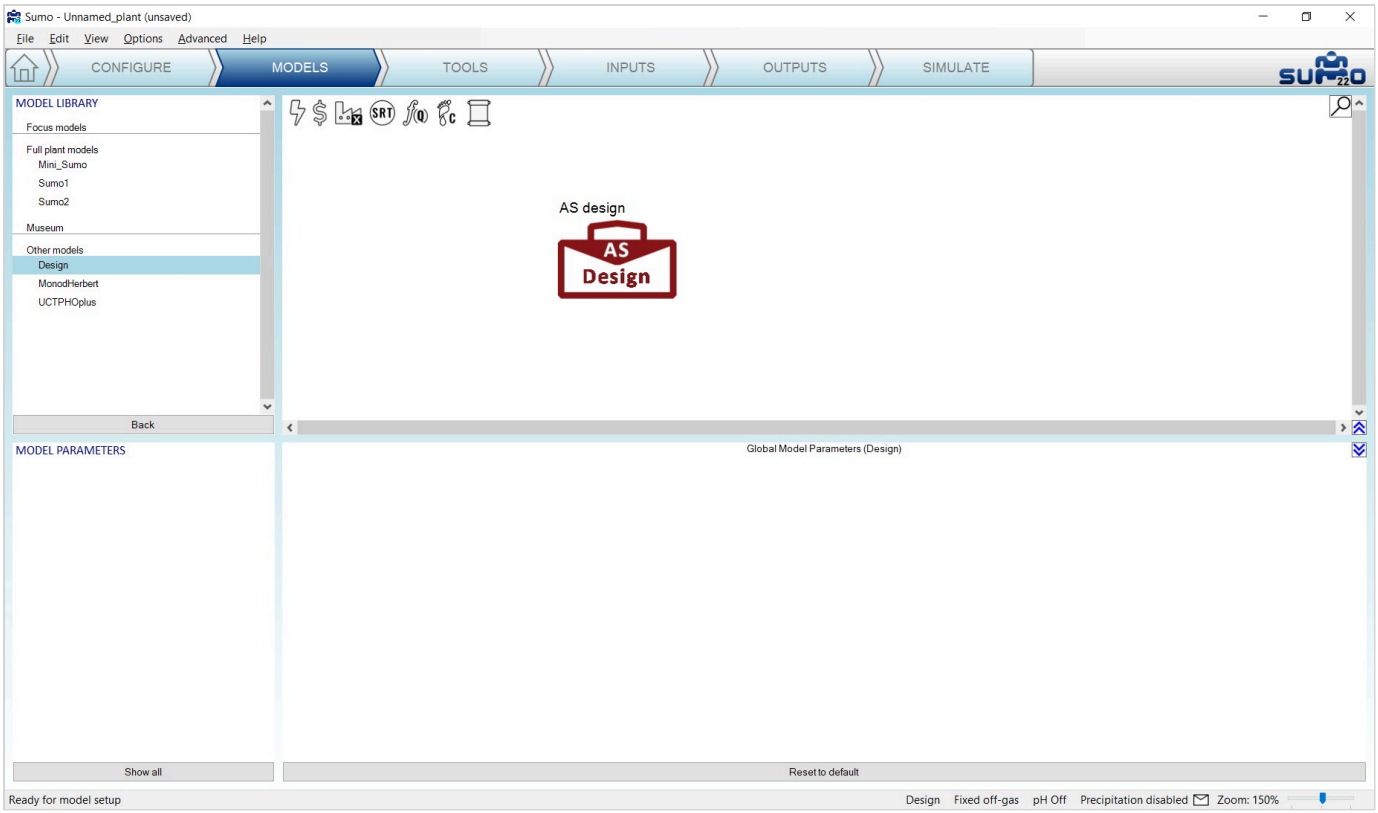


Figure 8.2 - AS design model selection

Inputs

On the *Inputs* tab, the main influent and design parameters can be set (Figure 8.3). By clicking on the *Show all* button, further details (such as COD and biomass fractions) can be added.

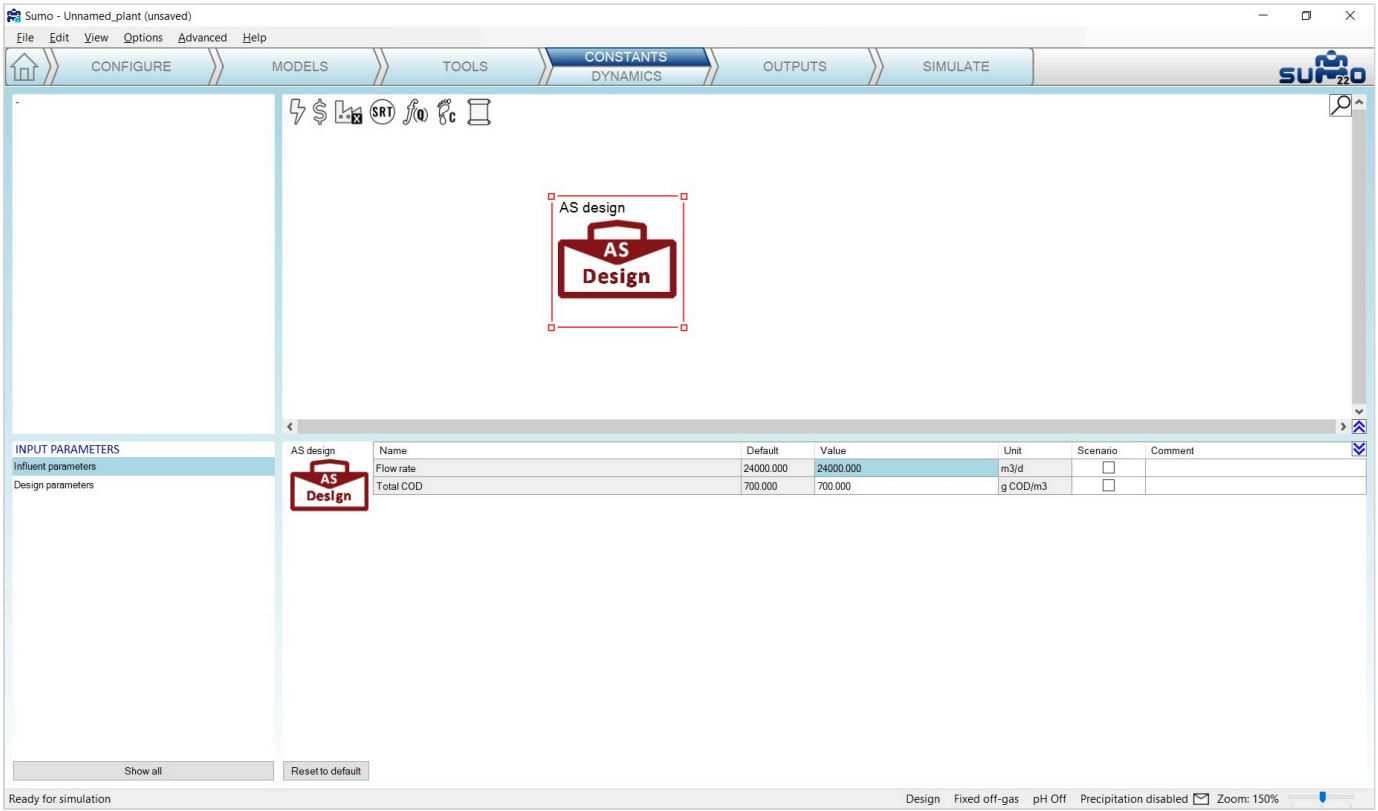


Figure 8.3 - AS design input setup

Outputs

Tables can be added here, similarly to the dynamic configurations (Figure 8.4).

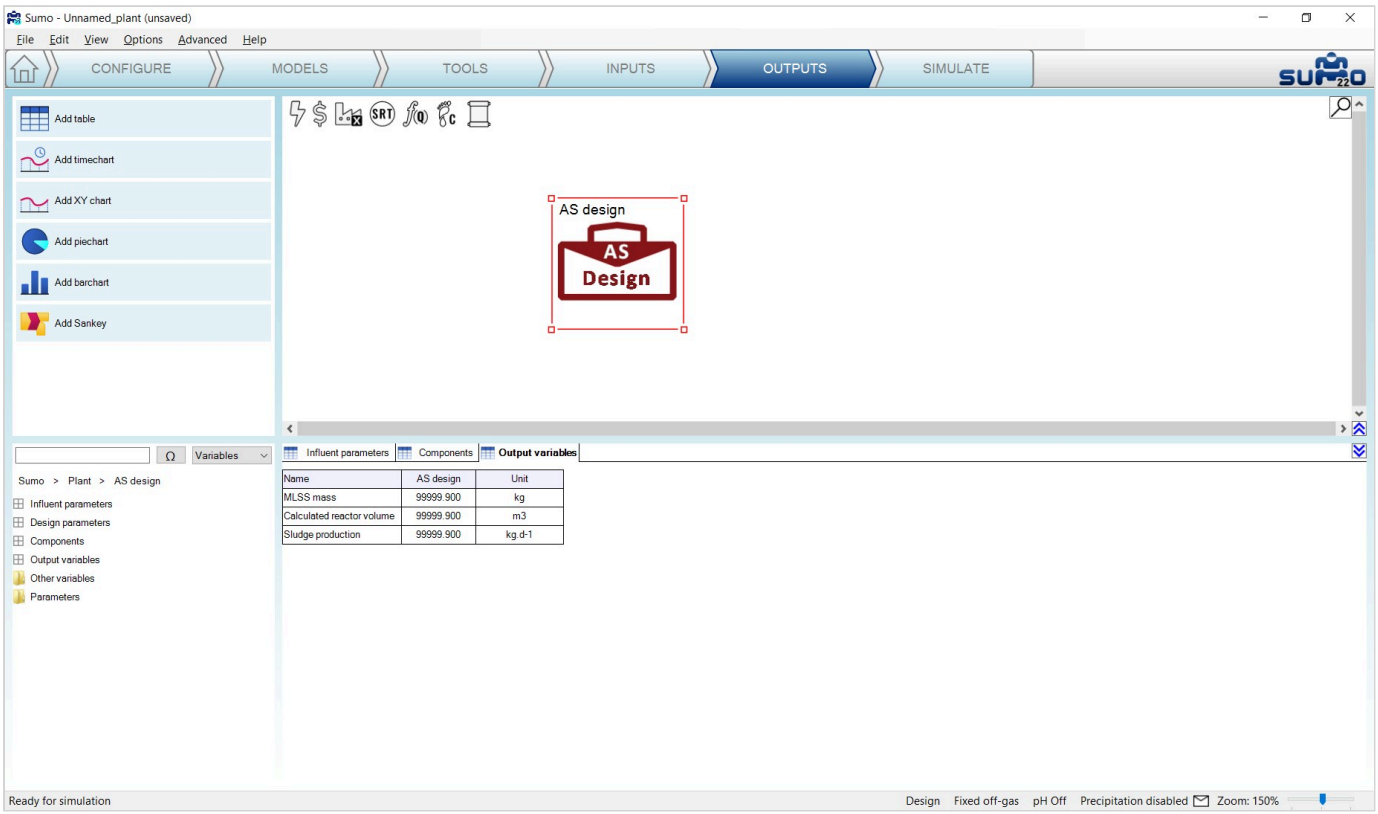


Figure 8.4 - AS design output setup

Simulate

On the *Simulation* tab, the *Algebraic* mode becomes active. Switching to this tab and clicking *Start Algebraic*, the desired calculations will be executed and a report can be written of the results. (Figure 8.5)

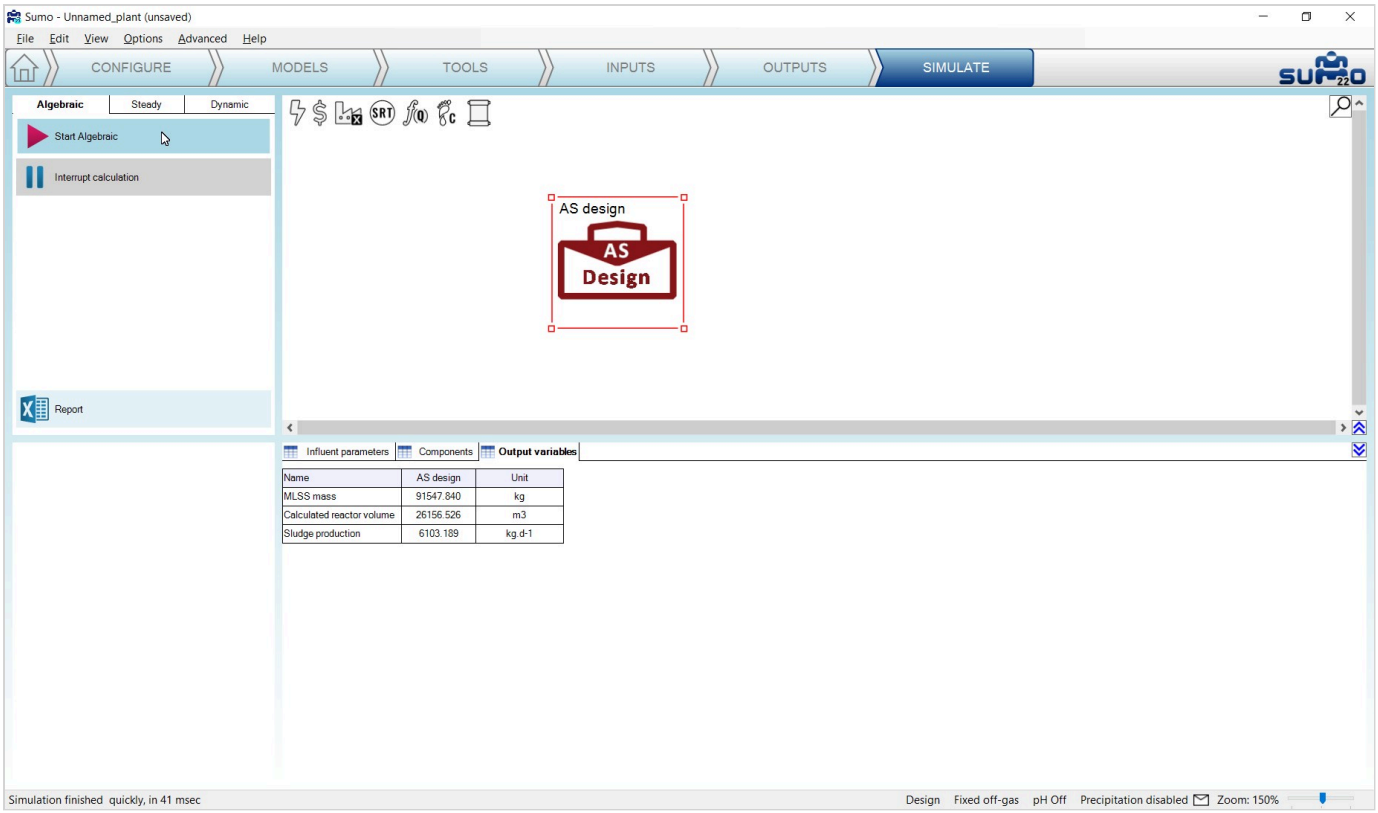


Figure 8.5 - AS design simulation

Technical reference

Process models in Sumo

List of process models available in Sumo with short description.

Introduction

The chapter provides a short description about the available process models in Sumo.

Full plant models

The full plant model contains models which are describing mainstream, digestion and sidestream processes in one model thus the whole operation of a wastewater treatment plant can be simulated.

Mini_Sumo

Dynamita, 2022

Full plant model for OUR and sludge production prediction considering only the following processes linked to the represented biomass groups:

- Ordinary heterotrophs, X_{OHO}:
  - BOD removal under aerobic conditions
  - denitrification in one step under anoxic conditions
  - fermentation of readily biodegradable substrate (S_B) under anaerobic conditions
- Nitrifiers, X_{NITO}:
  - 1 step nitrification from ammonia (S_{NHx}) to nitrate (S_{NOx}) under aerobic conditions
- Acidoclastic methanogens, X_{AMETO}:
  - methanogenesis from S_B under anaerobic conditions
- Hydrogenotrophic methanogens, X_{HMETO}:
  - methanogenesis based on dissolved hydrogen gas (S_{H2}) under anaerobic conditions
- Photosynthetic organisms, X_{ALGAE}:
  - growth on ammonia (S_{NHx}) and nitrate (S_{NOx}) in the presence of light (focused on pond model)
- Particulate biodegradable substrate (X_B) hydrolysis to S_B by heterotroph organisms (X_{HET}) formed by X_{OHO} and X_{AMETO}

The physio-chemical model considers:

- Chemical phosphorus removal (iron and alum dosing)

- No precipitates are considered
- No pH calculation is implemented
- Gas transfer focusing on Oxygen and Methane

Sumo1

Dynamita, 2022

Sumo1 is one step nitrification whole plant model considering different organism groups:

- Heterotrophs, X_{OHO}:
  - BOD removal under aerobic conditions
  - denitrification in one step under anoxic conditions
  - fermentation under anaerobic conditions
- Nitrifiers, X_{NITO}:
  - 1 step nitrification from ammonia (S_{NHx}) to nitrate (S_{NOx}) under aerobic conditions
- Carbon storing organisms, X_{CASTO}:
  - one biomass but the processes mimic phosphorus accumulating organisms (X_{PAO}) and gylcogen accumulating organisms (X_{GAO}) behavior
  - competing process between X_{GAO} and X_{PAO}: volatile fatty acids (S_{VFA}) storage
    - as glycogen (X_{GLY}) by X_{GAO} or
    - as polyhydroxyalkanoates (X_{PHA}) with phosphate release by X_{PAO} under anaerobic conditions
  - fermentation of readily biodegradable substrate (S_B) under anaerobic conditions by X_{PAO}
  - phosphate storage by consuming stored X_{PHA} by X_{PAO} under aerobic conditions
- Acidoclastic methanogens, X_{AMETO}:
  - methanogenesis from readily biodegradable substrate (S_B) under anaerobic conditions
- Hydrogenotrophic methanogens, X_{HMETO}:
  - methanogenesis is based on dissolved hydrogen gas (S_{H2}) under anaerobic conditions
- Photosynthetic organisms, X_{ALGAE}:
  - growth on ammonia (S_{NHx}) and nitrate (S_{NOx}) in the presence of light (focused on pond model)
- Particulate biodegradable substrate (X_B) hydrolysis to S_B by heterotroph organisms (X_{HET}) formed by X_{OHO} and X_{AMETO}

The physio-chemical model considers:

- Chemical phosphorus removal (iron dosing)
- Precipitations: calcium carbonate (X_{CaCO3}), Amorphous calcium phosphate (X_{ACP}), brushite (X_{BSH}), struvite (X_{STR}), vivianite (X_{Vivi})
- Chemical equilibrium (ionic speciation) for pH calculation and
- Detailed gas transfer with CO_2 and NH_3.

Varga et al. Recent Advances in Bio-P Modelling a new approach verified by full-scale observations, WRRmod2018 Session 1: Enhanced Biological Phosphorus Removal 47-60

Sumo2

Dynamita, 2022

Sumo2 is a two-step nitrification whole plant model extended from the Sumo1 model with the following modification:

- Two nitrifier biomass groups instead of X_{NITO}:
  - ammonia oxidizer bacteria (X_{AOB}) to oxidize S_{NHX} to nitrite (S_{NO2}) under aerobic conditions and
  - nitrite oxidizer bacteria (X_{NOB}) to oxidize S_{NO2} to nitrate (S_{NO3}) under aerobic conditions
- X_{OHO} denitrification process is extended to grow on nitrite too under anoxic conditions thus allowing shortcut nitrogen removal modeling
- Anammox organisms (X_{AMX}) biomass group is added to:
  - growth under autotrophic anaerobic environment using S_{NHx} and S_{NO2} as substrate to produce nitrogen gas (S_{N2})

Focus models

Focus models are special full plant models developed in Sumo to highlight processes in more detailed way.

Sumo2C

Dynamita, 2016

Sumo2C is an extension of Sumo2 for carbon capture technologies, by describing colloidal material and EPS generation, flocculation, and storage in all typical units of a water resource and recovery facility (WRRF).

Hauduc H., Al-Omari A., Wett B., Jimenez J., De Clippeleir H, Rahman A., Wadhawan T., Takacs I. (2018) Colloids, Flocculation and Carbon Capture A Comprehensive Plant-wide Model. Water Science and Technology, 79(1), 15-25

Sumo2S

Dynamita, 2021

Sumo2S is an extension of Sumo2 whole plant model with main sulfur reactions:

- 3 sulfur oxidation states as state variables: Sulfate (SO_4), elemental sulfur (S°) and hydrogen sulfide (H_2S)
- 2 step biological sulfur oxidation by SOO

- 2 step chemical oxidation of sulfur
- Sulfate reduction into hydrogen sulfide by 2 anaerobic biomasses: ASRO and HSRO
- interactions of sulfur cycle with phosphorus and iron cycles: precipitation of vivianite and FeS

Hauduc H., Wadhawan T., Johnson B., Bott C., Ward M., Takács I. (2018) Incorporating Sulfur Reactions and Interactions with Iron into a General Plantwide Model. Water Science and Technology, 79(1), 26-34.

Sumo4N

Dynamita, 2021

Sumo4N is an extension of Sumo2 whole plant model extended with 4 step nitrification (Pocquet et al., 2016) and 4 step denitrification models (Hiatt & Grady, 2008), including N_2O formation.

Hiatt, W.C., Grady, C.P.L. Jr., 2008. An updated process model for carbon oxidation, nitrification, and denitrification. Water Environ. Res. 80(11), 2145-2156.

Pocquet, M., Wu, Z., Queinnec, I., Spérandio, M., 2016. A two pathway model for N2O emissions by ammonium oxidizing bacteria supported by the NO/N2O variation. Water Res. 88, 948-959.

Museum models

Museum models are the representation of widely known historical models of the wastewater treatment.

ASM1

The classic model from 1986 that started it all. Influent inorganics added to be able to calculate TSS (required for certain phase separation units). Nitrification/denitrification model, for estimation of OUR and sludge production in BNR configurations.

Henze M., Grady C. P. L. Jr, Gujer W., Marais G. v. R. and Matsuo T. (2000) Activated Sludge Model No. 1, IWA Publishing, Scientific and Technical Report No. 9, London

ASM2D

Bio-P model based on ASM1 with modifications.

Henze M., Gujer W., Mino T., Matsuo T., Wentzel M. C., Marais G.v.R., and van Loosdrecht M.C.M. (2000). Activated Sludge Model No. 2d, IWA Publishing, Scientific and Technical Report No. 9, London IWA.

ASM2D_TUD

ASM2D with the TUD metabolic bio-P model.

Meijer, S. C. F. (2004). Theoretical and practical aspects of modelling activated sludge processes. Department of Biotechnological Engineering. Delft University of Technology, The Netherlands: 218

ASM3

Nitrification/denitrification model, with substrate storage.

Henze M., Gujer W., Mino T., Matsuo T., Wentzel M. C., Marais G.v.R., and van Loosdrecht M.C.M. (2000). Activated Sludge Model No. 2d, IWA Publishing, Scientific and Technical Report No. 9, London IWA.

ASM3_BioP

ASM3 with bio-P component added.

Rieger L., Koch G., Kühni M., Gujer W. and Siegrist H. (2001) The EAWAG bio-P module for activated sludge model No.3. Wat. Res., 35 (16), 3887-3903.

Barker-Dold

Nitrification/denitrification/bio-P model (modified ASM1 and Wentzel bio-P based).

Barker P.S. and Dold, P.L. (1997). General model for biological nutrient removal activated-sludge systems: model presentation, Wat. Env. Res., 69 (5), 969-984.

Other models

Other models are examples for researchers and developers to highlight the possibilities of Sumo.

Design

Model for design calculations and algebraic model development.

MonodHerbert

A simple model to demonstrate the model development logic on base ofmaterialsone-step Monod-Herbert process rate expressions.

UCTPHOplus

Hu, Z. R., M. C. Wentzel, et al. (2007). A general kinetic model for biological nutrient removal activated sludge systems: Model development. Biotechnology and Bioengineering 98(6): 1242-1258.

Nitrification/denitrification/bio-P model.

Components and processes

List of component used in Sumo model followed by detailed process descriptions.

Introduction

The chapter gives detailed insights into the components and processes of Sumo models. This information helps the user to understand the interactions between components, indicates the model logic and consideration behind the mathematical description.

Components in Sumo models

There are five symbols that distinguish the types of components, also referred to as state variables (SVs):

- soluble (S),
- colloidal (C),
- particulate (X),
- gaseous (G),
- and enthalpy (H).

The soluble SVs are transported through water, and colloidal SVs and particulate SV become part of the sludge which then can be separated from water through the settling process.

	Components			
Symbol	Name	Model	Definition	Unit
S_{VFA}	Volatile fatty acids (VFA)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A fermented product representing a combination of acetate and other volatile fatty acids produced in an anaerobic environment from S_B. It is available for biological removal by OHOs, CASTOs (PAOs, GAOs), and AMETOs and chemical removal during HFO reduction.	g COD.m^{-3}
S_B	Readily biodegradable substrate (non-VFA)	Mini_Sumo, Sumo1, Sumo2, Sumo2S, Sumo4N	Non-VFA organic material that can be fermented to VFA, it represents a group of readily biodegradable organic material present in wastewater.	g COD.m^{-3}
$S_{B,mono}$	Readily biodegradable substrate as monomers (non-VFA)	Sumo2C	Small molecular weight substrate mainly consumed by AHOs in 1st stage of high-rate process.	g COD.m^{-3}
$S_{B,poly}$	Readily biodegradable substrate as polymers	Sumo2C	Readily biodegradable substrate that is not degraded in 1st stage of a high-rate process. Consumed by OHOs in 2nd stage.	g COD.m^{-3}
S_{MEOL}	Methanol (MEOL)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A methyl alcohol or the simplest alcohol. A commonly used external carbon source for denitrification.	g COD.m^{-3}

	Components			
Symbol	Name	Model	Definition	Unit
C_B	Colloidal biodegradable substrate	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A biodegradable organic component, flocculates to form X_B. Analytically can be approximated by flocculation or filtration (larger than 0.1 micron but smaller than 1.2 micron)	g COD.m^{-3}
X_B	Slowly biodegradable substrate	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	High molecular weight particulates that are hydrolyzed by extracellular enzymes to release S_B. They are introduced directly from the influent and released during the bacterial decay process in death-regeneration concept models.	g COD.m^{-3}
S_U	Soluble unbiodegradable organics	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A soluble organic material that is not degraded biologically or chemically in wastewater and leaves in the effluent. Typically, measured by performing a flocculated filtration test on the effluent of a nitrifying plant. It also has a nitrogen and phosphorus content. There is only one process, the Thermal Hydrolysis Process, which generates S_U from X_U in the model.	g COD.m^{-3}
C_U	Colloidal unbiodegradable organics	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A non-biodegradable organic material, flocculates to form X_U and leaves the plant in the WAS or cake. Analytically can be approximated by flocculation or filtration (larger than 0.1 micron but smaller than 1.2 micron)	g COD.m^{-3}
X_U	Particulate unbiodegradable organics	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A non-biodegradable organic material that is larger than 1.2 micron. It is not hydrolysed and remains untransformed due to biological and chemical reactions. The thermal hydrolysis process model is the only unit that converts a portion of X_U to S_U.	g COD.m^{-3}
X_{STO}	Storage product of AHOs	Sumo2C	An internal cell storage organic material stored by AHOs in low SRT systems using $S_{B,mono}$ and S_{VFA}. Its production doesn't involve any energy and growth.	g COD.m^{-3}
X_{PHA}	Stored polyhydroxyalkanoates (PHA)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Poly-hydroxy alkanoates considered as an internal organic cellular storage product of CASTOs (PAOs). The composition of alkanoates is represented as poly-β-hydroxybutyrate.	g COD.m^{-3}

	Components			
Symbol	Name	Model	Definition	Unit
X_{GLY}	Stored glycogen (GLY)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Internal organic cellular storage product of CASTOs (GAOs).	g COD.m^{-3}
X_E	Endogenous decay products	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	An organic material released during cell lysis under aerobic and anoxic environment, it has an extremely slow conversion rate of 0.07 per day and it converts to X_B while releasing S_{NHx} and S_{PO4}. The X_E builds in a system with increasing SRT.	g COD.m^{-3}
$X_{E,ana}$	Anaerobic endogenous decay products	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	An organic material released on cell lysis under anaerobic environment and hydrolysed in aerobic environment to release S_B, S_{NHx}, and S_{PO4}. This component is responsible for the additional VS destruction observed in a post aerobic digestion process.	g COD.m^{-3}
X_{OHO}	Ordinary heterotrophic organisms (OHO)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Generalist facultative ordinary hetrotrophic organisms that consume different soluble biodegradable organics including S_B, S_{VFA}, and X_{MEOL} and can perform biological removal under aerobic, anoxic, and anaerobic environments. They are also responsible for hydrolysis of the particulates. In MiniSumo and Sumo1, they perform one step denitrification, meaning from S_{NOx} to S_{N2}. In other models they follow two steps, S_{NO3} reduction to S_{NO2}, and S_{NO2} reduction to S_{N2}.	g COD.m^{-3}
X_{CASTO}	Carbon storing organisms (CASTO)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A special group of carbon storing heterotrophic organisms representing a combination of both PAOs and GAOs. The process conditions dictate the ratio of PAO to GAO achieved in the process model. They are responsible for taking part in the EBPR process. They store PHA and/or GLY during the anaerobic conditions, and consume stored carbon during anoxic and aerobic environments to generate polyphosphate (X_{PP}). In Sumo1, they perform one step denitrification, meaning from S_{NOx} to S_{N2}. Is other models they follow two steps, S_{NO3} reduction to S_{NO2}, and S_{NO2} reduction to S_{N2}.	g COD.m^{-3}
X_{MEOLO}	Anoxic methanol utilizers (MEOLO)	Sumo1, Sumo2, Sumo2C, Sumo2S,	Specialist heterotrophic organisms responsible for removal of X_{MEOL}.	g COD.m^{-3}

	Components			
Symbol	Name	Model	Definition	Unit
		Sumo4N	Only found in systems with methanol addition and compete with OHOs during denitrification process. In Sumo1, they perform one step denitrification, meaning from S_{NOx} to S_{N2}. Is other models they follow two steps, S_{NO3} reduction to S_{NO2}, and S_{NO2} reduction to S_{N2}.	
X_{AHO}	Carbon adsorption heterotroph organisms (AHO)	Sumo2C	Heterotrophic organisms storing readily biodegradable small molecular weight components represented as $S_{B,mono}$ and volatile fatty acids (S_{VFA}) into X_{STO}. The growth rate of AHOs is higher than that of the OHOs and outgrow them in a short SRT system of <2 days. They only carry out aerobic consumption of the X_{STO} and are expected to be seeded from the influent.	g COD.m^{-3}
X_{NITO}	Aerobic nitrifying organisms (NITO)	Mini_Sumo, Sumo1	Obligate aerobic autotrophic organism responsible for complete nitrification, from S_{NHx} to S_{NOx}. It represents a combination of AOBs and NOBs for simplification in the referred models.	g COD.m^{-3}
X_{AOB}	Aerobic ammonia oxidizers (AOB)	Sumo2, Sumo2C, Sumo2S, Sumo4N	Obligate aerobic autotrophic organism responsible for the first step in nitrification, from SNHx to SNO2.	g COD.m^{-3}
X_{NOB}	Nitrite oxidizers (NOB)	Sumo2, Sumo2C, Sumo2S, Sumo4N	Obligate aerobic autotrophic organism responsible for the second step in nitrification, from S_{NO2} to S_{NO3}.	g COD.m^{-3}
X_{AMX}	Anammox organisms (AMX)	Sumo2, Sumo2C, Sumo2S, Sumo4N	A chemoautotrophic anaerobic bacteria that oxidizes ammonium with nitrite as the electron acceptor and with CO2 as the main carbon source. They are slow growers and have a long doubling time.	g COD.m^{-3}
X_{AMETO}	Acidoclastic methanogens (AMETO)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Anaerobic archea that consume S_{VFA} to produce S_{CH4} and S_{CO2} as a metabolic by-product and don't grow under aerobic conditions.	g COD.m^{-3}
X_{HMETO}	Hydrogenotrophic methanogens (HMETO)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Anaerobic archea that consume S_{H2} and S_{CO2} to produce S_{CH4} as a metabolic by-product and don't grow under aerobic conditions.	g COD.m^{-3}
X_{ASRO}	Acidoclastic sulfate-reducing organisms (ASRO)	Sumo2S	A group of bacteria and archaea that perform anaerobic	g COD.m^{-3}

	Components			
Symbol	Name	Model	Definition	Unit
			respiration utilizing S_{SO4} and S_{VFA}, reducing it to S_{H2S} and generating S_{CO2}. They compete with AMETOs for S_{VFA} and negatively impact performance of a digester.	
X_{HSRO}	Hydrogenotrophic sulfate-reducing organisms (HSRO)	Sumo2S	A group of bacteria and archaea that perform anaerobic respiration utilizing S_{SO4} and S_{H2}, reducing it to S_{H2S}. They compete with HMETOs for S_{H2} consumption and negatively impact performance of a digester.	g COD.m^{-3}
X_{SOO}	Sulfur-oxidizing organisms (SOO)	Sumo2S	They oxidize S_{H2S} in two steps under aerobic and anoxic environments, first from S_{H2S} to X_S (elemental sulfur) and second from X_S to S_{SO4}.	g COD.m^{-3}
X_{ALGAE}	Photosynthetic organisms (ALGAE)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A group of photosynthetic organisms which grow, assimilate nutrients, S_{CO2} and generate S_{O2} in the presence of light. They consume S_{O2} through respiration.	g COD.m^{-3}
S_{NHx}	Total ammonia (NH_x)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Total ammonia nitrogen is a sum of ammonium and free ammonia. An essential nutrient for the biokinetic growth reactions.	g N.m^{-3}
S_{NH2OH}	Hydroxylamine (NH_2OH)	Sumo4N	An intermediate product produced by AOB from S_{NHx}. It is then oxidized to S_{NO} under aerobic environments. It is also reduced to form S_{N2O} under anoxic environments.	g N.m^{-3}
S_{NOx}	Nitrate and nitrite (NO_x)	Mini_Sumo, Sumo1	A sum of nitrate and nitrite, and electron acceptor for anoxic reactions. In the referred Models it is considered nitrate for all COD conservation purposes.	g N.m^{-3}
S_{NO2}	Nitrite (NO_2)	Sumo2, Sumo2C, Sumo2S, Sumo4N	A sum of nitrous acid and nitrate ion and electron acceptor for anoxic reactions.	g N.m^{-3}
S_{NO3}	Nitrate (NO_3)	Sumo2, Sumo2C, Sumo2S, Sumo4N	An electron acceptor for anoxic reactions.	g N.m^{-3}
$S_{NO,AOB}$	Nitric oxide of AOB (NO)	Sumo4N	Nitric oxide generated by AOBs from S_{NH2OH} and either oxidized to S_{NO2} and reduced to S_{N2O}. It is considered as an internal product.	g N.m-3
$S_{NO,OHO}$	Nitric oxide of OHO (NO)	Sumo4N	Nitric oxide generated by OHOs during S_{NO2} reduction. It is considered as an internal product.	g N.m-3

	Components			
Symbol	Name	Model	Definition	Unit
S_{N2O}	Nitrous oxide (N_2O)	Sumo4N	Generated by OHOs from $S_{NO,OHO}$ and by AOBs from $S_{NO,AOB}$.	g N.m-3
S_{N2}	Dissolved nitrogen (N_2)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Only nitrogenous product of denitrification except for in Sumo4N model and is subject to gas transfer.	g $N.m^{-3}$
$S_{N,B}$	Soluble biodegradable organic N (from SB)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A nitrogen containing soluble organic material (urea, amino acids, amines, and others) that releases nitrogen as total ammonia on ammonification in wastewater treatment. In the model it doesn't have COD associated.	g $N.m^{-3}$
$X_{N,B}$	Particulate biodegradable organic N (from X_B)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A nitrogen containing particulate organic material (proteins and others) that releases $S_{N,B}$ on hydrolysis in wastewater treatment. In the model it doesn't have COD.	g $N.m^{-3}$
$X_{N,U}$	Particulate unbiodegradable organic N	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A nitrogen containing particulate organic material that is not biologically or chemically degraded in the plant and leaves with the cake solids. The only process that degrades $X_{N,U}$ to S_{NHx} is the thermal hydrolysis process.	g $N.m^{-3}$
S_{PO4}	Orthophosphate (PO_4)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Soluble inorganic phosphorus, represents a combination of Phosphoric acid, Dihydrogen phosphate ion, Hydrogen phosphate ion, Phosphate ion. An essential nutrient for the biokinetic growth reactions.	g $P.m^{-3}$
X_{PP}	Stored polyphosphate (PP)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Poly-phosphate considered as an internal inorganic cellular storage product of CASTOs (PAOs). The composition of X_{PP} is $(Ca_{0.1}K_{0.1}Mg_{0.35}PO_3)_n$.	g $P.m^{-3}$
$S_{P,B}$	Soluble biodegradable organic P (from SB)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A phosphorus containing soluble organic material that releases phosphorus as S_{PO4} in wastewater treatment. In the model it doesn't have COD.	g $P.m^{-3}$
$X_{P,B}$	Particulate biodegradable organic P (from X_B)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A phosphorus containing particulate organic material that releases $S_{P,B}$ on hydrolysis in wastewater treatment. In the model it doesn't have COD.	g $P.m^{-3}$
$X_{P,U}$	Particulate unbiodegradable organic P	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A phosphorus containing particulate organic material that is not biologically or chemically	g $P.m^{-3}$

	Components			
Symbol	Name	Model	Definition	Unit
			degraded in the plant and leaves with the cake solids. The only process that degrades $X_{P,U}$ to S_{PO4} is the process model of thermal hydrolysis process.	
S_{O2}	Dissolved oxygen (O_2)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Dissolved oxygen is major electron acceptor for aerobic system and is subjected to gas transfer.	g O_2.m^{-3}
S_{CH4}	Dissolved methane (CH_4)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Dissolved methane is the most reduced form of carbon and end product of methanogensis. They are subjected to gas transfer.	g COD.m^{-3}
S_{H2}	Dissolved hydrogen (H_2)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Dissolved hydrogen is generated during fermentation and transformed to S_{CH4} during methanogensis. They are subjected to gas transfer.	g COD.m^{-3}
S_{ALK}	Alkalinity (ALK)	MiniSumo	Assumed to be bicarbonate and used for appropriate conversion of electric charges in the biokinetic reactions.	eq ALK.L^{-1}
S_{CO2}	Total inorganic carbon (CO_2)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A sum of carbonic acid, bicarbonate ion, carbonate ion. It is end product of many biological reactions. As bicarbonate it is a substrate for nitrification and also consumed during methanogenesis.	g TIC.m^{-3}
X_{INORG}	Inorganics in influent and biomass	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	It represents the inorganic inerts present in influent and the biomass (0.11 g TSS.g COD^{-1}). It has a S_{Na}, S_{Cl}, S_{Ca} and S_{Mg} content.	g TSS.m^{-3}
S_{CAT}	Other strong cations (as Na^+)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Represented as sodium and is an essential element for biomass. It participates in pH and precipitation reactions.	g Na.m^{-3}
S_{AN}	Other strong anions (as Cl^-)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Represented as chloride and is an essential element for biomass. It participates in pH and precipitation reactions.	g Cl.m^{-3}
S_{Ca}	Calcium	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	An essential element for biomass and X_{PP} and participates in pH and precipitation reactions.	g Ca.m^{-3}
S_{Mg}	Magnesium	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	An essential element for biomass and X_{PP}. It participates in pH and precipitation reactions.	g Mg.m^{-3}
S_K	Potassium	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	An essential element for biomass and X_{PP}. It participates in pH and precipitation reactions.	g K.m^{-3}

	Components			
Symbol	Name	Model	Definition	Unit
S_{H2S}	Hydrogen sulfide (H_2S)	Sumo2S	Dissolved hydrogen sulfide gas, its subjected to gas transfer, biological and chemical reactions.	g S.m^{-3}
S_{SO4}	Sulfate (SO_4)	Sumo2S	An end product of S_{H2S} oxidation. It participates in pH determination	g S.m^{-3}
X_S	Particulate elemental sulfur (S)	Sumo2S	An intermediary product of partial S_{H2S} oxidation.	g S.m^{-3}
X_{FeOH}	Ferric hydroxide compounds (FeOH)	MiniSumo	Phosphorus-binding capacity of ferric hydroxides	g Fe.m^{-3}
X_{FeP}	Ferric phosphate compounds (FeP)	MiniSumo	This component results from binding phosphorus to the X_{FeOH}.	g Fe.m^{-3}
X_{AlOH}	Aluminium hydroxide compounds (AlOH)	MiniSumo	It stands for phosphorus-binding capacity of possible Al hydroxides	g Al.m^{-3}
X_{AlP}	Aluminium phosphate compounds (AlP)	MiniSumo	This component results from binding phosphorus to the X_{AlOH}.	g Al.m^{-3}
S_{Fe2}	Ferrous ion (Fe_2)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Ferrous ion oxidized to ferric ion and then participates in X_{HFO} formation. It precipiates S_{H2S} to X_{FeS} and S_{PO4} to X_{Vivi} under anaerobic environments.	g Fe.m^{-3}
$X_{HFO,H}$	Active hydrous ferric oxide, high surface (HFO,H)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A ferric hydroxide with high surface area and high capacity to bind S_{PO4}. Higher mixing condition results in more $X_{HFO,H}$ formation compared to $X_{HFO,L}$.	g Fe.m^{-3}
$X_{HFO,L}$	Active hydrous ferric oxide, low surface (HFO,L)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A ferric hydroxide with low surface area and low capacity to bind S_{PO4}. Poor mixing condition results in more $X_{HFO,L}$ formation compared to $X_{HFO,H}$.	g Fe.m^{-3}
$X_{HFO,old}$	Aged unused hydrous ferric oxide (HFO,old)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	When there is excess ferric addition and not much S_{PO4} is available then $X_{HFO,H}$ and $X_{HFO,L}$ formed age into $X_{HFO,old}$. These are incapable of removing S_{PO4}.	g Fe.m^{-3}
$X_{HFO,H,P}$	P-bound hydrous ferric oxide, high surface (HFO,H,P)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	The Fe-S_{PO4} complex formed with $X_{HFO,H}$.	g Fe.m^{-3}
$X_{HFO,L,P}$	P-bound hydrous ferric oxide, low surface (HFO,L,P)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	The Fe-S_{PO4} complex formed with $X_{HFO,L}$.	g Fe.m^{-3}
$X_{HFO,H,P,old}$	Aged P-bound hydrous ferric oxide, high surface (HFO,H,P,old)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Aged form of $X_{HFO,H,P}$.	g Fe.m^{-3}
$X_{HFO,L,P,old}$	Aged P-bound hydrous ferric oxide, low surface	Sumo1, Sumo2, Sumo2C, Sumo2S,	Aged form of $X_{HFO,L,P}$.	g Fe.m^{-3}

	Components			
Symbol	Name	Model	Definition	Unit
	(HFO,L,P,old)	Sumo4N		
$X_{HAO,H}$	Active hydrous aluminium oxide, high surface (HAO,H)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Aluminium hydroxide with high surface area and high capacity to bind S_{PO4}. Higher mixing condition results in more $X_{HAO,H}$ formation compared to $X_{HAO,L}$.	g Al.m^{-3}
$X_{HAO,L}$	Active hydrous aluminium oxide, low surface (HAO,L)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Aluminium hydroxide with low surface area and low capacity to bind S_{PO4}. Poor mixing condition results in more $X_{HAO,L}$ formation compared to $X_{HAO,H}$.	g Al.m^{-3}
$X_{HAO,old}$	Aged unused hydrous aluminium oxide (HAO,old)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	When there is excess X_{HAO} and not much S_{PO4} is available then XHAO and $X_{HAO,L}$ formed age into $X_{HAO,old}$. These are incapable of removing S_{PO4}.	g Al.m^{-3}
$X_{HAO,H,P}$	P-bound hydrous aluminium oxide, high surface (HAO,H,P)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	The Al-S_{PO4} complex formed with $X_{HAO,H}$.	g Al.m^{-3}
$X_{HAO,L,P}$	P-bound hydrous aluminium oxide, low surface (HAO,L,P)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	The Al-S_{PO4} complex formed with $X_{HAO,L}$.	g Al.m^{-3}
$X_{HAO,H,P,old}$	Aged P-bound hydrous aluminium oxide, high surface (HAO,H,P,old)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Aged form of $X_{HAO,H,P}$.	g Al.m^{-3}
$X_{HAO,L,P,old}$	Aged P-bound hydrous aluminium oxide, low surface (HAO,L,P,old)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Aged form of $X_{HAO,L,P}$.	g Al.m^{-3}
X_{CaCO3}	Calcium carbonate ($CaCO_3$)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Essential chemical for pH control - a precipitate that forms readily	g TSS.m^{-3}
X_{ACP}	Amorphous calcium phosphate (ACP)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Elemental composition of $Ca_3(PO_4)_2 * 4H_2O$.	g TSS.m^{-3}
X_{BSH}	Brushite (BSH)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Elemental composition of $CaHPO_4 * 2H_2O$. Forms at lower pH values than Struvite	g TSS.m^{-3}
X_{STR}	Struvite (STR)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Formed under anaerobic environments and has an elemental composition of $MgNH_4PO_4 * 6H_2O$.	g TSS.m^{-3}
X_{Vivi}	Vivianite (Vivi)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Formed under anaerobic environments and has an elemental composition of $Fe_3(PO_4)_2 * 8H_2O$.	g TSS.m^{-3}
X_{FeS}	Iron sulfide (FeS)	Sumo2S	Formed under anaerobic environments and is a precursor for pyrite formation.	g TSS.m^{-3}

	Components			
Symbol	Name	Model	Definition	Unit
H	Enthalpy	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	An energy-like property that is used to calculate temperature of a system. It flows from the influent unit to the plant.	$MJ.m^{-3}$
S_{ALPHA}	Alpha indicator	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A surrogate representing the surfactant composition in the wastewater.	unitless
$S_{ORPswitch}$	ORP driver for CASTO activity switches	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	A surrogate switch to calculate the activity of CASTOs.	unitless
G_{CO2}	Carbon dioxide gas (CO_2)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Gaseous form represented in bubbles of wastewater system.	g $TIC.m^{-3}$
G_{CH4}	Methane gas (CH_4)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Gaseous form represented in bubbles of wastewater system.	g $COD.m^{-3}$
G_{H2}	Hydrogen gas (H_2)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Gaseous form represented in bubbles of wastewater system.	g $COD.m^{-3}$
G_{O2}	Oxygen gas (O_2)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Gaseous form represented in bubbles of wastewater system.	g $O_2.m^{-3}$
G_{NH3}	Ammonia gas (NH_3)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Gaseous form represented in bubbles of wastewater system.	g $N.m^{-3}$
G_{N2}	Nitrogen gas (N_2)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Gaseous form represented in bubbles of wastewater system.	g $N.m^{-3}$
G_{NO}	Nitric oxide gas (NO)	Sumo4N	Gaseous form represented in bubbles of wastewater system.	g $N.m^{-3}$
G_{N2O}	Nitrous oxide gas (N_2O)	Sumo4N	Gaseous form represented in bubbles of wastewater system.	g $N.m^{-3}$
G_{H2S}	Hydrogen sulfide gas (H_2S)	Sumo2S	Gaseous form represented in bubbles of wastewater system.	g $S.m^{-3}$
$G_{CO2,atm}$	Carbon dioxide gas (CO2)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Gaseous form represented in the atmosphere around wastewater systems.	%v/v
$G_{CH4,atm}$	Methane gas (CH_4)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Gaseous form represented in the atmosphere around wastewater systems.	%v/v
$G_{H2,atm}$	Hydrogen gas (H_2)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Gaseous form represented in the atmosphere around wastewater systems.	%v/v
$G_{O2,atm}$	Oxygen gas (O_2)	Mini_Sumo, Sumo1, Sumo2, Sumo2C,	Gaseous form represented in the atmosphere around wastewater	%v/v

	Components			
Symbol	Name	Model	Definition	Unit
		Sumo2S, Sumo4N	systems.	
$G_{NH3,atm}$	Ammonia gas (NH3)	Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Gaseous form represented in the atmosphere around wastewater systems.	%v/v
$G_{N2,atm}$	Nitrogen gas (N_2)	Mini_Sumo, Sumo1, Sumo2, Sumo2C, Sumo2S, Sumo4N	Gaseous form represented in the atmosphere around wastewater systems.	%v/v
$G_{NO,atm}$	Nitric oxide gas (NO)	Sumo4N	Gaseous form represented in the atmosphere around wastewater systems.	%v/v
$G_{N2O,atm}$	Nitrous oxide gas (N_2O)	Sumo4N	Gaseous form represented in the atmosphere around wastewater systems.	%v/v
$G_{H2S,atm}$	Hydrogen sulfide gas (H_2S)	Sumo2S	Gaseous form represented in the atmosphere around wastewater systems.	%v/v
$S_{MM,index}$	Methyl mercaptan production index	Sumo2S	A surrogate for indicating the potential for odor generation at a wastewater facility.	Unitless

Biological processes

BOD removal

BOD removal from is characterized as soluble substrate component uptake by biomass and used for growth and respiration.

The colloidal biodegradable components are flocculated into particulate components (see Flocculation paragraph). The particulate components are hydrolyzed into soluble components thus biomass can grow on them (see Hydrolysis paragraph).

Biomasses involved in BOD removal

Ordinary heterotrophic organisms, X_{OHO}

Generalist facultative ordinary hetrotrophic organisms that consume different soluble biodegradable organics including S_B, S_{VFA}, and X_{MEOL} and can perform biological removal under aerobic, anoxic, and anaerobic environments. They are also responsible for hydrolysis of the particulates. In MiniSumo and Sumo1, they perform one step denitrification, meaning from S_{NOx} to S_{N2}. In other models they follow two steps, S_{NO3} reduction to S_{NO2}, and S_{NO2} reduction to S_{N2}.

Biological processes	Concepts description
Aerobic growth on VFA, O_2	Growth on S_{VFA} under aerobic conditions. Requires S_{O2}, nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH.
Anoxic growth on VFA, NO_2^-	Growth on S_{VFA} under anoxic conditions. This is the second step of denitrification in Sumo2, Sumo2C and Sumo2S), S_{NO2} is reduced into S_{N2}.

Biological processes	Concepts description
	This process is not described in Sumo1 and MiniSumo. Requires S_{NO2}, nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH.
Anoxic growth on VFA, NO_3^-	Growth on S_{VFA} under anoxic conditions. This is the denitrification process in Sumo1 and MiniSumo: S_{NO3} is reduced in S_{N2}. This is the first step of denitrification in Sumo2, Sumo2C and Sumo2S): S_{NO3} is reduced into S_{NO2}. Requires S_{NO3}, nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH.
Aerobic growth on S_B, O_2	Growth on S_B under aerobic conditions. Requires S_{O2}, nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH
Anoxic growth on S_B, NO_2^-	Growth on S_B under anoxic conditions. This is the second step of denitrification in Sumo2, Sumo2C and Sumo2S), S_{NO2} is reduced into S_{N2}. This process is not described in Sumo1 and MiniSumo. Requires S_{NO2}, nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH
Anoxic growth on S_B, NO_3^-	Growth on S_B under anoxic conditions. This is the denitrification process in Sumo1 and MiniSumo: S_{NO3} is reduced in S_{N2}. This is the first step of denitrification in Sumo2, Sumo2C and Sumo2S): S_{NO3} is reduced into S_{NO2}. Requires S_{NO3}, nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH.
S_B fermentation with high VFA (OHO growth, anaerobic)	Growth on S_B under anaerobic conditions. OHO Fermenters have different growth rate of 0.3 d^{-1} and digesters have different $K_{SB,ana}$ of 350 mgCOD/L Produce S_{VFA} as fermentation product and S_{H2}. Under high S_{VFA} concentration, the yield of S_{H2} production is higher (less S_{VFA} produced). Requires nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH.

Biological processes	Concepts description
S_B fermentation with low VFA (OHO growth, anaerobic)	Growth on S_B under anaerobic conditions. OHO Fermenters have different growth rate of 0.3 d^{-1} and digesters have different $K_{SB,ana}$ of 350 mgCOD/L Produce S_{VFA} as fermentation product and S_{H2}. Under low S_{VFA} concentration, the yield of S_{H2} production is lower (more S_{VFA} produced). Requires nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH.
Aerobic growth on S_{MEOL}, O_2	OHO aerobic growth on methanol in order to consum any residual methanol from anoxic carbon dosage for denitrification. Requires S_{O2}, nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH.
OHO decay	OHO decay process under anoxic and aerobic conditions. This process release X_B and X_E (death-regeneration concept).
OHO anaerobic decay	OHO decay process under anaerobic conditions. This process release X_B and $X_{E,ana}$ (death-regeneration concept).

Anoxic methanol utilizers, X_{MEOLO}

Specialist heterotrophic organisms responsible for removal of X_{MEOL}. Only found in systems with methanol addition and compete with OHOs during denitrification process. In Sumo1, they perform one step denitrification, meaning from S_{NOx} to S_{N2}. Is other models they follow two steps, S_{NO3} reduction to S_{NO2}, and S_{NO2} reduction to S_{N2}.

Biological processes	Concepts description
MEOLO growth, NO_2	Growth on SMEOL under anoxic conditions. This is the second step of denitrification in Sumo2, Sumo2C and Sumo2S), S_{NO2} is reduced into S_{N2}. This process is not described in Sumo1 and MiniSumo. Requires S_{NO2}, nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH
MEOLO growth, NO_3	Growth on SMEOL under anoxic conditions. This is the denitrification process in Sumo1 and MiniSumo: S_{NO3} is reduced in S_{N2}. This is the first step of denitrification in Sumo2, Sumo2C and Sumo2S): S_{NO3} is reduced into S_{NO2}. Requires S_{NO3}, nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH.

Biological processes	Concepts description
MEOLO decay	MEOLO decay process under anoxic and aerobic conditions. This process release X_B and X_E (death-regeneration concept).
MEOLO anaerobic decay	MEOLO decay process under anaerobic conditions. This process release X_B and $X_{E,ana}$ (death-regeneration concept).

Nitrogen removal

Nitrification model

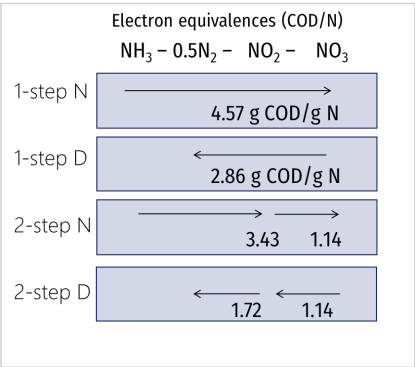
Nitrification rate is the most important parameter in design and reliable simulation of BNR (Biological Nutrient Removal) plants. The maximum specific growth rate of nitrifiers ranges from 0.2 to 1 d^{-1} for different wastewater. This parameter should be considered as part of wastewater characterization.

There are three models available in Sumo to describe the process on three layer of details:

1. Mini_Sumo and Sumo1 – one step nitrification process
   - one nitrifying organism (X_{NITO}),
   - ammonia (S_{NHx}) and nitrate (S_{NOx}) as nutrients
2. Sumo2, Sumo2C, and Sumo2S – two step nitrification process
   - Three organisms
     - ammonia oxidizing bacteria (X_{AOB})
     - nitrite oxidizing bacteria (X_{NOB})
     - Anamox organisms (X_{AMX})
   - Three nutrients
     - Ammonia (S_{NHx}), nitrite (S_{NO2}), nitrate (S_{NO3})
   - X_{AOB} kinetics are the first step and rate limiting
3. Sumo4N - detailed nitrification and GHG emission model

- 4-step nitrification model from Pocquet *et al.*, 2016
- 4-step denitrification model from Hiatt and Grady, 2008
- NO considered as cell internal intermediate

Sumo4N model is describe in details in Focus models mechanisms chapter.



Nitrogen removal Figure 1: Electron equivalence of nitrogen species involved in 1-step and 2-step ntritrification and denitrification

Biomasses involved in nitrification

Aerobic nitrifying organisms, X_{NITO}

Obligate aerobic autotrophic organism responsible for complete nitrification, from S_{NHx} to S_{NOx} in MiniSumo and Sumo1. It represents a combination of AOBs and NOBs for simplification in the referred models.

Biological processes	Concepts description
NITO growth	NITO growth process, using S_{NHx} as electron donor. S_{NHx} is oxidized in S_{NO3} in one step. S_{CO2} is used as carbon source. Requires S_{O2}, nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH.
NITO decay	NITO decay process under anoxic and aerobic conditions. This process release X_B and X_E.
NITO anaerobic decay	NITO decay process under anaerobic conditions. This process release X_B and $X_{E,ana}$.

Aerobic ammonia oxidizers, X_{AOB}

Obligate aerobic autotrophic organism responsible for the first step in nitrification, from S_{NHx} to S_{NO2} in Sumo2, Sumo2C and Sumo2S.

Biological processes	Concepts description
AOB growth	AOB growth process, using S_{NHx} as electron donor. This is the first step of nitrification: S_{NHx} is oxidized in S_{NO2} S_{CO2} is used as carbon source. Requires S_{O2}, nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH.
AOB decay	AOB decay process under anoxic and aerobic conditions. This process release X_B and X_E.
AOB anaerobic decay	AOB decay process under anaerobic conditions. This process release X_B and $X_{E,ana}$.

Nitrite oxidizers, X_{NOB}

Obligate aerobic autotrophic organism responsible for the second step in nitrification, from S_{NO2} to S_{NO3} in Sumo2, Sumo2C and Sumo2S.

Biological processes	Concepts description
NOB growth	NOB growth process, using S_{NO2} as electron donor. This is the second step of nitrification: S_{NO2} is oxidized in S_{NO3} S_{CO2} is used as carbon source. Requires S_{O2}, nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}).

Biological processes	Concepts description
	Bell shape inhibition function on pH: BellinhpH.
NOB decay	NOB decay process under anoxic and aerobic conditions. This process release X_B and X_E.
NOB anaerobic decay	NOB decay process under anaerobic conditions. This process release X_B and $X_{E,ana}$.

Anammox organisms, X_{AMX}

Anammox is a chemoautotrophic anaerobic bacteria that oxidizes ammonium with nitrite as the electron acceptor and with CO2 as the main carbon source. They are implemented in Sumo2, Sumo2C, Sumo2S and Sumo4N models.

Anammox are slow growers and have a long doubling time. Their growth reaction stoichiometry is described by Strous (1998, 1999):

$NH_4^+ + 1.32\ NO_2^- + 0.066\ HCO_3^- + 0.13\ H^+ = 0.26\ NO_3^- + 1.02\ N_2 + 0.066\ CH_2O_{0.5}N_{0.15} + 2.03\ H_2O$

This reaction allows saving up to 63% of oxygen demand and 100% of carbon requirement (Figure 2.2) compared to a full nitrification and denitrification pathway for nitrogen removal (Figure 2.1).

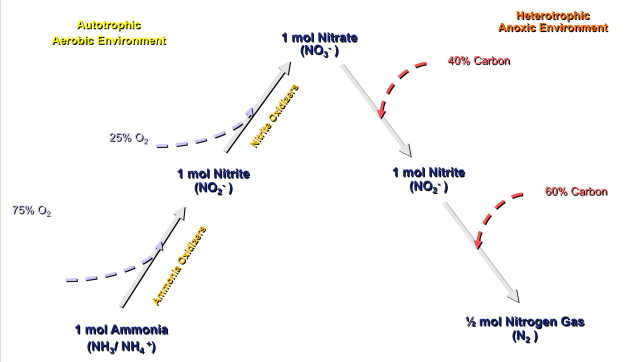


Figure 2.1 2-step full nitrification and denitrification reaction

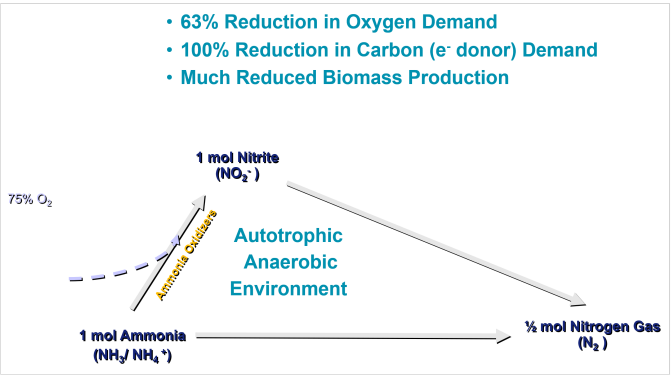


Figure 2.2 Anaerobic ammonia oxidation reaction

The Anammox organisms are modelled in Sumo2, Sumo2C, Sumo2S and Sumo4N models. The model includes description of anammox growth, decay and anaerobic decay.

The stoichiometry of Anammox growth in Sumo is derived from the stoichiometry proposed by Strous. Two stoichiometric parameters are introduced: the amount of nitrite utilised per mol of ammonia oxidized, and the amount of nitrate produced per mol of ammonia utilised.

$Y_{AMX,NO2}$	Yield of AMX on NO_2	1.32	mol NO2/mol NH4
$Y_{AMX,NO3}$	Yield of AMX on NO_3	0.26	mol NO3/mol NH4

The stoichiometric coefficient expressions are then obtained by applying the full elemental balance methodology from Takacs et al. (2007).

A generic biomass composition $Ca_CHa_HOa_ONa_N$ is considered. The theoretical oxygen demand of this biomass is by definition:

$Bio_{ThOD} = (a_C + a_H/4 - 3 * a_N/4 - a_O/2) * 2 * AM_O$

with AM_O as the atomic mass of oxygen.

Considering uncharged species, the Anammox reaction is set up as:

$(v_{NH3} + a_N) * NH_3 + v_{HNO2} * HNO_2 + a_C * CO2 = Ca_CHa_HOa_ONa_N + v_{N2} * N_2 + vHNO_3 * HNO_3 + vH_2O * H_2O$

With v_{NH3}, v_{HNO2}, v_{N2}, v_{HNO3} and v_{H2O} the stoichiometric coefficients of the ammonia oxidation with nitrite reaction.

Five equations can be derived from this reaction:

- Two equations for the definitions of the stoichiometric parameters that are chosen:
  - $Y_{NO2} = v_{HNO2} / v_{NH3}$
  - $Y_{NO3} = v_{HNO3} / v_{NH3}$
- Three mass balances can be expressed for hydrogen, nitrogen and oxygen:
  - H balance: $3 * (v_{NH3} + a_N) + v_{HNO2} = a_H + v_{HNO3} + 2 * v_{H2O}$
  - N balance: $v_{NH3} + v_{HNO2} = v_{HNO3} + 2 * v_{N2}$
  - O balance: $2 * v_{HNO2} + 2 * a_C = a_O + 3 * v_{HNO3} + v_{H2O}$

These 5 equations can be used to find the 5 unknowns: v_{NH3}, v_{HNO2}, v_{HNO3}, v_{N2} and v_{H2O}.The following code is executed in python for the symbolic resolution:

```
from sympy import symbols, solve, Eq

NH3, vNH3, HNO2, vHNO2, CO2, H3PO4, N2, vN2, HNO3, vHNO3, H2O, vH2O, YNO2, YNO3, aC, aH, aO, aN =
symbols('NH3, vNH3, HNO2, vHNO2, CO2, H3PO4, N2, vN2, HNO3, vHNO3, H2O, vH2O, YNO2, YNO3, aC, aH, aO, a

solve(( Eq(YNO2, vHNO2*N/(vNH3*N)), Eq(YNO3, vHNO3*N/(vNH3*N)), Eq( 3*(vNH3+aN)+vHNO2,aH+vHNO3+2*vH2O),
```

The result is (v_{H2O} is not shown as not included in the model):

$v_{NH3} = (4 * a_C + a_H - 3 * a_N - 2 * a_O) / (-3 * Y_{NO2} + 5 * Y_{NO3} + 3)$

$v_{HNO2} = Y_{NO2} * (4 * a_C + a_H - 3 * a_N - 2 * a_O) / (-3 * Y_{NO2} + 5 * Y_{NO3} + 3)$

$v_{HNO3} = Y_{NO3} * (4 * a_C + a_H - 3 * a_N - 2 * a_O) / (-3 * Y_{NO2} + 5 * Y_{NO3} + 3)$

$v_{N2} = (4 * Y_{NO2} * a_C + Y_{NO2} * a_H - 3 * Y_{NO2} * a_N - 2 * Y_{NO2} * a_O - 4 * Y_{NO3} * a_C - Y_{NO3} * a_H + 3 * Y_{NO3} * a_N + 2 * Y_{NO3} * a_O + 4 * a_C + a_H - 3 * a_N - 2 * a_O) / (2 * (-3 * Y_{NO2} + 5 * Y_{NO3} + 3))$

These coefficients must be converted per gram of biomass COD (arbitrary reference in all biomass growth reactions) and in g N. Then, v_{NH3}, v_{HNO2} and v_{HNO3} are multiplied by AM_N/Bio_{ThOD} and v_{N2} is multiplied by $2*AM_N/Bio_{ThOD}$. The coefficient a_N is the nitrogen content of the biomass, $i_{N,Bio}$. As nitrogen content of the biomass is explicitly expressed, the definition of the theoretical COD of the biomass is revised as:

$Bio_{ThOD}=(a_C+a_H/4-a_O/2)*2*AM_O$.

The convention of the negative signs for consumed components is also added. This results in the following stoichiometric coefficient expressions:

$v_{NH3} = -(3 * i_{N,BIO} * AM_O + 2 * AM_N) / (5 * Y_{AMX,NO3} + 3 - 3 * Y_{AMX,NO2}) / AM_O$

$v_{HNO2} = -Y_{AMX,NO2} / (5 * Y_{AMX,NO3} + 3 - 3 * Y_{AMX,NO2}) * (3 * i_{N,BIO} * AM_O + 2 * AM_N) / AM_O$

$v_{HNO3} = Y_{AMX,NO3} / (5 * Y_{AMX,NO3} + 3 - 3 * Y_{AMX,NO2}) * (3 * i_{N,BIO} * AM_O + 2 * AM_N) / AM_O$

$v_{N2} = 2 * (Y_{AMX,NO3} * AM_N - 1 * AM_N - 1 * Y_{AMX,NO2} * AM_N + 4 * Y_{AMX,NO3} * i_{N,BIO} * AM_O - -3 * Y_{AMX,NO2} * i_{N,BIO} * AM_O) / AM_O / (3 * Y_{AMX,NO2} - 5 * Y_{AMX,NO3} - 3)$

Biological processes	Concepts description
Growth	AMX growth process, using S_{NHx} as electron donor and S_{NO2} as electron acceptor. S_{NO3} and S_{N2} are produced by the reaction. The stoichiometry is described above. S_{CO2} is used as carbon source. Requires S_{NHx}, S_{NO2}, nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH.
Decay	AMX decay process under anoxic and aerobic conditions. This process release X_B and X_E.
Anaerobic decay	AMX decay process under anaerobic conditions. This process release X_B and $X_{E,ana}$.

Strous, M., Heijnen, J., Kuenen, J. et al. The sequencing batch reactor as a powerful tool for the study of slowly growing anaerobic ammonium-oxidizing microorganisms. Appl Microbiol Biotechnol 50, 589–596 (1998). https://doi.org/10.1007/s002530051340

Strous, M., Fuerst, J., Kramer, E. et al. Missing lithotroph identified as new planctomycete. Nature 400, 446–449 (1999). https://doi.org/10.1038/22749

Takács, I., Vanrolleghem, P.A., Wett, B., Murthy, S., 2007. Elemental balance based methodology to establish reaction stoichiometry in environmental modeling. Water Sci. Technol. 56, 37–41.

Impact of operating conditions and design on nitrification

Nitrification is impacted by:

- dissolved oxygen level
- liquid temperature
- pH and alkalinity
- Low mixing condition or floc size can cause diffusion issues and cause reduction in nitrification rate. Half saturation for oxygen for nitrifiers can be possible calibration factor to mimic this limitation.

If the ammonia level in the aerobic cell is close to half saturation, then its important to simulate the reactor as plug flow.

Sidestream and mainstream nitrification

Two types of process unit model options are available for selection on configure tab: Mainstream or Sidestream (these can be selected from the configure tab if i.e. the CSTR is selected)

The growth rate and half-saturation for sidestream reactors are different due to possible diffusion issues, inhibitory compounds in centrate, and temperature.

Measuring specific growth rate

Two different tests can be performed to measure nitrifiers growth rate:

1. High F/M test – 7 days
   - Batch test: Small initial nitrifier concentration combined with high initial ammonia concentration
   - Exponential response of NO_x to estimate growth rate
   - pH and alkalinity control are especially important
   - This can be done with different wastewater to identify possible inhibition, download and see the High FM.msumo example

2. Washout test – several days
   - Operating a flow through CSTR just at correct HRT initially filled with nitrifying sludge
   - Important step to identify flow rate to the CSTR just enough to cause a washout
   - There is little to no growth of nitrifiers during the test and test is performed using actual plant influent
   - See Washout test.msumo example

Denitrification model

Denitrification is the reduction process of oxidized forms of oxygen, used as electron acceptor in the growth process of heterotrophic organisms. If denitrification is complete, these electron acceptors are reduced sequentially to nitrogen gas (S_{N2}).

Impact of operating conditions and design on denitrification

Denitrification is impacted by the availability of a carbon source. **Knowing RBCOD concentration is extremely important for nitrogen removal design and modelling.** The denitrification rate is then controlled by:

- the concentration of readily biodegradable COD (SB plus SVFA) in raw wastewater
- the addition of an external carbon source
- the rate of hydrolysis under anoxic condition (when other carbon sources are depleted)

Model specifications under anoxic conditions

1. MiniSumo
   - One biomass involved in denitrification: OHOs
   - One step denitrification, S_{NO3} to S_{N2}
   - Growth of heterotrophic biomass on S_B reduced by reduction factor as nor S_{VFA} and neither methanol utilizers are part of the model
   - Decay of OHO also reduced under anoxic condition
   - Hydrolysis reduced under denitrification using the reduction factor
2. Sumo1
   - 3 biomasses involved in denitrification: OHOs, CASTOs and MEOLOs
   - One step denitrification, S_{NO3} to S_{N2}
   - Hydrolysis reduced under anoxic conditions
   - Growth of OHO on S_B and S_{VFA} is reduced under anoxic conditions
   - First substrate preference is S_{VFA} over S_B, reaction is reduced for S_B until S_{VFA} disappears
   - Methanol utilizers and their respective kinetics and stoichiometry is included
   - PAOs and GAOs perform denitrification on stored compounds and have a reduction factor
   - All biomass has reduction factor for decay even for methanol utilizers
3. Sumo2, Sumo2C and Sumo2S
   - 3 biomasses involved in denitrification: OHOs, CASTOs and MEOLOs
   - Two step denitrification: S_{NO3} to S_{NO2} to S_{N2}
   - All the reactions are same as Sumo1 but with 2 steps of denitrification
   - $K_{NO2}/(K_{NO2} + S_{NO2})$ switching function is on nitrate to nitrite reduction, meaning nitrite denitrification is preferred, prevents build-up of NO_2^- in simulation. This can depend on the NO_2^- in the effluent of the plant, complete reasons for nitrite build up during denitrification are not known and has to do with type and concentration of carbon dose.
   - Sumo2S - Sulphur-oxidizing organisms (SOO) are involved in denitrification in presence of H2S and elemental sulphur
4. Sumo4N

- Sumo4N model is describe in details in Focus models mechanisms chapter.

Key model details of the denitrification process

1. Under anoxic conditions, the yield coefficients are reduced (compared to aerobic conditions) and is particularly important for denitrification kinetics analysis.
2. Reduction factor for anoxic growth kinetic of OHOs
   - In Sumo the default value of 0.6 is used for denitrification while
     - In real plants it ranges from 0.3 to 0.85 and
     - it can depend on system design or operation, represents degree of removal rate and process SRT.
     - It can be used for calibration
   - Results in lower rate of substrate utilization and endogenous decay. This is because not all the biomass are facultative and don't participate in denitrification.
   - is implemented as relative energy generated is higher with O_2 as electron acceptor than with nitrate.
   - The actual value be determined by performing OUR and NUR test, see Anoxic reduction factor.msumo
   - Denitrification batch tests are done to identify the denitrification rate kinetics, see Denitrification test MLSS.msumo
3. Inhibition due to oxygen is simulated using an inverse Monod also referred as a switching function
   - $(K_{O2})/((K_{O2}) + (S_{O2}))$, dissolved oxygen inhibits denitrification reactions
   - This value is 0.15 g O_2/m^3, however, this is an important constant that can be used to calibrate denitrification performance, especially in case of large flocs, deep tanks, and not well mixed conditions.
   - A high value of the constant means, more denitrification under partially aerobic conditions, can be used for calibration
4. Specific denitrification rate (g N/g VSS/h) is not a model parameter but is a calculated variable

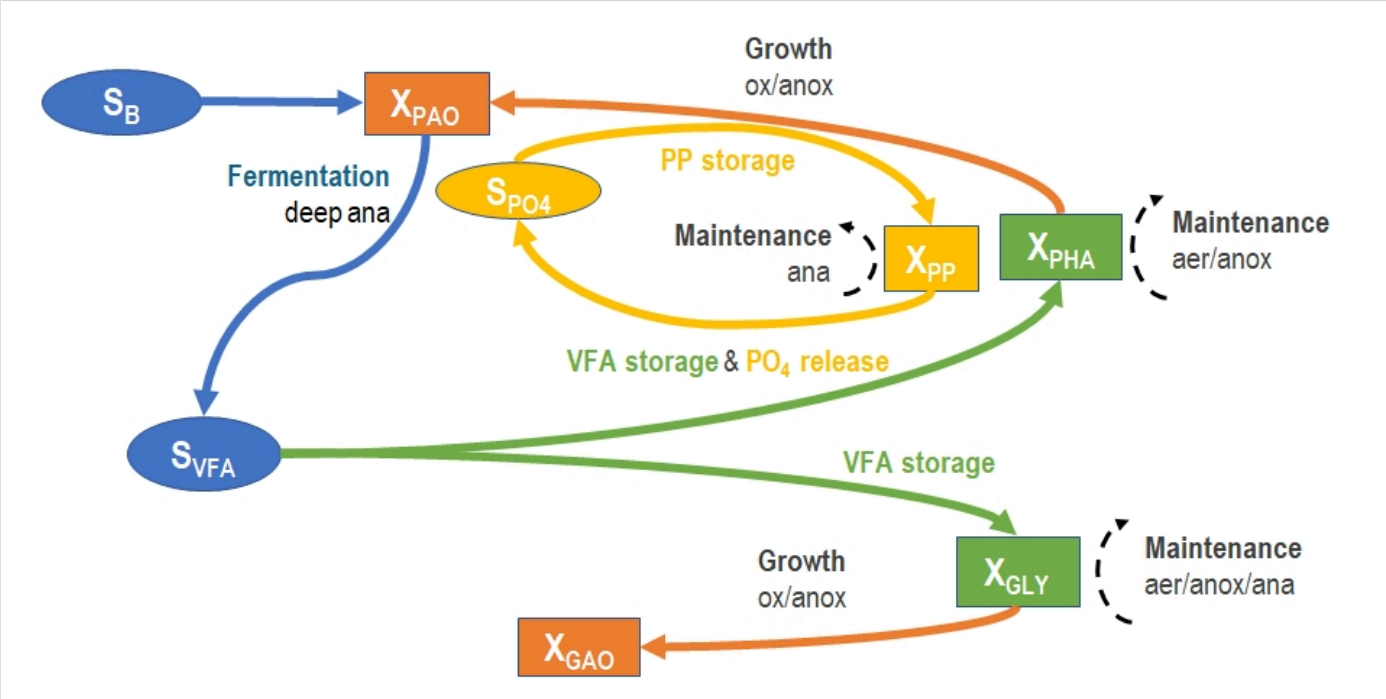
Phosphorus removal

Biological phosphorus removal is achieved in activated sludge processes via two main pathways:

1. Removal by biomass synthesis
   Incorporation into molecules building cell walls, DNA, ATP as 1-2% of these is phosphorus. This process can remove at least 30% of P from influent and transfer it to the sludge.
2. Enhanced biological P removal
   This chapter focuses on this process as the "luxury uptake" of polyphosphate once the conditions of the plant are set properly.

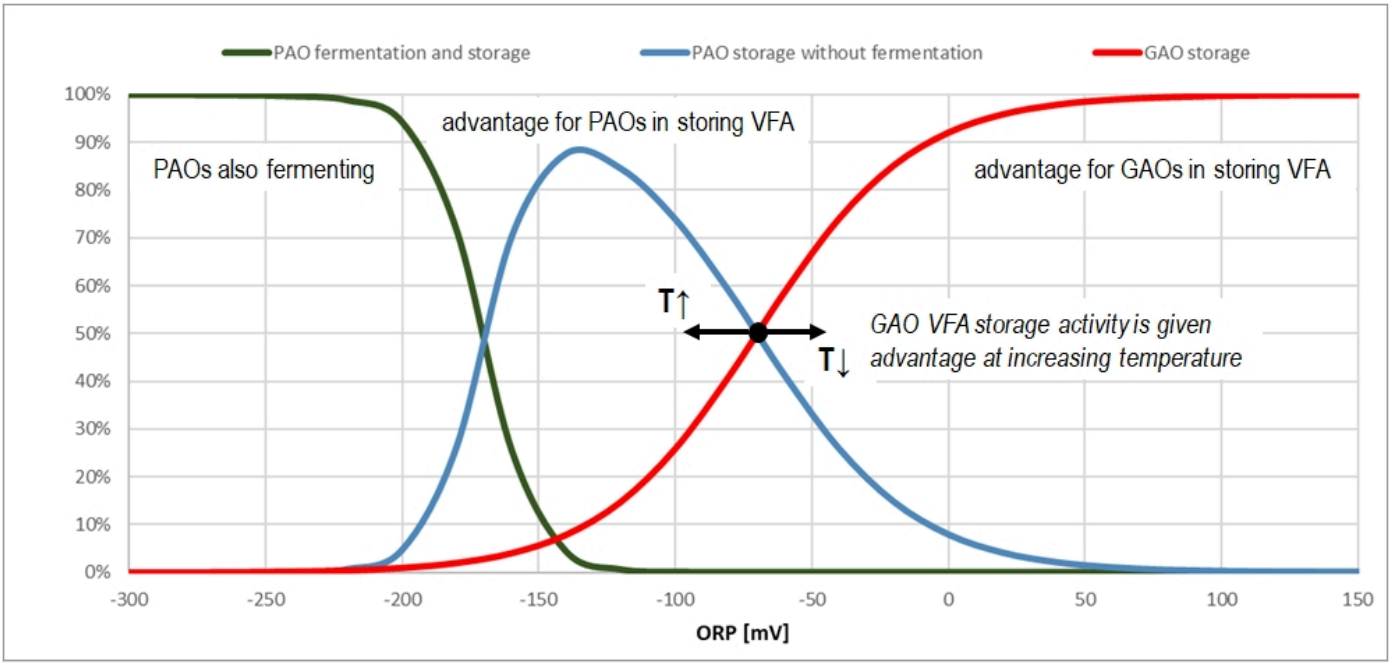
Enhanced biological phosphorus removal (EBPR) processes

Sumo uses a model where two biomass fractions compete for the volatile fatty acids (VFA): one of them storing phosphates (phosphorus accumulating organisms, PAO) and the other one storing glycogen (glycogen accumulating organisms, GAO). These biomass fractions are represented as one unified biomass (carbon storing organisms, CASTO) in the model, however the processes that are specific to PAO or GAO are differentiated when external (ambient conditions) or internal (metabolism) driving forces require. The proportion between GAOs and PAOs is tracked by the amount of stored glycogen (GLY) and poly-hydroxy-alkanoates (PHA) relative to all stored carbon (XSTC = XPHA + XGLY) in the system.



Bio-P model structure with main processes

A logistic ORP switch function is employed to control the competition between VFA storage by GAOs and PAOs: at low ORP, GAO storage is inhibited and PAO storage is favored. Another ORP switch function is used to control the fermentation activity of Tetrasphaera-like PAOs under deep ORP regime.



In order to account for the lag in the biomass response following a change in the ORP (which can happen rapidly), a regulating role state variable ($S_{ORPswitch}$, called as "ORP driver for CASTO activity switches") was introduced to the model, along with a new process that changes the value of this variable according to the following first-order kinetics:

$$dS_{ORPswitch}/dt = k_{ORPswitch} * (ORP + offset_{ORPswitch} - S_{ORPswitch})$$

where:

- ORP is the actual ORP derived from actual concentrations of O_2, NO_x, CH_4 and H_2 (as well as H_2S in models involving sulfur);
- $offset_{ORPswitch}$ is a simple constant value that transposes $S_{ORPswitch}$ values into the positive range (required by the solver algorithm);
- $k_{ORPswitch}$ is the kinetic rate that represents the ORP time lag.

The effect is that $S_{ORPswitch}$ follows ORP with a lag depending on the actual difference from the actual ORP. For small changes in the latter, $S_{ORPswitch}$ is quick to catch up, while for abrupt changes it takes time for $S_{ORPswitch}$ to catch up with ORP, resulting in a less hectic timeline of $S_{ORPswitch}$ compared to ORP. The response time can be adjusted by manipulating the $k_{ORPswitch}$ parameter.

The PAO/GAO VFA storage mechanisms have been set in all plantwide process models to be driven by the new $S_{ORPswitch}$ variable instead of ORP. The default value of the $k_{ORPswitch}$ parameter was chosen to be 1 d^{-1}, which matches the default CASTO growth rate parameter.

Biomass involved in BioP: Carbon storing organisms, X_{CASTO}

Biological processes	Concepts description
CASTO growth on PHA and GLY, O_2	PHA/GLY → CASTO Requires O_2. **Kinetic parameters** ▸ μ_{CASTO}: Maximum specific growth rate of CASTOs ▸ K_{STC}: Half-saturation of PHA and GLY for CASTOs ▸ $K_{O2,CASTO,AS}$: Half-saturation of O_2 for CASTOs (AS) **Kinetic rate limitation/inhibitions** ▸ Monod ratio saturation function on substrate: $MRsat_{XSTC,XCASTO,KSTC}$ ▸ Monod saturation function on electron acceptor: O_2 → $Msat_{SO2,KO2,CASTO}$ ▸ Monod saturation functions on nutrients: NH_x, PO_4, cations, anions, calcium and magnesium: $Msat_{SNHx,KNHx,OHO}$, $Msat_{SPO4,KPO4,BIO}$, $Msat_{SCAT,KCAT}$, $Msat_{SAN,KAN}$, $Msat_{SCa,KCa,PAO}$, $Msat_{SMg,KMg,PAO}$ ▸ Bell shape inhibition function on pH: $Bellinh_{pH}$

CASTO growth on PHA and GLY, NO_x/NO_2/NO_3	PHA/GLY → CASTO
	Requires NO_x/NO_2/NO_3.
	
	Kinetic parameters
	
	▸ μ_{CASTO}: Maximum specific growth rate of CASTOs
	▸ $\eta_{CASTO,anox}$: Reduction factor for anoxic growth of CASTOs on NO_x
	▸ K_{STC}: Half-saturation of PHA and GLY for CASTOs
	▸ $K_{NOx,CASTO,AS}$/$K_{NO2,CASTO,AS}$/$K_{NO3,CASTO,AS}$: Half-saturation of NO_x/NO_2/NO_3 for CASTOs (AS)
	▸ $K_{O2,CASTO,AS}$: Half-saturation of O_2 for CASTOs (AS)
	
	Kinetic rate limitation/inhibitions
	
	▸ Monod ratio saturation function on substrate: $MRsat_{XSTC,XCASTO,KSTC}$
	▸ Monod saturation function on electron acceptor:
	  ▸ NO_x → $Msat_{SNOx,KNOx,CASTO}$ (Mini_Sumo, Sumo1)
	  ▸ NO_2 → $Msat_{SNO2,KNO2,CASTO}$ (Sumo2, 2C, 2S)
	  ▸ NO_3 → $Msat_{SNO3,KNO3,CASTO}$ (Sumo2, 2C, 2S)
	▸ Monod inhibition function on O_2: $Minh_{SO2,KO2,CASTO}$
	▸ Monod inhibition function on NO_2: $Minh_{SNO2,KNO2,CASTO}$ (Sumo2, 2C, 2S)

Biological processes	Concepts description
	▸ Monod saturation functions on nutrients: NH_x, PO_4, cations, anions, calcium and magnesium: $Msat_{SNHx,KNHx,OHO}$, $Msat_{SPO4,KPO4,BIO}$, $Msat_{SCAT,KCAT}$, $Msat_{SAN,KAN}$, $Msat_{SCa,KCa,PAO}$, $Msat_{SMg,KMg,PAO}$ ▸ Bell shape inhibition function on pH: $Bellinh_{pH}$
PAO polyphosphate storage, O_2	$S_{PO4} \rightarrow X_{PP}$ Requires O_2. **Kinetic parameters** ▸ $q_{PAO,PP}$: Maximum polyphosphate uptake rate of PAOs ▸ $K_{O2,CASTO,AS}$: Half-saturation of O_2 for CASTOs (AS) ▸ $K_{PO4,PAO,AS}$: Half-saturation of PO4 for PAOs (AS) ▸ $Ki_{PP,PAO,max}$: Half-inhibition of maximum PP content of PAOs **Kinetic rate limitation/inhibitions** ▸ Monod saturation function on electron acceptor: $O_2 \rightarrow Msat_{SO2,KO2,CASTO}$ ▸ Logistic saturation function on substrate: $Logsat_{SPO4,KPO4,PAO}$ ▸ Logistic inhibition function on product: $Loginh_{XPP,XPAO,max}$ ▸ Monod saturation functions on nutrients as calcium, magnesium and potassium: $Msat_{SCa,KCa,PAO}$, $Msat_{SMg,KMg,PAO}$, $Msat_{SK,KK,PAO}$ ▸ Bell shape inhibition function on pH: $Bellinh_{pH}$
PAO polyphosphate storage, $NO_x/NO_2/NO_3$	$S_{PO4} \rightarrow X_{PP}$ Requires $NO_x/NO_2/NO_3$. **Kinetic parameters** ▸ $q_{PAO,PP}$: Maximum polyphosphate uptake rate of PAOs ▸ $\eta_{CASTO,anox}$: Reduction factor for anoxic growth of CASTOs ▸ $K_{NOx,CASTO,AS}/K_{NO2,CASTO,AS}/K_{NO3,CASTO,AS}$: Half-saturation of $NO_x/NO_2/NO_3$ for CASTOs (AS) ▸ $K_{O2,CASTO,AS}$: Half-saturation of O_2 for CASTOs (AS) ▸ $K_{PO4,PAO,AS}$: Half-saturation of PO_4 for PAOs (AS) ▸ $Ki_{PP,PAO,max}$: Half-inhibition of maximum PP content of PAOs **Kinetic rate limitation/inhibitions** ▸ Monod saturation function on electron acceptor: $O_2 \rightarrow Msat_{SO2,KO2,CASTO}$ ▸ Logistic saturation function on substrate: $Logsat_{SPO4,KPO4,PAO}$ ▸ Logistic inhibition function on product: $Loginh_{XPP,XPAO,max}$ ▸ Monod inhibition function on O_2: $Minh_{SO2,KO2,CASTO}$ ▸ Monod inhibition function on NO_2: $Minh_{SNO2,KNO2,CASTO}$ (Sumo2, 2C, 2S) ▸ Monod saturation functions on nutrients as calcium, magnesium and potassium: $Msat_{SCa,KCa,PAO}$, $Msat_{SMg,KMg,PAO}$, $Msat_{SK,KK,PAO}$ ▸ Bell shape inhibition function on pH: $Bellinh_{pH}$
PAO growth on PHA, O_2; PO_4 limited	PHA/GLY → CASTO Requires O_2 and PP. **Kinetic parameters**

Biological processes	Concepts description
	▸ $\mu_{PAO,lim}$: Maximum specific growth rate of CASTOs under P limited ▸ K_{PHA}: Half-saturation of PHA for PAOs ▸ $K_{O2,CASTO,AS}$: Half-saturation of O_2 for CASTOs (AS) ▸ $Ki_{PO4,lim,AS}$: Half-inhibition of PO4 for PAOs under PO4 limitation (AS) ▸ $K_{PP,lim}$: Half-saturation of PP (nutrient) for PAOs under PO_4 limitation (AS) **Kinetic rate limitation/inhibitions** ▸ Monod ratio saturation function on substrate: $MRsat_{XPHA,XPAO,KPHA}$ ▸ Monod saturation function on electron acceptor: O_2 → $Msat_{SO2,KO2,CASTO}$ ▸ Monod inhibition function on PO_4: $Minh_{SPO4,KiPO4,lim}$ ▸ Monod saturation function on X_{PP}: $Msat_{XPP,KPP,lim}$ ▸ Monod saturation functions on nutrients: NH_x, cations, anions, calcium and magnesium: $Msat_{SNHx,KNHx,OHO}$, $Msat_{SCAT,KCAT}$, $Msat_{SAN,KAN}$, $Msat_{SCa,KCa,PAO}$, $Msat_{SMg,KMg,PAO}$ ▸ Bell shape inhibition function on pH: $Bellinh_{pH}$

PAO growth on PHA, NO_x/NO_2/NO_3; PO_4 limited	PHA/GLY → CASTO
	Requires NO_x/NO_2/NO_3 and PP.
	Kinetic parameters
	▸ $\mu_{PAO,lim}$: Maximum specific growth rate of CASTOs under P limited
	▸ K_{PHA}: Half-saturation of PHA for PAOs
	▸ $K_{O2,CASTO,AS}$: Half-saturation of O_2 for CASTOs (AS)
	▸ $Ki_{PO4,lim,AS}$: Half-inhibition of PO4 for PAOs under PO4 limitation (AS)
	▸ $K_{PP,lim}$: Half-saturation of PP (nutrient) for PAOs under PO_4 limitation (AS)
	Kinetic rate limitation/inhibitions
	▸ Monod ratio saturation function on substrate: $MRsat_{XPHA,XPAO,KPHA}$
	▸ Monod saturation function on electron acceptor:
	  ▸ NO_x → $Msat_{SNOx,KNOx,CASTO}$ (Mini_Sumo, Sumo1)
	  ▸ NO_2 → $Msat_{SNO2,KNO2,CASTO}$ (Sumo2, 2C, 2S)
	  ▸ NO_3 → $Msat_{SNO3,KNO3,CASTO}$ (Sumo2, 2C, 2S)
	▸ Monod inhibition function on O_2: $Minh_{SO2,KO2,CASTO}$
	▸ Monod inhibition function on NO_2: $Minh_{SNO2,KNO2,CASTO}$ (Sumo2, 2C, 2S)
	▸ Monod inhibition function on PO_4: $Minh_{SPO4,KiPO4,lim}$
	▸ Monod saturation function on X_{PP}: $Msat_{XPP,KPP,lim}$
	▸ Monod saturation functions on nutrients: NH_x, cations, anions, calcium and magnesium: $Msat_{SNHx,KNHx,OHO}$, $Msat_{SCAT,KCAT}$, $Msat_{SAN,KAN}$, $Msat_{SCa,KCa,PAO}$, $Msat_{SMg,KMg,PAO}$
	▸ Bell shape inhibition function on pH: $Bellinh_{pH}$

Biological processes	Concepts description
PAO's PHA storage from VFAs and PO_4 release	VFA → PHA and X_{PP} → S_{PO4} **Kinetic parameters** ▸ $q_{PAO,PHA}$: Rate of VFA storage into PHA for PAOs ▸ $K_{VFA,CASTO,AS}$: Half-saturation of VFA storage for CASTOs (AS) ▸ K_{PP}: Half-saturation of PP for PAOs ▸ $Ki_{PHA,PAO,max}$: Half-inhibition of maximum PHA content of PAOs **Kinetic rate limitation/inhibitions** ▸ Monod saturation function on VFA: $Msat_{SVFA,KVFA,CASTO}$ ▸ Monod ratio saturation function on PP: $MRsat_{XPP,XPAO,KPP}$ ▸ Logistic inhibition function on product: $Loginh_{XPHA,XPAO,max}$
GAO's GLY storage from VFAs	PHA → CO_2 and GLY → CO_2 **Kinetic parameters** ▸ $q_{GAO,GLY}$: Rate of VFA storage into GLY for GAOs ▸ $K_{VFA,CASTO,AS}$: Half-saturation of VFA storage for CASTOs (AS) ▸ $Ki_{GLY,GAO,max}$: Half-inhibition of maximum GLY content of GAOs **Kinetic rate limitation/inhibitions** ▸ Monod saturation function on VFA: $Msat_{SVFA,KVFA,CASTO}$ ▸ Logistic inhibition function on product: $Loginh_{XGLY,XGAO,max}$
CASTO aerobic maintenance	PHA → CO_2 and GLY → CO_2 Requires O_2. **Kinetic parameters** ▸ b_{STC}: Rate of CASTOs maintenance on PHA and GLY ▸ $K_{O2,CASTO,AS}$: Half-saturation of O_2 for CASTOs (AS) ▸ K_{STC}: Half-saturation of PHA and GLY for PAOs **Kinetic rate limitation/inhibitions** ▸ Monod saturation function on electron acceptor: O_2 → $Msat_{SO2,KO2,CASTO}$ ▸ Monod ratio saturation function on STC: $MRsat_{XSTC,XCASTO,KSTC}$
CASTO anoxic maintenance, $NO_x/NO_2/NO_3$	PHA → CO_2 and GLY → CO_2 Requires $NO_x/NO_2/NO_3$. **Kinetic parameters** ▸ b_{STC}: Rate of CASTOs maintenance on PHA and GLY ▸ $\eta_{bSTC,anox}$: Reduction factor for anoxic maintenance of CASTOs on PHA and GLY ▸ $K_{O2,CASTO,AS}$: Half-saturation of O_2 for CASTOs (AS) ▸ $K_{NOx,CASTO,AS}/K_{NO2,CASTO,AS}/K_{NO3,CASTO,AS}$: Half-saturation of $NO_x/NO_2/NO_3$ for CASTOs (AS) ▸ K_{STC}: Half-saturation of PHA and GLY for PAOs

Biological processes	Concepts description
	Kinetic rate limitation/inhibitions ▸ Monod inhibition function on O_2: $Minh_{SO2,KO2,CASTO}$ ▸ Monod inhibition function on NO_2: $Minh_{SNO2,KNO2,CASTO}$ (Sumo2, 2C, 2S) ▸ Monod saturation function on electron acceptor: ▸ NO_x → $Msat_{SNOx,KNOx,CASTO}$ (Mini_Sumo, Sumo1) ▸ NO_2 → $Msat_{SNO2,KNO2,CASTO}$ (Sumo2, 2C, 2S) ▸ NO_3 → $Msat_{SNO3,KNO3,CASTO}$ (Sumo2, 2C, 2S) ▸ Monod ratio saturation function on STC: $MRsat_{XSTC,XCASTO,KSTC}$
GAO anaerobic maintenance	GLY → VFA **Kinetic parameters** ▸ b_{STC}: Rate of CASTOs maintenance on PHA and GLY ▸ $\eta_{bGLY,ana}$: Reduction factor for anoxic maintenance of CASTOs on PHA and GLY ▸ $K_{O2,CASTO,AS}$: Half-saturation of O_2 for CASTOs (AS) ▸ $K_{NOx,CASTO,AS}/K_{NO2,CASTO,AS}/K_{NO3,CASTO,AS}$: Half-saturation of $NO_x/NO_2/NO_3$ for CASTOs (AS) ▸ K_{STC}: Half-saturation of PHA and GLY for PAOs **Kinetic rate limitation/inhibitions** ▸ Monod inhibition function on O_2: $Minh_{SO2,KO2,CASTO}$ ▸ Monod inhibition function on: ▸ NO_x → $Minh_{SNOx,KNOx,CASTO}$ (Mini_Sumo, Sumo1) ▸ NO_2 → $Minh_{SNO2,KNO2,CASTO}$ (Sumo2, 2C, 2S) ▸ NO_3 → $Minh_{SNO3,KNO3,CASTO}$ (Sumo2, 2C, 2S) ▸ Monod ratio saturation function on STC: $MRsat_{XSTC,XCASTO,KSTC}$
PP cleavage for maintenance	PP → PO_4 Rate expression covers the aerobic, anoxic and anaerobic PP cleavage as follows (Sumo1, MODEL sheet, row 27, column CB): r24 = $b_{PP,ana,T}$ * X_{PAO} * $Logsat_{XPP,KPO4,PAO}$ * ($\eta_{bPP,aer}$ * $MR_{inhXPHA,XPAO,KPHA,cle}$ * $Msat_{SO2,KO2,CASTO}$ + $\eta b_{PP,anox}$ * $Minh_{SO2,KO2,CASTO}$ * $Msat_{SNOx,KNOx,CASTO}$ + $Minh_{SO2,KO2,CASTO}$ * $Minh_{SNOx,KNOx,CASTO}$) **Kinetic parameters** ▸ $b_{PP,ana}$: Rate of PAOs maintenance under anaerobic conditions (PP cleavage) ▸ $\eta_{bPP,aer}$: Reduction factor for aerobic maintenance of PAOs on PP ▸ $\eta_{bPP,aer}$: Reduction factor for aerobic maintenance of PAOs on PP ▸ $\eta_{bPP,anox}$: Reduction factor for anoxic maintenance of PAOs on PP ▸ $K_{PO4,PAO,AS}$: Half-saturation of PO4 for PAOs (AS) ▸ $K_{PHA,cle}$: Half-saturation of PHA for PAOs at PP cleavage ▸ $K_{O2,CASTO,AS}$: Half-saturation of O_2 for CASTOs (AS) ▸ $K_{NOx,CASTO,AS}/K_{NO2,CASTO,AS}/K_{NO3,CASTO,AS}$: Half-saturation of $NO_x/NO_2/NO_3$ for CASTOs (AS)

Biological processes	Concepts description
	Kinetic rate limitation/inhibitions ▸ Logistic saturation function on substrate: $Logsat_{XPP,KPO4,PAO}$ ▸ Monod ratio inhibition function on PHA: $MRinh_{XPHA,XPAO,KPHA,cle}$ ▸ Monod saturation function on O_2: $Msat_{SO2,KO2,CASTO}$ ▸ Monod saturation function on: ▸ $NO_x \rightarrow Msat_{SNOx,KNOx,CASTO}$ (Mini_Sumo, Sumo1) ▸ $NO_2 \rightarrow Msat_{SNO2,KNO2,CASTO}$ (Sumo2, 2C, 2S) ▸ $NO_3 \rightarrow Msat_{SNO3,KNO3,CASTO}$ (Sumo2, 2C, 2S) ▸ Monod inhibition function on O_2: $Minh_{SO2,KO2,CASTO}$ ▸ Monod inhibition function on: ▸ $NO_x \rightarrow Minh_{SNOx,KNOx,CASTO}$ (Mini_Sumo, Sumo1) ▸ $NO_2 \rightarrow Minh_{SNO2,KNO2,CASTO}$ (Sumo2, 2C, 2S) ▸ $NO_3 \rightarrow Minh_{SNO3,KNO3,CASTO}$ (Sumo2, 2C, 2S)
S_B fermentation with high VFA (PAO growth, anaerobic)	SB → VFA + CASTO **Kinetic parameters** ▸ $\mu_{FERM,PAO}$: Fermentation growth rate of PAOs **Activity limitation** ▸ $act_{FERM,PAO,ORP}$: Fermentation activity switch for ORP **Kinetic rate limitation/inhibitions** ▸ Logistic saturation function on VFA: $Logsat_{SVFA,KVFA,FERM}$ ▸ Monod saturation function on S_B: $Msat_{SB,KSB,ana}$ ▸ Monod saturation functions on nutrients: NH_x, PO_4, cations, anions, calcium and magnesium: $Msat_{SNHx,KNHx,BIO}$, $Msat_{SPO4,KPO4,BIO}$, $Msat_{SCAT,KCAT}$, $Msat_{SAN,KAN}$, $Msat_{SCa,KCa}$, $Msat_{SMg,KMg}$ ▸ Bell shape inhibition function on pH: $Bellinh_{pH}$
S_B fermentation with low VFA (PAO growth, anaerobic)	SB → VFA + CASTO **Kinetic parameters** ▸ $\mu_{FERM,PAO}$: Fermentation growth rate of PAOs **Activity limitation** ▸ $act_{FERM,PAO,ORP}$: Fermentation activity switch for ORP **Kinetic rate limitation/inhibitions** ▸ Logistic inhibition function on VFA: $Loginh_{SVFA,KVFA,FERM}$ ▸ Monod saturation function on S_B: $Msat_{SB,KSB,ana}$ ▸ Monod saturation functions on nutrients: NH_x, PO_4, cations, anions, calcium and magnesium: $Msat_{SNHx,KNHx,BIO}$, $Msat_{SPO4,KPO4,BIO}$, $Msat_{SCAT,KCAT}$, $Msat_{SAN,KAN}$, $Msat_{SCa,KCa}$, $Msat_{SMg,KMg}$ ▸ Monod saturation functions on CO_2: $Msat_{SCO2,KCO2,BIO}$ ▸ Bell shape inhibition function on pH: $Bellinh_{pH}$

Biological processes	Concepts description
CASTO decay	CASTO → X_B and X_E under anoxic and aerobic conditions. **Kinetic parameters** ▸ b_{CASTO}: Decay rate of CASTOs ▸ $\eta_{bCASTO,anox}$: Reduction factor for anoxic decay of CASTOs ▸ K_{STC}: Half-saturation of PHA and GLY for PAOs ▸ $K_{O2,CASTO,AS}$: Half-saturation of O_2 for CASTOs (AS) ▸ $K_{NOx,CASTO,AS}/K_{NO2,CASTO,AS}/K_{NO3,CASTO,AS}$: Half-saturation of $NO_x/NO_2/NO_3$ for CASTOs (AS) ▸ K_{PP}: Half-saturation of PP for PAOs **Kinetic rate limitation/inhibitions** ▸ Monod ratio inhibition function on STC: $MRinh_{XSTC,XCASTO,KSTC}$ ▸ Monod saturation function on O_2: $Msat_{SO2,KO2,CASTO}$ ▸ Monod ratio inhibition function on PP: $MRinh_{XPP,XPAO,KPP}$ ▸ Monod saturation function on: ▸ NO_x → $Msat_{SNOx,KNOx,CASTO}$ (Mini_Sumo, Sumo1) ▸ NO_2 → $Msat_{SNO2,KNO2,CASTO}$ (Sumo2, 2C, 2S) ▸ NO_3 → $Msat_{SNO3,KNO3,CASTO}$ (Sumo2, 2C, 2S) ▸ Monod inhibition function on O_2: $Minh_{SO2,KO2,CASTO}$ ▸ Monod inhibition function on: ▸ NO_x → $Minh_{SNOx,KNOx,CASTO}$ (Mini_Sumo, Sumo1) ▸ NO_2 → $Minh_{SNO2,KNO2,CASTO}$ (Sumo2, 2C, 2S) ▸ NO_3 → $Minh_{SNO3,KNO3,CASTO}$ (Sumo2, 2C, 2S)
CASTO anaerobic decay	CASTO → X_B and X_E under anaerobic conditions. **Kinetic parameters** ▸ b_{CASTO}: Decay rate of CASTOs ▸ $\eta_{bCASTO,ana}$: Reduction factor for anaerobic decay of CASTOs ▸ $K_{O2,CASTO,AS}$: Half-saturation of O_2 for CASTOs (AS) ▸ $K_{NOx,CASTO,AS}/K_{NO2,CASTO,AS}/K_{NO3,CASTO,AS}$: Half-saturation of $NO_x/NO_2/NO_3$ for CASTOs (AS) ▸ K_{PP}: Half-saturation of PP for PAOs ▸ K_{GLY}: Half-saturation of glycogen for GAOs (AS) ▸ $m_{tox,ana,max}$: Toxicity factor of aerobes under anaerobic conditions (maximum) **Kinetic rate limitation/inhibitions** ▸ Monod ratio inhibition function on GLY: $MRinh_{XGLY,XCGAO,KGLY}$ ▸ Monod ratio inhibition function on PP: $MRinh_{XPP,XPAO,KPP}$ ▸ Monod inhibition function on O_2: $Minh_{SO2,KO2,CASTO}$ ▸ Monod inhibition function on: ▸ NO_x → $Minh_{SNOx,KNOx,CASTO}$ (Mini_Sumo, Sumo1) ▸ NO_2 → $Minh_{SNO2,KNO2,CASTO}$ (Sumo2, 2C, 2S) ▸ NO_3 → $Minh_{SNO3,KNO3,CASTO}$ (Sumo2, 2C, 2S)

Biological processes	Concepts description
	▸ First order toxicity: $X_{CASTO} * m_{tox,ana}$

Chemical phosphorus removal

Phosphorus can be chemically removed by:

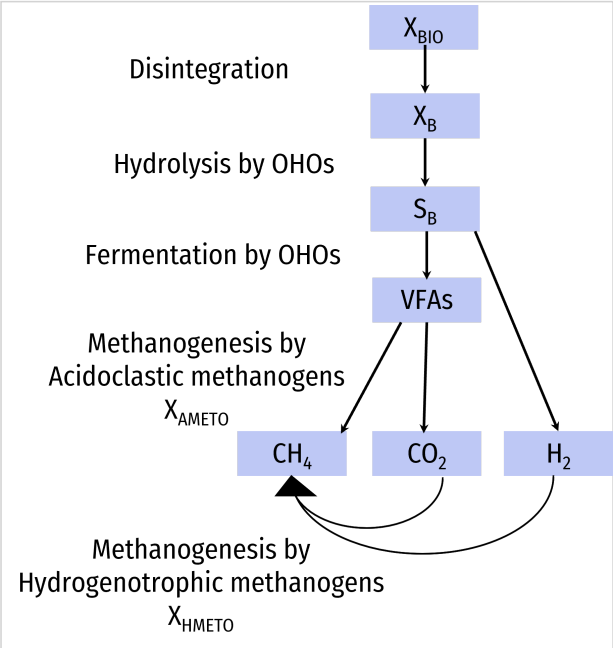
- metal salt addition (iron or aluminium). The chemical processes implemented in the model are described in a dedicated paragraph)
- natural or induced precipitation of:
  - Amorphous calcium phosphate ($Ca_3(PO_4)_2 * 4H_2O$)
  - Brushite ($CaHPO_4 * 2H_2O$)
  - Struvite ($MgNH_4PO_4 * 6H_2O$)
  - Vivianite ($Fe_3(PO_4)_2 * 8H_2O$)

The chemical precipitation model is described in a dedicated paragraph.

Anaerobic digestion processes

All Sumo models describe the anaerobic digestion processes involving 3 biomasses: the OHOs with fermentation process, Acidoclastic methanogens (AMETOs) and hydrogenotrophic methanogens (HMETOs).

The typical pathway of anaerobic digestion is the lysis of all biomasses (except OHOs and methanogens), hydrolysis of biodegradable particulate substrate, fermentation and methanogenesis, leading to methane production.



Typical anaerobic digestion processes pathway

The OHOs fermentation proces is described in BOD removal paragraph.

Methanogenesis

Acidoclastic methanogens, X_{AMETO}

Anaerobic archea that consume S_{VFA} to produce S_{CH4} and S_{CO2} as a metabolic by-product and don't grow under aerobic conditions.

Biological processes	Concepts description
AMETO growth	Substrate is S_{VFA} and produce S_{CH4}. Too much S_{VFA} results in a Haldane S_{VFA} inhibition Free ammonia inhibition Requires nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH.
AMETO decay	AMETO decay process under anoxic and aerobic conditions. This process release X_B and X_E (death-regeneration concept).
AMETO anaerobic decay	AMETO decay process under anaerobic conditions. This process release X_B and $X_{E,ana}$ (death-regeneration concept).

Hydrogenotrophic methanogens, X_{HMETO}

Anaerobic archea that consume S_{H2} and S_{CO2} to produce S_{CH4} as a metabolic by-product and don't grow under aerobic conditions.

Biological processes	Concepts description
HMETO growth	Substrate H2 and produce S_{CH4}. Requires nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH.
HMETO decay	HMETO decay process under anoxic and aerobic conditions. This process release X_B and X_E (death-regeneration concept).
HMETO anaerobic decay	HMETO decay process under anaerobic conditions. This process release X_B and $X_{E,ana}$ (death-regeneration concept).

Biological conversions

Flocculation

Flocculation is a process where colloidal components in liquid phase are aggregated into larger flocs thus behave as particulates. In Sumo models flocculation process is a conversion of colloidal components into particulates. The process rate is depending on the concentration of total biomass.

Hydrolysis

Hydrolysis is a process where larger molecules are broken into smaller molecules which are soluble in liquid phase. In Sumo hydrolysis is a biological process where particulate components are converted into soluble components. The process rate is depending on the concentration of heterotroph biomass.

Ammonification

The ammonification process is part of the nitrogen cycle when organic nitrogen is turned into soluble ammonia. In Sumo models soluble organic nitrogen compound is converted into ammonia. The process rate is depending on the concentration of heterotroph biomass.

Biological phosphorus conversion

Biological phosphorus conversion is similar to the ammonification process but in this process organic phosphorus is converted into phosphate. The process rate is depending on the concentration of heterotroph biomass.

Endogenous products conversion

In Sumo model this process is used to mimic the extreme slow hydrolysis of endogenous decay products by slowly converting X_E to particulate biodegradable substrate. The process rate is depending on the concentration of heterotroph biomass.

Anaerobic methanol conversion

Fermentation process of methanol utilizer organisms under anaerobic condition. The process rate depends on the methanol utilizer organisms concentration.

Nitrate/Nitrite assimilative reduction

Processes that occur only under limited ammonia availability. It ensures sufficient ammonia production for biomasses growth by reducing S_{NO3} and S_{NO2} into S_{NHx} with the biomasses as electron donors.

Photosynthesis processes

Photosynthetic processes are active only in the Gen3 pond process unit. The photosynthetic organisms (X_{ALGAE}) are considered as one biomass group which can grow, respire and decay.

Growth is dependent on the user input "Solar radiation for algal photosynthesis - depth averaged" which may vary depending on time of day (there is no sunlight at night), latitude and season, cloud cover as well as the depth of the pond. It is the user's responsibility to account for these factors when specifying the depth averaged solar radiation. Specifying diurnal and seasonal variations of solar radiation is possible using Input Dynamics.

The effect of shading in the water column due to influent particulate material, as well as algae itself, is accounted for using the parameter "TSS concentration for calculating light extinction switching factor". When the simulated TSS concentration in the water column approaches this value, the growth rate of algae switches to zero regardless of what the specified value is for "Solar radiation for algal photosynthesis - depth averaged".

Growth of algae is accompanied by assimilation of ammonia as a nutrient source unless ammonia becomes limiting in which case nitrate is assimilated. Phosphorus and carbon dioxide are also assimilated for growth.

Respiration of algae is simulated when oxygen is available. Respiration means the conversion of algae into water, CO2, ammonia and phosphate by oxydation using oxygen. In the absence of oxygen, the respiration rate switches to zero and decay of algae is switched on. Decay means the lysis of algae into particulate organic material, ammonia and phosphate and occurs in the pond sediments where oxygen is absent.

Mechanisms of focus models

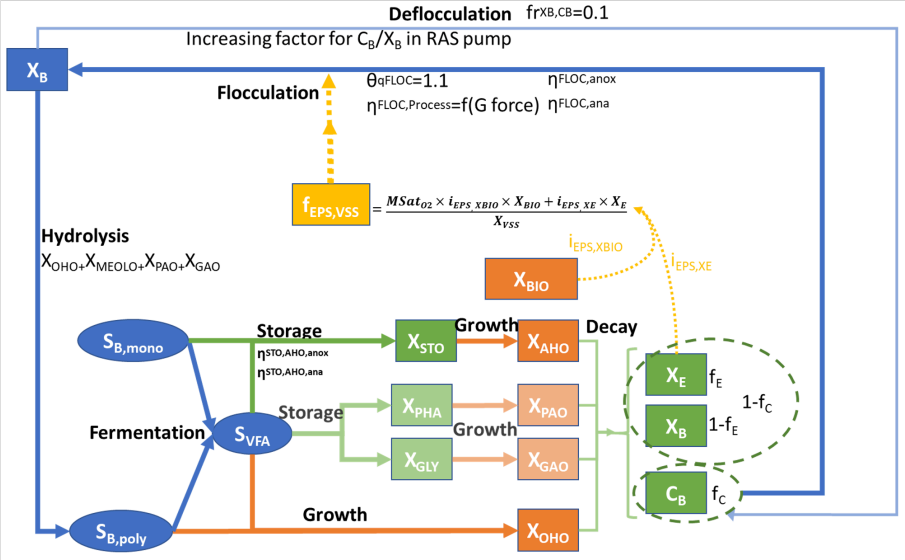
The chapter describes in details the model mechanisms and refers to publications.

Sumo2C

The whole-plant model SUMO2 (Dynamita, 2016, described in previous chapter) considering typical biological and physio-chemical model was modified to include the required components and processes in accordance with the critical review of existing models and experimental data, as

summarized in Sumo2C Figure 1:

- Readily biodegradable substrate (S_B) is split into monomers and polymers ($S_{B,mono}$ and $S_{B,poly}$).
- A new biomass, A-Stage Heterotrophic Organisms (AHO) is added. This biomass stores $S_{B,mono}$ and S_{VFA} into X_{STO} and has a high growth rate, while the Ordinary Heterotrophic Organisms consume only $S_{B,poly}$ and have a reduced growth rate.
- Hydrolysis process is performed only by low growth rate heterotrophic organisms (OHO, MEOLO, PAO and GAO) to simulate the low hydrolysis observed in A-Stage processes.
- Decay processes produce a fraction (f_C) of colloids, split into biodegradable and unbiodegradable colloids (CB and CU) in the same f_E proportion, as X_E (particulate endogenous decay products) and X_B (slowly biodegradable substrate) are generated in death-regeneration models.
- The modified model incorporates modeled EPS (X_{MEPS}) as a flocculation agent, calculated variable based on a weighted sum of biomasses (X_{BIO}) and particulate endogenous decay products (X_E) related to the particulate COD (X_{COD}), with a saturation function on oxygen, meaning that under low DO, EPS are less produced (Nogaj et al., 2015). The calculated X_{MEPS} is an indicator of EPS production, but the calculated values results depending on the analysis method used by different authors.
- The kinetic rate of flocculation processes are first order reactions that depend on the calculated X_{MEPS} concentration. The rate is reduced under anoxic and anaerobic conditions to match with experimental observations. Furthermore, the flocculation rate is sensitive to temperature and to mixing intensity, represented in the model with a flocculation factor (F_f in %) that can be vary in each reactor depending on the aeration and mixing technology (F_f=0.1 for mechanical mixing, 0.5 for coarse bubbles, 0.75 for anaerobic processes).
- An empirical pump process unit is implemented to simulate the deflocculation processes occurring at pumping. The factor for the increase in C_B/X_B and C_U/X_U ratio can be adjusted depending on the pump technology.



Sumo2C Figure 1 - Biological processes added and modified for the removal and capture of organics in the modified model

Carbon absorption heterotroph organisms, X_{AHO}

Heterotrophic organisms storing readily biodegradable small molecular weight components represented as $S_{B,mono}$ and volatile fatty acids (S_{VFA}) into X_{STO}. The growth rate of AHOs is higher than that of the OHOs and outgrow them in a short SRT system of <2 days. They only carry out aerobic consumption of the X_{STO} and are expected to be seeded from the influent.

Biological processes	Concepts description
AHO storage of $S_{B,mono}$	Storage of $S_{B,mono}$ into X_{STO} without any energy required
AHO storage of S_{VFA}	Storage of S_{VFA} into X_{STO} without any energy required
AHO growth on X_{STO}, O_2	Requires O_2, X_{STO} and nutrients. This is the AHO growth process.
AHO decay	Decay process of AHO under anoxic and aerobic conditions, resulting in X_B, C_B and X_E release. X_{STO} is also considered to be released in the proportion of X_{STO}/X_{AHO}.
AHO anaerobic decay	Decay process of AHO under anaerobic conditions, resulting in X_B, C_B and $X_{E,ana}$ release.

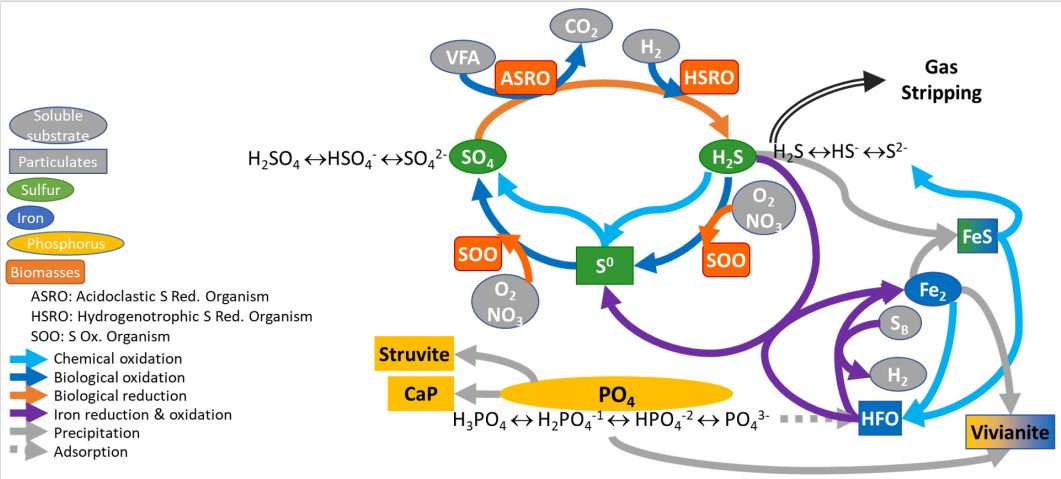
Biological processes	Concepts description
	X_{STO} is also considered to be released in the proportion of X_{STO}/X_{AHO}.

Haider, S., Svardal, K., Vanrolleghem, P.A., Kroiss, H., 2003. The effect of low sludge age on wastewater fractionation (S(S), S(I)). Water Sci. Technol. J. Int. Assoc. Water Pollut. Res. 47, 203–209.

Nogaj, T., Randall, A., Jimenez, J., Takacs, I., Bott, C., Miller, M., Murthy, S., Wett, B., 2015. Modeling of organic substrate transformation in the high-rate activated sludge process. Water Sci. Technol. 71, 971–979. https://doi.org/10.2166/wst.2015.051

Sumo2S

Biology and chemistry was extended with required components, species and reactions in accordance to the following literature review. Sumo2S Figure 1 synthesizes the sulfur cycle implemented in Sumo© models (Dynamita 2018) and the interactions with phosphorus and iron cycles.



Sumo2S Figure 1 - Phosphorus, sulfur and iron cycles interaction implemented in the plant-wide model.

General sulfur and iron model

The sulfur model included in Sumo includes three oxidation states of sulfur: Sulfate (SO_4^{-2}) as S_{SO4}, elemental sulfur (S^0) as X_S, and sulfide (S^-) as S_{H2S}.

Considering iron, two oxidation states are included in the model. Hydrous ferric oxides (HFO) species are already included in the base model for the chemical phosphorus treatment. These state variables ($X_{HFO,H}$, $X_{HFO,L}$, $X_{HFO,old}$, $X_{HFO,H,P}$, $X_{HFO,L,P}$, $X_{HFO,H,P,old}$ and $X_{HFO,L,P,old}$ depending on the floc size and P-bound status) are considered to be the only ferric (Fe^{3+}) species in the model, as ferric iron is only minimally soluble in water (Hauduc et al., 2015). X_{HFO} is a calculated variable being the sum of the seven HFO state variables. For the ferrous iron (Fe^{2+}), a new state variable is included in the model as S_{Fe2}, and ferrous oxides are not considered.

These states are considered to interact with other wastewater components as described below.

FeS precipitation and iron interaction

Reduction of Fe^{3+}, sulfide as electron donor

A chemical reduction of Fe^{3+} by sulfide occurs under reducing conditions. In this reaction, sulfide is oxidized into colloidal elemental sulfur which precipitates (Firer et al., 2008; Nielsen et al., 2005):

$$2\ Fe^{3+} + HS^- \rightarrow 2\ Fe^{2+} + S^0 + H^+$$

Implementation in the whole plant model: Elemental sulfur has been added as a particulate state variable (X_S), as elemental sulfur has a low solubility and flocculates easily. The hydrous ferric oxides (X_{HFO}) are reduced by H_2S in a single process into ferrous iron (S_{Fe2}) and elemental sulfur (X_S) with adequate stoichiometric coefficient to balance the redox reaction and a first order rate with respect to the X_{HFO} concentration.

Reduction of Fe^{3+}, organic matter as electron donor

Hydrous ferric oxides are reduced in digesters into soluble Fe^{2+} which precipitates into iron sulfide [FeS], and release bounded phosphates (Ge et al., 2013), that can further precipitate into vivianite [$Fe_3(PO_4)_2,8H_2O$] (Cheng et al., 2015). This biological process is performed by Fe^{3+} reducing bacteria, using organic matter as electron donors (Lovley and Phillips, 1988).

Implementation in the whole plant model: To keep the model simple, this new iron reducing biomass and the associated growth is not introduced in the model. The soluble biodegradable substrate (S_B) and volatile acids (S_{VFA}) are considered as electron donor and a first order kinetic rate expression with respect to the hydrous ferric oxide (X_{HFO}) concentration is used.

FeS precipitation

Fe^{2+} precipitates with sulfide into iron sulfide, FeS (Firer et al., 2008; Nielsen et al., 2005):

$$Fe^{2+} + HS^- \rightarrow FeS + H^+$$

Implementation in the whole plant model: The acid-base reactions of the sulfate and sulfide species are added in the pH model for speciation (equilibrium model). The precipitation is modelled following Koutsoukos et al (1980) kinetic expression with a solubility product $K_{sp,FeS}=3.7*10^{-19}$ (Nielsen et al., 2005).

Oxidation of Fe^{2+}

According to Gutierrez et al. (2010), the precipitated iron sulfide (FeS) is re-oxidized into ferric oxides and sulfate in an aerobic zone.

Implementation in the whole plant model: Both oxidation of ferrous iron (S_{Fe2}) and precipitated iron sulfide (X_{FeS}) are considered in the model with oxygen as electron acceptor with adequate stoichiometric coefficient to balance the redox reaction and a first order rate with respect to the S_{Fe2} and X_{FeS} concentrations respectively.

Reduction of sulfate

The biological sulfate reduction is the main process step in sulfur biotreatment, often combined with a chemical step or a metal precipitation step (Hao et al., 2014). The biological sulfate reduction is performed by sulfate reducing organisms (SRO), which can use either hydrogen or organic compounds as electron donor. These bacteria are directly in competition with hydrogenotrophic and acetoclastic methanogens respectively in anaerobic bioprocesses (Chou et al., 2008; Hao et al., 2014; Kalyuzhnyi and Fedorovich, 1998) and in sewer sediments (Liu et al., 2016). Models for sewer system usually neglect the biomass growth whereas models for anaerobic digestion always consider it. These models consider different kind of substrates. Knobel and Lewis (2002), Liu et al. (2015) and Fedorovich et al. (2003) consider 5 or 4 substrates respectively (different volatile fatty acids and H_2), whereas Batstone (2006) suggests considering only hydrogenotrophic sulfate reducer bacteria if S/COD ratio is below 0.1 mg S/mg COD. The best compromise seems to be the model from Barrera et al. (2015) and Poinapen and Ekama (2010) who consider H_2, acetate and propionate as substrates. The WATS model for sewer processes (Hvitved-Jacobsen et al., 2013) consider only soluble substrate for sulfate reduction biological processes.

Implementation in the whole plant model: Considering the actual structure of the extended version of Sumo model, S_{VFA} and S_{H2} have been chosen as substrate for sulfate reducing organisms (SRO), resulting in competition with the AMETO and HMETO, which would be similar to what is suggested by Barrera (2015) and in accordance with Kalyuzhnyi and Federovich (1998). Similarly to the methanogenesis implementation, two biomasses are introduced: ASRO (Acidoclastic Sulfate-Reducing Organisms) and HSRO (Hydrogenotrophic Sulfate-Reducing Organisms). This leads to 4 additional processes to consider growth and decay of both biomasses. Stoichiometric and kinetic values from Barrera (2015) are used. The produced sulfide is inhibitory (Utgikar et al. 2002). It has been considered in the kinetic rate expression through Haldane functions when sulfide is a reactant of the process, otherwise through Monod limitation function term.

Oxidation of sulfide

Biological oxidation

The biological oxidation of sulfide into sulfate is performed through intermediate species. The oxidation may use either oxygen, nitrite or nitrate as electron acceptor. In the literature, the biological oxidation of sulfide is mainly modelled in one or two steps, elemental sulfur (S^0) being the intermediate. The oxidation of elemental sulfur to sulfate is the limiting step (Buisman, et al., 1991; Jiang et al., 2009; Tichy et al., 1998). According to several authors, when sulfide is oxidized in a digester at limited oxygen levels, it reacts to elemental sulfur which precipitates, making it less available for further biological reduction (Diaz and Fdz-Polanco 2012; Jenicek et al. 2008).

Implementation in the whole plant model: A Sulfur Oxidizing Organism (X_{SOO}) has been introduced in the model with four oxidation processes to consider the two steps of sulfide oxidation and two possible oxidants (O_2 and NO_3). The parameter values from Mannucci et al (2012) are used as first estimation.

Chemical oxidation

At high SOO activity, chemical oxidation is negligible (Luther et al., 2011) but must be considered in case of sewer processes with lower biomass concentration as the oxygen consumption for sulfide oxidation count significantly in the OUR (Nielsen et al., 2003). The literature reports kinetic laws with different orders and a wide range of oxidation rate parameters, however the rate of the two steps of oxidation are not determined independently (Buisman et al., 1990; Hvitved-Jacobsen et al., 2013; Klok et al., 2013; Luther et al., 2011; Nielsen et al., 2003).

Implementation in the whole plant model: Two processes for oxidation of S_{H2S} by oxygen in two steps ($S_{H2S} \rightarrow X_S \rightarrow S_{SO4}$) is added. All the oxidation intermediates are considered through the elemental sulfur state variable (X_S), whereas the second oxidation step ($X_S \rightarrow S_{SO4}$) is much slower (Nielsen et al., 2003). To simplify the model, first order reactions with respect to sulfide and to elemental sulfur has been implemented for both steps of the oxidation process.

Biomasses involved in sulfur reactions

Acidoclastic sulfate-reducing organisms, X_{ASRO}

A group of bacteria and archaea that perform anaerobic respiration utilizing S_{SO4} and S_{VFA}, reducing it to S_{H2S} and generating S_{CO2}. They compete with AMETOs for S_{VFA} and negatively impact performance of a digester.

Biological processes	Concepts description
ASRO growth - SO_4 reduction with S_{VFA}	ASRO growth process on S_{VFA}, using S_{SO4} as electron acceptor. S_{H2S} is produced. Requires S_{SO4} and nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH.
ASRO decay	ASRO decay process under anoxic and aerobic conditions. This process release X_B and X_E (death-regeneration concept).
ASRO anaerobic decay	ASRO decay process under anaerobic conditions. This process release X_B and $X_{E,ana}$ (death-regeneration concept).

Hydrogenotrophic sulfate-reducing organisms, X_{HSRO}

A group of bacteria and archaea that perform anaerobic respiration utilizing S_{SO4} and S_{H2}, reducing it to S_{H2S}. They compete with HMETOs for S_{H2} consumption and negatively impact performance of a digester.

Biological processes	Concepts description
HSRO growth - SO_4 reduction with S_{H2}	HSRO growth process on S_{H2}, using S_{SO4} as electron acceptor. S_{H2S} is produced. Requires S_{SO4} and nutrients (S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}). Bell shape inhibition function on pH: BellinhpH.
HSRO decay	HSRO decay process under anoxic and aerobic conditions. This process release X_B and X_E (death-regeneration concept).

Biological processes	Concepts description
HSRO anaerobic decay	HSRO decay process under anaerobic conditions. This process release X_B and $X_{E,ana}$ (death-regeneration concept).

Sulfur-oxidizing organisms, X_{SOO}

Sulfur-oxidizing organisms (SOO) oxidize S_{H2S} in two steps under aerobic and anoxic environments, first from S_{H2S} to X_S (elemental sulfur) and second from X_S to S_{SO4}.

Biological processes	Concepts description
SOO growth on H_2S, O_2	SOO aerobic growth, using S_{H2S} as electron donor. S_{H2S} is oxidised into elemental sulfur X_S with S_{O2} as electron acceptor. Requires S_{H2S}, S_{O2} and nutrients (S_{H2S}, S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}).
SOO growth on H_2S, NO_2	SOO anoxic growth, using S_{H2S} as electron donor. S_{H2S} is oxidised into elemental sulfur X_S with S_{NO2} as electron acceptor. Requires S_{H2S}, S_{NO2} and nutrients (S_{H2S}, S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}).
SOO growth on H_2S, NO_3	SOO anoxic growth, using S_{H2S} as electron donor. S_{H2S} is oxidised into elemental sulfur X_S with S_{NO2} as electron acceptor. Requires S_{H2S}, S_{NO2} and nutrients (S_{H2S}, S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}).
SOO growth on S°, O_2	SOO aerobic growth, using elemental sulfur X_S as electron donor. X_S is oxidised into sulfate S_{SO4} with S_{O2} as electron acceptor. Requires X_S, S_{O2} and nutrients (S_{H2S}, S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}).
SOO growth on S°, NO_2	SOO anoxic growth, using elemental sulfur X_S as electron donor. X_S is oxidised into sulfate S_{SO4} with S_{NO2} as electron acceptor. Requires X_S, S_{NO2} and nutrients (S_{H2S}, S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}).
SOO growth on S°, NO_3	SOO anoxic growth, using elemental sulfur X_S as electron donor. X_S is oxidised into sulfate S_{SO4} with S_{NO3} as electron acceptor. Requires X_S, S_{NO3} and nutrients (S_{H2S}, S_{NHx}, S_{PO4}, S_{CAT}, S_{AN}, S_{Ca}, S_{Mg}).
SOO decay	SOO decay process under anoxic and aerobic conditions. This process release X_B and X_E (death-regeneration concept).
SOO anaerobic decay	SOO decay process under anaerobic conditions. This process release X_B and $X_{E,ana}$ (death-regeneration concept).

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*Barrera, E. L., Spanjers, H., Solon, K., Amerlinck, Y., Nopens, I., and Dewulf, J. (2015) Modeling the anaerobic digestion of cane-molasses vinasse: Extension of the Anaerobic Digestion Model No. 1 (ADM1) with sulfate reduction for a very high strength and sulfate rich wastewater. Water Research, **71**, 42–54.*

Batstone, D. J. (2006) Mathematical Modelling of Anaerobic Reactors Treating Domestic Wastewater: Rational Criteria for Model Use. Reviews in Environmental Science and Bio/Technology, ***5****(1), 57–71.*

Buisman, C., Ijspeert, P., Hof, A., Janssen, A., Tenhagen, R., and Lettinga, G. (1991) Kinetic-Parameters of a Mixed Culture Oxidizing Sulfide and Sulfur with Oxygen. Biotechnology and Bioengineering, ***38****(8), 813–820.*

Buisman, C., Uspeert, P., Janssen, A., and Lettinga, G. (1990) Kinetics of chemical and biological sulphide oxidation in aqueous solutions. Water Research, ***24****(5), 667–671.*

Chou, H.-H., Huang, J.-S., Chen, W.-G., and Ohara, R. (2008) Competitive reaction kinetics of sulfate-reducing bacteria and methanogenic bacteria in anaerobic filters. Bioresource Technology, ***99****(17), 8061–8067.*

Díaz, I. & Fdz-Polanco, M. 2012 Robustness of the microaerobic removal of hydrogen sulfide from biogas. Water Science and Technology ***65****, 1368–1374.*

Fedorovich, V., Lens, P., and Kalyuzhnyi, S. (2003) Extension of Anaerobic Digestion Model No. 1 with Processes of Sulfate Reduction. Applied Biochemistry and Biotechnology, ***109****(1-3), 33–46.*

Firer, D., Friedler, E., and Lahav, O. (2008) Control of sulfide in sewer systems by dosage of iron salts: Comparison between theoretical and experimental results, and practical implications. Science of the Total Environment, ***392****(1), 145–156.*

Gutierrez, O., Park, D., Sharma, K. R., and Yuan, Z. (2010) Iron salts dosage for sulfide control in sewers induces chemical phosphorus removal during wastewater treatment. Water Research, ***44****(11), 3467–3475.*

Hao, T., Xiang, P., Mackey, H. R., Chi, K., Lu, H., Chui, H., van Loosdrecht, M. C. M., and Chen, G.-H. (2014) A review of biological sulfate conversions in wastewater treatment. Water Research, ***65****, 1–21.*

Hauduc, H., Takács, I., Smith, S., Szabo, A., Murthy, S., Daigger, G.T., Spérandio, M., 2015. A dynamic physico-chemical model for chemical phosphorus removal. Water Research. ***73****, 157–170.*

Hvitved-Jacobsen, T., Vollertsen, J., and Nielsen, A. H. (2013) Sewer Processes: Microbial and Chemical Process Engineering of Sewer Networks, Second Edition, CRC Press.

Jenicek, P., Keclik, F., Maca, J. & Bindzar, J. 2008 Use of microaerobic conditions for the improvement of anaerobic digestion of solid wastes. Water Science and Technology ***58****,1491–1496.*

Jiang, G., Sharma, K. R., Guisasola, A., Keller, J., and Yuan, Z. (2009) Sulfur transformation in rising main sewers receiving nitrate dosage. Water Research, ***43****(17), 4430–4440.*

Kalyuzhnyi, S. V. and Fedorovich, V. V. (1998) Mathematical modelling of competition between sulphate reduction and methanogenesis in anaerobic reactors. Bioresource Technology, ***65****(3), 227–242.*

Klok, J. B. M., de Graaff, M., van den Bosch, P. L. F., Boelee, N. C., Keesman, K. J., and Janssen, A. J. H. (2013) A physiologically based kinetic model for bacterial sulfide oxidation. Water Research, ***47****(2), 483–492.*

Knobel, A. N. and Lewis, A. E. (2002) A mathematical model of a high sulphate wastewater anaerobic treatment system. Water Research, ***36****(1), 257–265.*

Liu, Y., Tugtas, A. E., Sharma, K. R., Ni, B.-J., and Yuan, Z. (2016) Sulfide and methane production in sewer sediments: Field survey and model evaluation. Water Research, ***89****, 142–150.*

Liu, Y., Zhang, Y., and Ni, B.-J. (2015) Evaluating Enhanced Sulfate Reduction and Optimized Volatile Fatty Acids (VFA) Composition in Anaerobic Reactor by Fe (III) Addition. Environmental Science & Technology, ***49****(4), 2123–2131.*

Luther, G. W., Findlay, A. J., MacDonald, D. J., Owings, S. M., Hanson, T. E., Beinart, R. A., and Girguis, P. R. (2011) Thermodynamics and Kinetics of Sulfide Oxidation by Oxygen: A Look at Inorganically Controlled Reactions and Biologically Mediated Processes in the Environment. Frontiers in Microbiology, ***2****:62.*

Mannucci, A., Munz, G., Mori, G., Lubello, C., 2012. Biomass accumulation modelling in a highly loaded biotrickling filter for hydrogen sulphide removal. Chemosphere 88, 712–717.

Nielsen, A. H., Lens, P., Vollertsen, J., and Hvitved-Jacobsen, T. (2005) Sulfide-iron interactions in domestic wastewater from a gravity sewer. Water Research, ***39****(12), 2747–2755.*

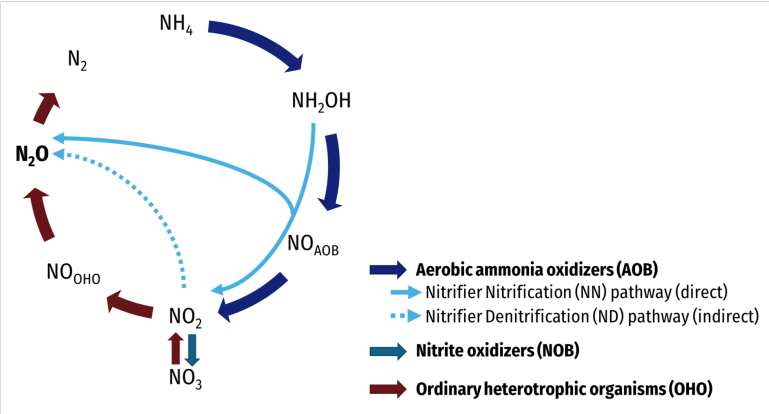
Nielsen, A. H., Vollertsen, J., and Hvitved-Jacobsen, T. (2003) Determination of kinetics and stoichiometry of chemical sulfide oxidation in wastewater of sewer networks. Environmental Science & Technology, ***37****(17), 3853–3858.*

*Poinapen, J. and Ekama, G. A. (2010) Biological sulphate reduction with primary sewage sludge in an upflow anaerobic sludge bed reactor - Part 5: Steady-state model. Water SA, **36**(3), 193–202.*

*Tichy, R., Janssen, A., Grotenhuis, J. T. C., Van Abswoude, R., and Lettinga, G. (1998) Oxidation of biologically-produced sulphur in a continuous mixed-suspension reactor. Water Research, **32**(3), 701–710.*

Sumo4N

To identify N_2O formation pathways on various wastewater treatment processes, several attempts to describe nitrification and denitrification intermediates in dynamic models have been published in the last decade. However, there is no clear consensus on the N_2O production modelling concepts yet. The combination of the 4-step denitrification model from Hiatt & Grady (2008) and the 2-P model for ammonium oxidizing bacteria from Pocquet et al. (2016) has been used in recent studies and seems promising (Mampaey et al, 2019; Fiat et al., 2019).



Sumo4N Figure 1 - Biological processes of the N cycle

What we know about N_2O production so far:

- The contribution of ND pathway is usually higher than the contribution of NN pathway
- The contribution of ND pathway increases at low DO under 1 mg O_2/L (Peng et al.,2014).
- The contribution of the ND pathway increases with high nitrite at low DO level (Wunderlin et al., 2013).
- The contribution of NN pathway increases with the DO (Peng et al.,2014).

4-step denitrification: Anoxic growth of OHOs from Hiatt&Grady (2008, only for OHO denitrification on S_B and S_{VFA})

- Reduction factor for anoxic growth from Hiatt&Grady, 2008
- Half-saturation for substrates and O_2 kept at Sumo2 values
- Half saturation for NO_3 and NO_2 from Hiatt&Grady2008
- Same anoxic yield than in Hiatt&Grady (0.54), although the aerobic yield in Sumo is higher than in Hiatt&Grady (respectively 0.67 and 0.54)
- In Sumo2 some inhibition terms on NO_2 make sure that the denitrification reactions are occurring successively. These terms are not used in Hiatt&Grady and have been removed.
- Assimilative nitrate/nitrite reduction to ammonia coded differently in Sumo2 (and kept as is): $NO_3^- \rightarrow NH_4^+$ and $NO_2^- \rightarrow NH_4^+$ directly, biomasses are used as electron donors instead of substrate
- Mixotrophic growth of NOB not implemented

These parameters take into consideration the fraction of heterotrophic bacteria accomplishing each step of denitrification and the reduced maximum specific growth rate under anoxic conditions.

This results into 8 denitrification processes:

2	**r2**	OHO growth on VFAs, NO_3
3	**r3**	OHO growth on VFAs, NO_2
4	**r4**	OHO growth on VFAs, NO
5	**r5**	OHO growth on VFAs, N_2O

7	**r7**	OHO growth on S_B, NO_3
8	**r8**	OHO growth on S_B, NO_2
9	**r9**	OHO growth on S_B, NO
10	**r10**	OHO growth on S_B, N_2O

Growth processes on volatile fatty acids (S_{VFA}) or readily biodegradable substrate (S_B) are similar and occurs successively thanks to the switch functions:

- $Msat_{VFA,KVFA}$ used for growth on VFA processes
- $Msat_{SB,KSB}$*$Minh_{SVFA,KVFA}$ used for growth on readily biodegradable processes

Biological processes	Concepts description
OHO growth with NO_3	Reduction $NO_3^- \rightarrow NO_2^-$ **Kinetic parameters** ▸ μ_{OHO}: Maximum specific growth rate of OHOs ▸ $\eta_{OHO,NO3}$: Reduction factor for anoxic growth of OHOs on NO_3 ▸ $K_{VFA,NO3,AS}$: Half-saturation of VFA for OHOs on NO_3 (AS) ▸ $K_{SB,NO3,AS}$: Half-saturation of readily biodegradable substrate for OHOs on NO_3 (AS) ▸ $K_{O2,OHO,NO3,AS}$: Half-saturation of O_2 for OHOs on NO_3 (AS) ▸ $K_{NO3,OHO,AS}$: Half-saturation of NO_3 for OHOs (AS) **Kinetic rate limitation/inhibitions** ▸ Monod saturation function on substrate: $Msat_{VFA,KVFA}$ or $Msat_{SB,KSB}$*$Minh_{SVFA,KVFA}$ ▸ Monod saturation function on electron acceptor: NO_3 => $Msat_{SNO3,KNO3,OHO}$ ▸ Monod inhibition function on O_2: $Minh_{SO2,KO2,OHO,NO3}$ ▸ Monod saturation functions on nutrients: NH_x, PO_4, cations, anions, calcium and magnesium: $Msat_{SNHx,KNHx,OHO}$, $Msat_{SPO4,KPO4,BIO}$, $Msat_{SCAT,KCAT}$, $Msat_{SAN,KAN}$, $Msat_{SCa,KCa}$, $Msat_{SMg,KMg}$ ▸ Bell shape inhibition function on pH: BellinhpH
OHO growth with NO_2	Reduction $NO_2^- \rightarrow NO_{,OHO}$ (NO considered as cell-internal intermediate) Inhibited by NO **Kinetic parameters** ▸ μ_{OHO}: Maximum specific growth rate of OHOs ▸ $\eta_{OHO,NO2}$: Reduction factor for anoxic growth of OHOs on NO_2 ▸ $K_{VFA,NO2,AS}$: Half-saturation of VFA for OHOs on NO_2 (AS) ▸ $K_{SB,NO2,AS}$: Half-saturation of readily biodegradable substrate for OHOs on NO_2 (AS) ▸ $K_{NO2,OHO,AS}$: Half-saturation of NO_2 for OHOs (AS) ▸ $K_{O2,OHO,NO2,AS}$: Half-saturation of O_2 for OHOs on NO_2 (AS) ▸ $Ki_{NO,OHO,NO2,AS}$: Half-inhibition of NO for OHOs denitrification of NO_2 (AS) **Kinetic rate limitation/inhibitions**

Biological processes	Concepts description
	▸ Monod saturation function on substrate: $Msat_{VFA,KVFA}$ or $Msat_{SB,KSB}$*$Minh_{SVFA,KVFA}$ ▸ Monod saturation function on electron acceptor: NO_2 => $Msat_{SNO2,KNO2,OHO}$ ▸ Monod inhibition function on O_2: $Minh_{SO2,KO2,OHO,NO2}$ ▸ Monod inhibition function on NO: $Minh_{SNO,KiNO,OHO,NO2}$ ▸ Monod saturation functions on nutrients: NH_x, PO_4, cations, anions, calcium and magnesium: $Msat_{SNHx,KNHx,OHO}$, $Msat_{SPO4,KPO4,BIO}$, $Msat_{SCAT,KCAT}$, $Msat_{SAN,KAN}$, $Msat_{SCa,KCa}$, $Msat_{SMg,KMg}$ ▸ Bell shape inhibition function on pH: BellinhpH
OHO growth with NO	Reduction $NO_{,OHO}$→N_2O (NO considered as cell-internal intermediate) Inhibited by NO **Kinetic parameters** ▸ μ_{OHO}: Maximum specific growth rate of OHOs ▸ $\eta_{OHO,NO}$: Reduction factor for anoxic growth of OHOs on NO ▸ $K_{VFA,NO,AS}$: Half-saturation of VFA for OHOs on NO (AS) ▸ $K_{SB,NO,AS}$: Half-saturation of readily biodegradable substrate for OHOs on NO (AS) ▸ $K_{NO,OHO,AS}$: Half-saturation of NO for OHOs (AS) ▸ $K_{O2,OHO,NO,AS}$: Half-saturation of O_2 for OHOs on NO (AS) ▸ $Ki_{NO,OHO,NO,AS}$: Half-inhibition of NO for OHOs denitrification of NO (AS) **Kinetic rate limitation/inhibitions** ▸ Monod saturation function on substrate: $Msat_{VFA,KVFA}$ or $Msat_{SB,KSB}$*$Minh_{SVFA,KVFA}$ ▸ Haldane functions on electron acceptor: NO => $Hsat_{SNO,KNO,OHO}$ ▸ Monod inhibition function on O_2: $Minh_{SO2,KO2,OHO,NO2}$ ▸ Monod saturation functions on nutrients: NH_x, PO_4, cations, anions, calcium and magnesium: $Msat_{SNHx,KNHx,OHO}$, $Msat_{SPO4,KPO4,BIO}$, $Msat_{SCAT,KCAT}$, $Msat_{SAN,KAN}$, $Msat_{SCa,KCa}$, $Msat_{SMg,KMg}$ ▸ Bell shape inhibition function on pH: BellinhpH
OHO growth with N_2O	Reduction N_2O→N_2 Inhibited by NO **Kinetic parameters** ▸ μ_{OHO}: Maximum specific growth rate of OHOs ▸ $\eta_{OHO,N2O}$: Reduction factor for anoxic growth of OHOs on N_2O ▸ $K_{VFA,N2O,AS}$: Half-saturation of VFA for OHOs on N_2O (AS) ▸ $K_{SB,N2O,AS}$: Half-saturation of readily biodegradable substrate for OHOs on N_2O (AS) ▸ $K_{N2O,OHO,AS}$: Half-saturation of N_2O for OHOs (AS) ▸ $K_{O2,OHO,N2O,AS}$: Half-saturation of O_2 for OHOs on N_2O (AS) ▸ $Ki_{NO,OHO,NO2,AS}$: Half-inhibition of NO for OHOs denitrification of N_2O (AS)

Biological processes	Concepts description
	Kinetic rate limitation/inhibitions ▸ Monod saturation function on substrate: $Msat_{VFA,KVFA}$ or $Msat_{SB,KSB}$*$Minh_{SVFA,KVFA}$ ▸ Monod saturation function on electron acceptor: N_2O => $Msat_{SN2O,KN2O,OHO}$ ▸ Monod inhibition function on O_2: $Minh_{SO2,KO2,OHO,NO2}$ ▸ Monod inhibition function on NO: $Minh_{SNO,KiNO,OHO,N2O}$ ▸ Monod saturation functions on nutrients: NH_x, PO_4, cations, anions, calcium and magnesium: $Msat_{SNHx,KNHx,OHO}$, $Msat_{SPO4,KPO4,BIO}$, $Msat_{SCAT,KCAT}$, $Msat_{SAN,KAN}$, $Msat_{SCa,KCa}$, $Msat_{SMg,KMg}$ ▸ Bell shape inhibition function on pH: BellinhpH

4-step AOB nitrification: From Pocquet et al. 2016

Five processes are included in the model. Nitric oxide (NO) is considered to be a metabolism intermediate and thus unlikely being released in the bulk and stripped. Consequently, the correction factor for mass transfer of NO parameter ($f_{kL,GNO}$) is set to zero.

- AOB decay kept as in Sumo2
- NOB growth and decay kept as in Sumo2

Biological processes	Concepts description
AOB NH_x oxidation to NH_2OH	Requires O_2. The Monod term in the original model (Pocquet et al, 2016) is on free ammonia. It has been replaced by a term on total ammonia for more stability of the model under normal pH range. **Kinetic parameters** The maximum rate is the maximum specific growth rate of AOBs divided by the AOB yield (μ_{AOB}/Y_{AOB}) to keep the same substrate utilization rate than for the AOB growth process (AOB NH_2OH oxidation to NO process) ▸ μ_{AOB}: Maximum specific growth rate of AOBs ▸ $K_{O2,NHx,AOB,AS}$: Half-saturation of O_2 for NH_x oxydation by AOBs (AS) ▸ $K_{O2,NHx,AOB,Sidestream}$: Half-saturation of O_2 for NH_x oxydation by AOBs (Sidestream) ▸ $K_{NHx,NH2OH,AOB,AS}$: Half-saturation of NH_x to NH_2OH for AOBs (AS) **Kinetic rate limitation/inhibitions** ▸ Monod saturation functions on electron acceptor: O_2 => $Msat_{SO2,KO2,NHx,AOB}$ ▸ Monod saturation functions on electron donor: NHx => $Msat_{SNHx,KNHx,NH2OH,AOB}$
AOB NH_2OH oxidation to NO	Requires O_2. This is the AOB growth process. **Kinetic parameters** ▸ μ_{AOB}: Maximum specific growth rate of AOBs

Biological processes	Concepts description
	▸ $K_{O2,NH2OH,AOB,AS}$: Half-saturation of O_2 for NH_2OH oxidation by AOBs (AS) ▸ $K_{O2,NH2OH,AOB,sidestream}$: Half-saturation of O_2 for NH_2OH oxidation by AOBs (Sidestream) ▸ $K_{NH2OH,AOB,AS}$: Half-saturation of NH_2OH for AOBs (AS) ▸ $K_{NHx,\ AOB,AS}$: Half-saturation of NH_x for AOBs (AS) **Kinetic rate limitation/inhibitions** ▸ Monod saturation functions on electron donor: NH_2OH => $Msat_{SNH2OH,KNH2OH,AOB}$ ▸ Monod saturation functions on electron acceptor: O_2 => $Msat_{SO2,KO2,NH2OH,AOB}$ ▸ Logistic switch on bicarbonates, pH dependent: $LogsatpH_{CO2,AOB}$ ▸ Monod saturation functions on nutrients: NH_x, PO_4, cations, anions, calcium and magnesium: $Msat_{SNHx,KNHx,AOB}$, $Msat_{SPO4,KPO4,BIO}$, $Msat_{SCAT,KCAT}$, $Msat_{SAN,KAN}$, $Msat_{SCa,KCa}$, $Msat_{SMg,KMg}$ ▸ Bell shape inhibition function on pH: BellinhpH
AOB NO oxidation to NO2	Requires O_2. **Kinetic parameters** The maximum rate is the maximum specific growth rate of AOBs divided by the AOB yield (μ_{AOB}/Y_{AOB}) to keep the same substrate utilization rate than for the AOB growth process (AOB NH_2OH oxidation to NO process) ▸ μ_{AOB}: Maximum specific growth rate of AOBs ▸ $K_{O2,NH2OH,AOB,AS}$: Half-saturation of O_2 for NH_2OH oxidation by AOBs (AS) ▸ $K_{O2,NH2OH,AOB,sidestream}$: Half-saturation of O_2 for NH_2OH oxidation by AOBs (Sidestream) $K_{NO,NO2,AOB,AS}$: Half-saturation of NO to NO_2 for AOBs (AS) **Kinetic rate limitation/inhibitions** ▸ Monod saturation functions on electron acceptor: O_2 => $Msat_{SO2,KO2,NH2OH,AOB}$ ▸ Monod saturation functions on electron donor: NO => $Msat_{SNO,KNO,NO2,AOB}$
AOB NO reduction to N2O (NN pathway)	Direct pathway of N_2O production (or NN pathway): NO reduction to N_2O by the enzyme “Nor” coupled with the hydroxylamine oxidation to nitrite **Kinetic parameters** The maximum rate is the maximum specific growth rate of AOBs divided by the AOB yield (μ_{AOB}/Y_{AOB}), reduced by a reduction factor for NO reduction to N_2O by AOBs (NN pathway) ($\eta_{AOB,NO,N2O}$) ▸ μ_{AOB}: Maximum specific growth rate of AOBs ▸ $\eta_{AOB,NO,N2O}$: Reduction factor for NO reduction to N_2O by AOBs (NN pathway) ▸ $K_{NH2OH,AOB,AS}$: Half-saturation of NH_2OH for AOBs (AS)

Biological processes	Concepts description
	▸ $K_{NO,N2O,AOB,AS}$: Half-saturation of NO to N2O for AOBs (AS) **Kinetic rate limitation/inhibitions** ▸ Monod saturation functions on electron donor: NH2OH => $Msat_{SNH2OH,KNH2OH,AOB}$ ▸ Monod saturation functions on electron acceptor: NO => $Msat_{SNO,KNO,N2O,AOB}$
AOB HNO2 reduction to N2O (ND pathway)	Indirect pathway of N_2O production (or ND pathway): HNO_2 reduction to N_2O coupled with NH_2OH oxidation to nitrite. Originally this ND pathway considers 2 steps: NO_2 reduction to NO (NirK enzyme), then NO reduction to N_2O (Nor enzyme) (Mampaey et al., 2013; Ni et al., 2011). These two processes are merged in this single one to avoid the NO loop with the AOB NO oxidation to NO_2 process (Pocquet et al., 2016). the Haldane-type term on O2 is replaced with a simple Monod inhibition term. This results in a limitation of this process under anoxic conditions with hydroxylamine, what is observed by some authors (Domingo-Félez and Smets, 2016) **Stoichiometric parameters** ▸ Y_{AOB}: Yield of AOBs on NH_x **Kinetic parameters** The maximum rate is the maximum specific growth rate of AOBs divided by the AOB yield (μ_{AOB}/Y_{AOB}), reduced by a reduction factor for HNO_2 reduction to N_2O by AOBs (ND pathway) ($\eta_{AOB,NO2,N2O}$) ▸ μ_{AOB}: Maximum specific growth rate of AOBs ▸ $\eta_{AOB,NO2,N2O}$: Reduction factor for HNO2 reduction to N2O by AOBs (ND pathway) ▸ $K_{NH2OH,AOB,AS}$: Half-saturation of NH_2OH for AOBs (AS) ▸ $K_{HNO2,AOB,AS}$: Half-saturation of HNO_2 for AOBs (AS) ▸ $K_{iO2,AOB,AS}$: Half-inhibition of O_2 for N_2O production by AOBs (AS) **Kinetic rate limitation/inhibitions** ▸ Monod saturation functions on electron donor: NH_2OH => $Msat_{SNH2OH,KNH2OH,AOB}$ ▸ Monod saturation functions on electron acceptor: HNO_2 => $Msat_{SHNO2,KHNO2,AOB}$ ▸ This process contribution increase at low DO: Monod inhibition term on O_2 => $Minh_{SO2,KiO2,AOB}$

Fiat, J., Filali, A., Fayolle, Y., Bernier, J., Rocher, V., Spérandio, M., Gillot, S., 2019. Considering the plug-flow behavior of the gas phase in nitrifying BAF models significantly improves the prediction of N2O emissions. Water Res. 156, 337–346. https://doi.org/10.1016/j.watres.2019.03.047

Hiatt, W.C., Grady, C.P.L. Jr., 2008. An updated process model for carbon oxidation, nitrification, and denitrification. Water Environ. Res. 80(11), 2145-2156.

Houweling, Dwight; Constantine, Tim; Eriksen Søren; Uri Carreño, Nerea; Holmen Andersen, Mikkel. 2016. N2O Emissions from Sidestream Deammonification: Using Latest Generation Models to Guide Optimization. 2016 WEFTEC Proceedings

Ni, B.-J., Law, Y., Guo, J., Yuan, Z. 2014. Modeling of Nitrous Oxide Production by Autotrophic Ammonia-Oxidizing Bacteria with Multiple Production Pathways. Environmental Science and Technology, 48(7):3916-24.

Mampaey, K.E., Spérandio, M., van Loosdrecht, M.C.M., Volcke, E.I.P., 2019. Dynamic simulation of N2O emissions from a full-scale partial nitritation reactor. Biochem. Eng. J. 152, 107356. https://doi.org/10.1016/j.bej.2019.107356

Pocquet, M., Wu, Z., Queinnec, I., Spérandio, M., 2016. A two pathway model for N2O emissions by ammonium oxidizing bacteria supported by the NO/N2O variation. Water Res. 88, 948-959.

Uri, Nerea; Nielson, Per H.; Holmen Andersen, Mikkel; Hafner, Sasha; Li, Zheqin; Chandran, Kartik. 2017. Continuous Aeration Control to Reduce N2O Emissions in a Full-Scale Sidestream Deammonification Reactor. 2017 WEFTEC Proceedings

Physico-chemical processes

pH and alkalinity

The first mechanistic models (e.g. ASM1) did alkalinity accounting to estimate running out of alkalinity and the detrimental effect on nitrification through lack of bicarbonate and low pH. Starting from ADM1 and all modern software today calculate pH instead based on chemical equilibrium and determine alkalinity by "virtual" titration.

There are three different methods to calculate pH:
1) Kinetic approach such as the Musvoto (2000) - this is easy to implement in existing Gujer matrix tools, but computationally very inefficient due to the large difference between the rates of protonation-deprotonation and biological reactions.

2) Tableau - this is a standard chemical method, easy to extend, but it requires solving a multidimensional non-linear problem involving key species. It is quite OK for determining pH of one solution, but when we have 1000 locations in the plant model, some within recycle loops etc., the problem dimension may easily become hundred thousand and unfeasible to solve efficiently every single timestep.

3) The one most software uses: Solve pH, alkalinity and ionic strength. If pH and ionic strength (IS) were known, each ionic species concentration can be calculated from the total component concentration (i.e. total ammonia+ammonium can be split at a certain pH and IS to undissociated ammonia and ammonium ions). The method is based on guessing a pH and IS value, calculating ionic species, checking the charge balance and the IS error, and using Newton-Raphson method to vary pH and IS until both charge balance and IS error are zero.

The advantage of this method is that the variables to be solved are limited (2 in the base case). Disadvantage is that the equations for species calculation must be developed manually for each species (though symbolic solvers are available such as Maple or SymPy Python library). After a certain complexity of the pH model (e.g. in the case of many species and ionic pairs) the equations can become unsolvable symbolically. In this case the problem dimension will be increased by adding one central species (such as Fe^{3+} or HCO_3^-) to pH and IS (so solving three variables instead of two). This drastically reduces the complexity of the equations and only marginally increases the solution time.

Consider a simple example for ammonia in distilled water, in a simple chemical model.

Components definition

On the components tab of the model each state variable is defined and its total component concentrations (i.e. total ammonia + ammonium for S_{NHx}) is setup in “Initial concentration” column. This is equivalent to the “Input setup” task of the GUI, see user manual for details.

	State variables				
Symbol	Name	Influent	Initial concentration	Unit	Decimals
S_{NHx}	Ammonia ($NH_4 + NH_3$)	3	1.4	g $N.m^{-3}$	2
S_{NOx}	Nitrate and nitrite ($NO_3 + NO_2$) (considered to be NO_3 only for stoichiometry)	15	0	g $N.m^{-3}$	2
S_{CO2}	Total dissolved inorganic carbon	0.01	0	$mol.L^{-1}$	4
S_{CAT}	Strong cations	0.01	0	$mol.L^{-1}$	4
S_{AN}	Strong anions	0.003	0	$mol.L^{-1}$	4

... Components | Species | pH | Calculated variables | other parameters

Speciation expressions

In a solution of pure ammonia, we have two dissociation/ionization reactions and a mass balance:
Water dissociation: $[H^+] * [OH^-] = k_W$
Ammonia ionization: $[H^+] * [NH_3] / [NH_4^+] = K_{iNH3}$
Mass balance: $S_{NHx} = [NH_3] + [NH_4^+]$

Three equations can be solved for three variables to calculate the speciation of ammonia:
$[OH^-] = k_W / [H^+]$
$[NH_3] = (K_{iNH3} * S_{NHx})/([H^+] + K_{iNH3})$
$[NH_4^+] = ([H^+] * S_{NHx})/([H^+] + K_{iNH3})$

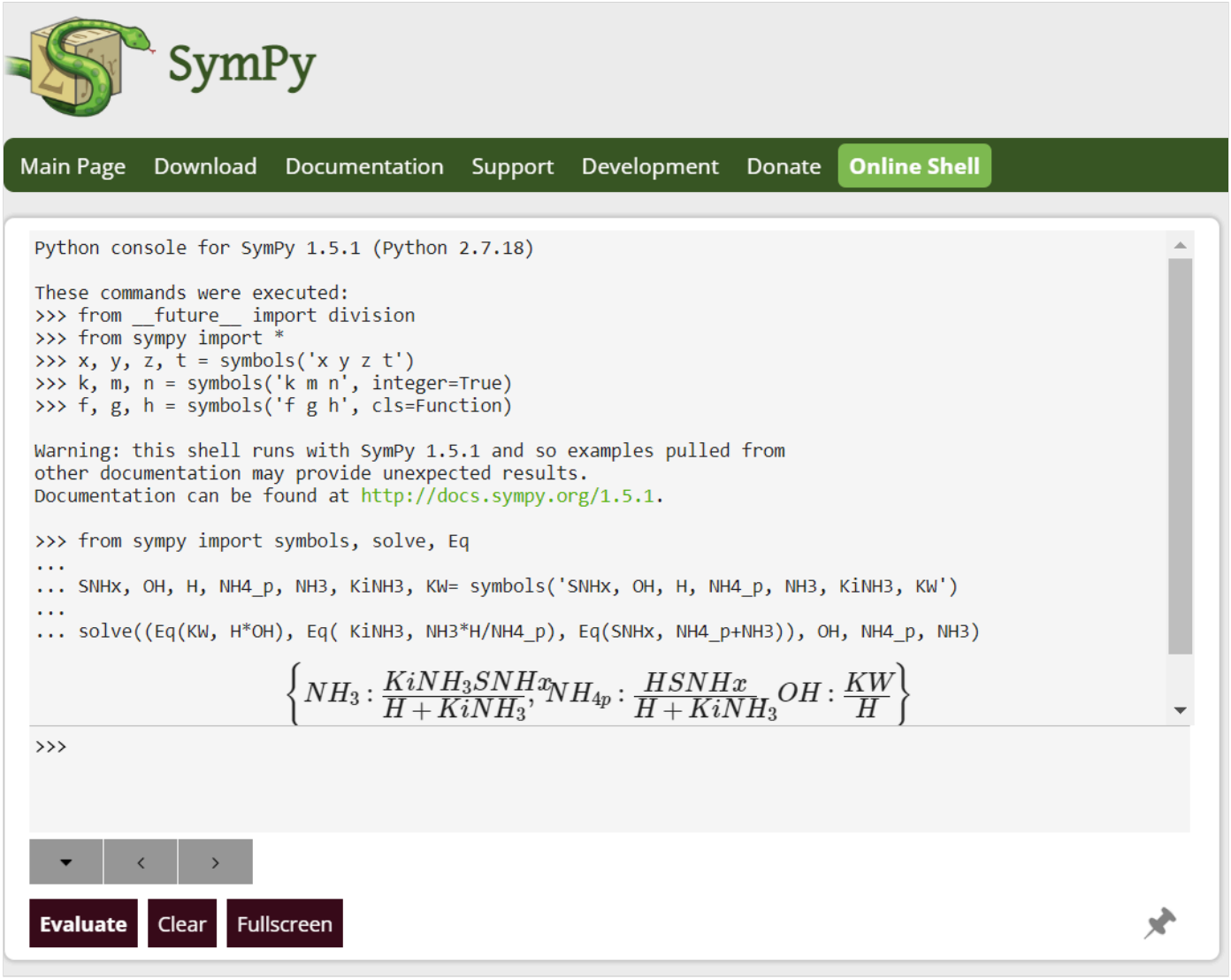
This can be solved through a symbolic solver, especially in case of more complex systems (carbonates, phosphates, ion pairing…). Sympy is a Python library for symbolic mathematics and can be used online (http://live.sympy.org/). The above system for ammonia speciation can be solved with the following code:

```
from sympy import symbols, solve, Eq
SNHx, OH, H, NH4_p, NH3, KiNH3, KW= symbols('SNHx, OH, H, NH4_p, NH3, KiNH3, KW')
solve((Eq(KW, H*OH), Eq( KiNH3, NH3*H/NH4_p), Eq(SNHx, NH4_p+NH3)), OH, NH4_p, NH3)
```

where

from sympy import symbols, solve, Eq	Loads the appropriate libraries and functions
SNHx, OH, H, NH4_p, NH3, KiNH3, KW=symbols('SNHx, OH, H, NH4_p, NH3, KiNH3, KW')	Declares the variables and parameters
solve((Eq(KW, H*OH), Eq(KiNH3, NH3*H/NH4_p), Eq(SNHx, NH4_p+NH3)), OH, NH4_p, NH3)	Provides the system of 3 equations (comma meaning “=” sign) And the 3 unknown variables

The results will be:



Knowing the definition of pH

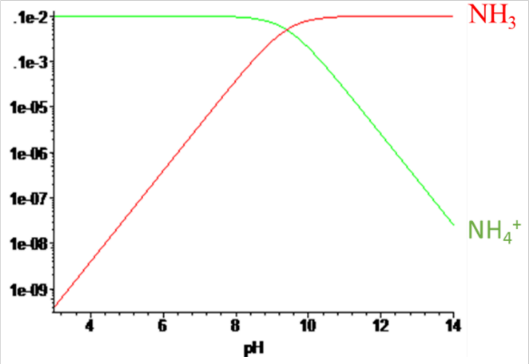
$$[H^+] = 10^{(-pH)}$$

These equations are entered into the pH table in the Sumo model file, in the pH sheet:

	Equilibrium matrix	Type(Equilibrium)			
Symbol	Name	$[H^+]$	$[OH^-]$	$[NH_3]$	$[NH_4^+]$
$diss_{H2O}$	Dissociation of water	10^(-pH)	$K_W/[H^+]$		
ion_{amm}	Ionization of ammonia			$(S_{NHx}/(AM_N*1000))*Ki_{NH3}/([H^+]+Ki_{NH3})$	$(S_{NHx}/(AM_N*1000))*[H^+]/([H^+]+Ki_{NH3})$

S_{NHx} needs to be converted from g/m^3 (equivalent to mg/L, used in the kinetic model) to mol/L (used in the equilibrium model), therefore divided by the atomic mass of N (AM_N * 1000 = 14000 mg/mol). Sumo constructs the necessary equation system and solver setup from this information automatically.

These species plotted as a function of pH provide the dissociation curves, we know (for 0.0001 molar pure ammonia solution):



It is possible to make a **pH and ionic strength guess** (i.e. pH=7.0, IS=0.0001 mol/kg)

Dissociation and acidity constants

The dissociation and acidity constants used for the speciation calculations are sensitive to the temperature and ionic strength. They are corrected in the calculated variables of the model:

- **For temperature**

For water dissociation constants the Van't Hoff equation is used to correct the constant value for temperature. For other compounds, empirical equations are used when available.

	Standard enthalpy change of reactions	**Type(Algebraic)**		
Symbol	**Name**	**Expression**	**Value**	**Unit**
$dH_{diss,H2O}$	Standard enthalpy change of dissociation of water	$(H_{OHm}+H_{H3Op}) - 2*H_{H2O}$	58032.2	$J.mol^{-1}$
	Dissociation constants - temperature correction	**Type(Algebraic)**		
Symbol	**Name**	**Expression**	**Value**	**Unit**
$K_{W,T}$	Water dissociation	$K_{W,param}*Exp(dH_{diss,H2O}/R*(1/T_{std}-1/T_K))$	1.007E-14	unitless
$K_{C1,T}$	Carbonate first step	$10^{(-(3404.7/T_K-14.8435+T_K*0.03279))}$	4.44367E-07	unitless
$K_{C2,T}$	Carbonate second step	$10^{(-(2902.4/T_K-6.498+T_K*0.02379))}$	4.68074E-11	unitless
Ki_{NH3}	Ammonia ionization	$10^{(-(2835.8/T_K - 0.6322 + 0.00123*T_K))}$	5.67748E-10	unitless
	Temperature	**Type(Algebraic)**		
Symbol	**Name**	**Expression**	**Value**	**Unit**
T_K	Temperature [K]	$T+T_{null}$	298.15	K

- **For ionic strength**

In a non-ideal aqueous phase, such as typical wastewater, the ions interact due to molecular attraction and repelling, and those interactions increase with the total charge concentration. These interactions reduce the number of ions that are available (active) for reactions. Therefore, the measured concentration must be corrected in order to get the activities the ions would have under ideal conditions.

Sumo is using Davies corrections equations for ionic strength, which is valid from ionic strength in the range of 0 – 0.5 mol/kg (Tait et al., 2012). The activity correction coefficient (f_{mono}, f_{di} and f_{tri} for monovalent, divalent and trivalent ions respectively) allows correcting ion concentrations for non-ideal aqueous phase.

In Sumo those activity coefficients are used to correct directly the dissociations constants, so that the calculated ion concentrations (in Species sheet) are directly the concentration measured by the operator, and this simplify the expressions in the equilibrium table.

As example, for water dissociation:

$$[H+]*f_{mono} * [OH-]*f_{mono} = K_W$$

Is equivalent to:

$$[H+] * [OH-] = K_W/f_{mono}^2$$

	Activity coefficients	Type(Algebraic)		
Symbol	**Name**	**Expression**	**Value**	**Unit**
A_{Davies}	Davies correction coefficient	1.82483*10^6*ρ^(0.5)*(ε*T_K)^(-1.5)	0.509	
ε	dielectric constant	2727.586+0.6224107*T_K-466.9151*Ln(T_K)-(52000.87/T_K)	78.452	
ρ	solution density	1-(T-3.9863)^2*(T+288.9414)/(508929.2*(T+68.12963))+0.0	0.997	g. cm^{-3}
IS_{lim}	IS limited for activity coefficient calculations	Min(IS; 0.3)	0.001	ISunit
f_{mono}	Monovalent activity coefficient	10^(-A_{Davies}*1^(2)*(IS_{lim}^(0.5)/(1+1.5*IS_{lim}^(0.5))-0.3*IS_{lim}))	0.966	unitless
f_{di}	Divalent activity coefficient	10^(-A_{Davies}*2^(2)*(IS_{lim}^(0.5)/(1+1.5*IS_{lim}^(0.5))-0.3*IS_{lim}))	0.869	unitless
f_{tri}	Trivalent activity coefficient	10^(-A_{Davies}*3^(2)*(IS_{lim}^(0.5)/(1+1.5*IS_{lim}^(0.5))-0.3*IS_{lim}))	0.729	unitless

	Dissociation constants - activity correction	Type(Algebraic)		
Symbol	**Name**	**Expression**	**Value**	**Unit**
K_W	Water dissociation	$K_{W,T}/f_{mono}$^2	1.08E-14	unitless
K_{C1}	Carbonate first step	$K_{C1,T}/f_{mono}$^2	4.77E-07	unitless
K_{C2}	Carbonate second step	$K_{C2,T}/f_{di}$	5.39E-11	unitless

The values for these corrections coefficients are **first calculated based on the ionic strength guess.**

Speciation calculation

Now the dissociation and activity constants are corrected based on ionic strength guess, the speciation of the components can be calculated:

[H^+] concentration is 1e-7 mol/L, k_W at 25°C is 1.08e-14, therefore

$$[OH^-] = 1e\text{-}14/1e\text{-}7 = 1.08e\text{-}7$$

pK of ammonia is 9.244, that is K_{iNH3} is 1e-9.244.

Let us take total ammonia (S_{NHx}) concentration as 1.4 mgN/L = 0.1 mmol/L = 0.0001 mol/L

[NH_3] = 0.0001 * 1e-9.244 /(1.08e-7 + 1e-9.244) = 5.64273e-7 mol/L
[NH_4^+] = 0.0001 * 1.08e-7 /(1.08e-7 + 1e-9.244) = 9.93879e-5 mol/L (that is at pH 7 most ammonia is ionized)

Those calculations can be found on the pH sheet:

	Equilibrium matrix	Type(Equilibrium)			
	Name	**[H^+]**	**[OH^-]**	**[NH_3]**	**[NH_4^+]**
$diss_{H2O}$	Dissociation of water	0.0000001	1.08E-07	0	0
ion_{amm}	Ionization of ammonia	0	0	5.64273E-07	9.93879E-05

Charge balance, ionic strength and alkalinity calculation

Knowing this speciation, the total charge balance error and the ionic strength can be calculated. On the pH sheet, the charge balance and ionic strength table contains the appropriate number of charges for the charge balance calculation, and the appropriate coefficient to calculate the ionic strength, being calculated as follow:

$$I=\frac{1}{2}\sum [i]\, z_i^2$$

where z_i is the charge of the species.

	Equilibrium matrix	Type(Equilibrium)					
Symbol	Name	$[H^+]$	$[OH^-]$	$[NH_3]$	$[NH_4^+]$	Value	Unit
$diss_{H2O}$	Dissociation of water	10^(-pH)	$K_W/[H^+]$				$mol.L^{-1}$
ion_{amm}	Ionization of ammonia			$(S_{NHx}/(AM_N*1000))*Ki_{NH3}/([H^+]+Ki_{NH3})$	$(S_{NHx}/(AM_N*1000))*[H^+]/([H^+]+Ki_{NH3})$		$mol.L^{-1}$

	Charge balance and ionic strength	Type(Chargebalance)					
Symbol	Name	$[H^+]$	$[OH^-]$	$[NH_3]$	$[NH_4^+]$	Value	Unit
chargebalance	Charge balance	1	-1	0	1	0.000099	$mol.L^{-1}$
IS_{calc}	Ionic strength	0.5*(1)^2	0.5*(-1)^2	0	0.5*(1)^2	0.000050	$mol.L^{-1}$

Charge balance calculation

The concentration of each species is multiplied by its corresponding charge, which are summed for all species to calculate the global charge balance. Here, we should have:

Charge balance: $[H^+] + [NH_4^+] = [OH^-]$

Ionic strength calculation

The concentration of each species is multiplied by its corresponding ionic strength coefficient ($0.5*z_i^2$), which are summed for all species to calculate the total ionic strength.

Alkalinity calculation

Alkalinity is essentially the amount of monovalent acid we have to add to bring the pH to the equivalence point, about pH 4.1. In this simple example it will be essentially the hydroxyl ion concentration (minus the insignificant proton concentration), adjusted by the free ammonia which will (for practical purposes) all be ionized at pH 4.
$S_{ALK} = [OH^-] + [NH_3] - [H^+]$

These calculations can be found in the Sumo models on the calculated variables tab for the complete system we deal with, plus the chemical matrix on the pH tab.

Resolution of charge balance, ionic strength and alkalinity

As described in the paragraph above, these three variables and the pH are all correlated thus all cannot be set by the user.

On the ammonia solution example, the charge balance calculation is:

$[H^+] + [NH_4^+] = [OH^-] = 1e\text{-}7 + 9.93879e\text{-}5$

This does not equal to 1.08e-7 so we have a charge balance error (charge balance = 0.000099 mol/L), the pH of a 0.1 mmol/L ammonia solution is not 7. Furthermore, the calculated ionic strength is 0.00005 mol/L, which is different from our guess (0.00001 mol/L).

The task of the Newton-Raphson solver is to solve this system, depending on the options chosen by the user (for influent only, in other process units the second case is used):

Rules	pH Specification (option available in configure mode for influents)	Input variables	Variables solved	Targets
pHSet	Input pH and alkalinity	pH S_{ALK}	$S_{CAT,NET}$ IS S_{CO2}	Chargebalanceerror IServror SCO2error
NonpHSet	Input ions and CO_2	S_{CO2} S_{CAT} S_{AN}	pH IS	Chargebalanceerror IServror

Input pH and alkalinity (pH Set)

If the pH 7 is set by the user and a low alkalinity (0.5 mg CaCO3/L) is set, then a charge balance, alkalinity and IS error means that some ions are missing in the solutions. The Newton-Raphson solver will adjust CO_2 concentration and calculate the net missing cations until all the errors are close to zero. Then the initial cation or anion concentration is adjusted with the calculated net missing cations as described in the following table:

	Cations and anions calculation revised	**Type(Equilibrium)**
Symbol	**Name**	**Expression**
S_{CAT}	Cations concentration	If((S_{CAT}_0 + $S_{CAT,NET}$) > 0; S_{CAT}_0 + $S_{CAT,NET}$; S_{CAT}_0)
S_{AN}	Anions concentration	If((S_{CAT}_0 + $S_{CAT,NET}$) > 0; S_{AN}_0; S_{AN}_0 - $S_{CAT,NET}$)

On this example the calculated S_{CO2} concentration is 0.53 g TIC.m^{-3} and the $S_{CAT,NET}$ calculated is -0.09 mmol.L^{-1} to counterbalance the ammonium. This leads to the following results:

Name	Value	Unit
IS	9.97E-05	ISunit
S_{CO2}	0.53	mg TIC/L
S_{ALK}	0.5	mg $CaCO_3$/L
S_{CAT_NET}	-0.090	mmol/L
S_{CAT}	0.00	mmol/L
S_{AN}	0.090	mmol/L
S_{NHx}	1.4	g N/m^3
[NH_4^+]	0.100	mmol/L
[NH_3]	0.00039	mmol/L
chargebalanceerror	4E-15	eq.L^{-1}
ISerror	2E-15	ISunit
SCO2error	-2E-10	mg $CaCO_3$/L

Input ions and CO_2 (NonpHSet)

All the ionic composition is defined by the user. The Newton-Raphson solver will adjust pH and IS until charge balance error and IS error are close to zero.

The actual pH, with proper molar mass of N, pK values and ionic strength correction in Sumo is 9.79 in this unbuffered solution at 20°C. This leads to the following results:

Name	Value	Unit
pH	9.79	pHunit
IS	2.89E-05	ISunit
S_{CO2}	0	mg TIC/L
S_{ALK}	5.0	mg $CaCO_3$/L
S_{CAT}	0.000	mmol/L
S_{AN}	0.000	mmol/L
S_{NHx}	1.4	g N/m^3
[NH_4^+]	0.029	mmol/L
[NH_3]	0.071	mmol/L
chargebalanceerror	-2E-13	eq.L^{-1}
ISerror	-2E-13	ISunit
SCO2error	nd	mg $CaCO_3$/L

Musvoto, E., Wentzel, M., Loewenthal, R., Ekama, G., 2000. Integrated chemical-physical processes modelling - I. Development of a kinetic-based model for mixed weak acid/base systems. Water Res. 34, 1857–1867. doi:10.1016/S0043-1354(99)00334-6

Tait, S., Solon, K., Volcke, E.I.P., Batstone, D.J., 2012. A unified approach to modelling wastewater chemistry: model corrections, in: Conference Proceedings: 3rd IWA/WEF Wastewater Treatment Modelling Seminar, WWTmod 2012. Presented at the 3rd Wastewater Treatment Modelling Seminar (WWTmod2012), pp. 51–62.

Chemical phosphorus removal with metal salts addition (iron or aluminium)

The precipitation of amorphous ferric oxide (HFO, considered to be $Fe(OH)_3(s)$ by Smith et al. (2011)) provides a number of adsorption sites for ions on its surface, which allow both adsorption and co-precipitation of ions with HFO. The model concepts are developed focusing only on phosphates adsorption and co-precipitation.

The model is based on the concept of reactive site density (named active site factor, ASF expressed as sites/mole of HFO), consisting of oxygen binding sites on HFO for which phosphate species and protons are competing. An equilibrium model, the Surface Complexation Model has already been developed on this basis by Smith et al. (2011, 2008). The total number of available sites per unit of volume (SiteT in $mol.m^{-3}$) is defined as the product of the mean number of active site factors of HFO (ASF_{HFO}) and the amount of precipitated HFO (X_{HFO} in mol $Fe.L^{-1}$). Each site has the ability to form bidentate and monodentate surface complexes with HPO_4^{2-}, $H_2PO_4^-$ and H_3PO_4 (MUSIC model, (Hiemstra and VanRiemsdijk, 1996)). Bidentate species means that phosphate species ($H_2PO_4^-$ or H_3PO_4) are bound to two sites owning two metal atoms. To keep the model simple, only one kind of phosphate (without specification of its speciation) is considered to bind onto HFO. The value of the parameter representing the number of active site factors may thus have to be adjusted compared to those used in Surface Complexation Model.

The mean number of active site factors of HFO (ASF_{HFO}) has been found to depend on mixing intensity and HFO aging (Smith et al., 2008; Szabo et al., 2008). Furthermore this equilibrium model was not designed to describe the experimental results observed by Szabo et al. (2008), such as kinetic behaviour of phosphorus removal consisting of an initial fast removal followed by slow removal, and the influence of HFO aging (loss of active surface sites). A detailed dynamic physicochemical model for chemical phosphorus removal with HFO was developed by Hauduc et al (2015). This model is based on the equilibrium model from Smith et al. (2008).

The kinetic model developed in Sumo aims to catch this dynamic behaviour, while keeping the model as simple as possible. The modelling concepts are schematically synthesized on Figure 3 and detailed in the following paragraphs for the main processes considered:

- HFO precipitation
- Phosphorus binding on HFO
- HFO aging
- Phosphorus desorption
- Phosphorus dissolution

HFO precipitation

To simplify the model, the kinetic of HFO precipitation is not considered and aluminium is considered to enter in the reactors of the treatment process directly in the form of HFO. However, the mixing conditions at the dosage point highly impact the size of the flocs. Well mixed metal dosage point will result in smaller flocs. Smaller flocs have higher active site factors, meaning a higher reactive surface compare to the size.

To represent the flocs populations, the model includes 3 flocs types:

- Active hydrous aluminium oxide, high surface (HFO,H) with an active site factor of $i_{ASF,HFO,H}$
- Active hydrous aluminium oxide, low surface (HFO,L) with an active site factor of $i_{ASF,HFO,H}$
- Aged hydrous aluminium oxide (HFO,old) with no active sites

Consequently, the split of the iron dose between the different HFO is considered in the Influent process unit code:

Symbol	Name	Expression	Unit
$X_{HFO,H}$	Active hydrous ferric oxide, high surface (HFO,H)	$G/(K_G+G)$	g $Fe.m^{-3}$
$X_{HFO,L}$	Active hydrous ferric oxide, low surface (HFO,L)	$S_{Fe}-X_{HFO,H}$	g $Fe.m^{-3}$

Table 1 Calculation of HFO,H and HFO,L in Influent process unit code (see definition of parameters in Table 2)

The concentration of active hydrous ferric oxide depends on the impact of mixing intensity, considered through the Monod-type factor: $G/(K_G+G)$, with G the average velocity gradient in mixing tank (in s^{-1}) and K_G the half saturation coefficient for G value. This factor has a value between 0 and 1 and has a value close to 1 in well mixed conditions.

The parameters for influent process units are the following:

Symbol	Name	Default	Unit
S_{Fe}_M	$Fe(OH)_3$	0.0	$mg.L^{-1}$
G	Average velocity gradient in mixing tank	50	s^{-1}
K_G	Half saturation coefficient for G value	10	s^{-1}

Table 2 Influent parameters for aluminium and flocculent dosage

Phosphorus binding on HFO

Phosphate is considered to bound on HFO. The stoichiometric coefficients of the binding processes can be found in Table 3 and Table 3 Stoichiometry of HFO aging processes (with $T_{HFO,H} = X_{HFO,H} + X_{HFO,H,P}$ and $T_{HFO,L} = X_{HFO,L} + X_{HFO,L,P}$):

Name	$XHFO_{,H}$	$XHFO_{,L}$	$XHFO_{,old}$	$XHFO_{,H,P}$	$XHFO_{,L,P}$	$XHFO_{,H,P,old}$	$XHFO_{,L,P,old}$
Aging of active HFO,H	$-\frac{X_{HFO,H}}{T_{HFO,H}}$	$\frac{X_{HFO,H}}{T_{HFO,H}}$		$-\frac{X_{HFO,H,P}}{T_{HFO,H}}$		$\frac{X_{HFO,H,P}}{T_{HFO,H}}$	
Aging of active HFO,L		$-\frac{X_{HFO,L}}{T_{HFO,L}}$	$\frac{X_{HFO,L}}{T_{HFO,L}}$		$-\frac{X_{HFO,L,P}}{T_{HFO,L}}$		$\frac{X_{HFO,L,P}}{T_{HFO,L}}$

Table 3 Stoichiometry of HFO aging processes

Table 4 with the stoichiometric parameters listed in Table 7, and the kinetic rate expression can be found in Table 6 with the kinetic parameters listed in Table 8.

The model considers the following processes:

- Fast binding of P on active HFO,H to form HFO,H,P
- Slow binding of P on active HFO,L to form HFO,L,P

The kinetic rate expressions are first order to the concentration of free binding sites and a Monod saturation term on the involved phosphorus component ensures the mathematical stability of the model.

Phosphorus desorption

Phosphorus desorption processes are used in the model to reproduce the observed equilibrium between bound and free phosphorus (Smith et al., 2011, 2008). The stoichiometric coefficient can be found in Table 4 with the stoichiometric parameters listed in Table 7, and the kinetic rate expression can be found in Table 6 with the kinetic parameters listed in Table 8. The processes are the reverse of the binding processes:

- Desorption of P on active HFO,H,P to form HFO,H and free phosphate
- Desorption of P on active HFO,L,P to form HFO,L and free phosphate

The kinetic rate expressions are first order to the concentration of each used HFO component and a Monod saturation term on the involved phosphorus component bound on HFO ensures the mathematical stability of the model.

HFO aging

As the model consider only 3 HFO types (High, Low and old). HFO flocs with or without bound phosphate are considered to have the same aging kinetic. Consequently, only 2 aging processes are required, but each includes 3 conversions:

- Fast binding of P on active HFO,H:

HFO,H => HFO,L	non-used active hydrous aluminium oxide, high surface is turned into active hydrous aluminium oxide, low surface
HFO,H,P=>HFO,H,P,old	P-bound hydrous aluminium oxide, high surface is turned into aged P-bound hydrous aluminium oxide, high surface

The kinetic rate expression is first order to the total HFO,H components ($X_{HFO,H}+X_{HFO,H,P}$)

- Slow binding of P on active HFO,L

HFO,L => HFO,old	**non-used active hydrous aluminium oxide, low surface is turned into aged unused hydrous aluminium oxide**
HFO,L,P=>HFO,L,P,old	**P-bound hydrous aluminium oxide, low surface is turned into aged P-bound hydrous aluminium oxide, low surface**

The kinetic rate expression is first order to the total HFO,L components ($X_{HFO,L}+X_{HFO,L,P}$)

Aged used hydrous aluminium oxide are considered inert, meaning that the phosphorus is definitely entrapped in the floc structure, except for HFO,H,P,old and HFO,L,P,old in the phosphorus dissolution process (see next paragraph) for a mathematical purpose.

The stoichiometric coefficient can be found in Table 3 with the stoichiometric parameters listed in Table 7, and the kinetic rate expression can be found in Table 6 with the kinetic parameters listed in Table 8.

Phosphorus dissolution

The phosphorus dissolution process is included in the model to ensure that phosphate will never be depleted for biomass growth. It ensures that below a free phosphate concentration, any bound phosphate on aged HFO will be released, as this bound phosphate cannot be desorbed. The kinetic rate expression is then first order to the total phosphate bound on aged HFO ($X_{HFO,H,P,old}$+$X_{HFO,L,P,old}$) and the switch on/off of this process is managed through a logarithm saturation expression that depends on the soluble phosphate concentration.

The stoichiometric coefficient can be found in Table 5 with the stoichiometric parameters listed in Table 7, and the kinetic rate expression can be found in Table 6 with the kinetic parameters listed in Table 8.

Name	S_{PO4}	$X_{HFO,H}$	$X_{HFO,L}$	$X_{HFO,H,P}$	$X_{HFO,L,P}$
Fast binding of P on active HFO,H	-1	$-\frac{1}{ASF_{HFO,H} * \left(\frac{AM_P}{AM_{Fe}}\right)}$		$\frac{1}{ASF_{HAO,H} * \left(\frac{AM_P}{AM_{Al}}\right)}$	
Slow binding of P on active HFO,L	-1		$-\frac{1}{ASF_{HFO,L} * \left(\frac{AM_P}{AM_{Fe}}\right)}$		$\frac{1}{ASF_{HFO,L} * \left(\frac{AM_P}{AM_{Fe}}\right)}$
Desorption of P from $X_{HFO,H,P}$	$ASF_{HFO,H} \times \frac{AM_P}{AM_{Fe}}$	1		-1	
Desorption of P from $X_{HFO,L,P}$	$ASF_{HFO,L} \times \frac{AM_P}{AM_{Fe}}$		1		-1

Table 4 Stoichiometry of phosphate binding and desorption on HFO

Name	S_{PO4}	$X_{HFO,old}$	$X_{HFO,H,P,old}$	$X_{HFO,L,P,old}$
Dissolution of P from $X_{HFO,H,P,old}$ and $X_{HFO,L,P,old}$	$ASF_{HFO,H} \times \frac{AM_P}{AM_{Fe}} \times \frac{X_{HFO,H,P,old}}{X_{HFO,H,P,old} + X_{HFO,L,P,old}}$ $+ASF_{HFO,L} \times \frac{AM_P}{AM_{Fe}} \times \frac{X_{HFO,L,P,old}}{X_{HFO,H,P,old} + X_{HFO,L,P,old}}$	1	$\frac{-X_{HFO,H,P,old}}{X_{HFO,H,P,old} + X_{HFO,L,P,old}}$	$\frac{-X_{HFO,L,P,old}}{X_{HFO,H,P,old} + X_{HFO,L,P,old}}$

Table 5 Stoichiometry of bound phosphorus dissolution

Name	Rate
Aging of active HFO,H	$q_{HFOH,AGING}$ *($X_{HFO,H}$+$X_{HFO,H,P}$)
Aging of active HFO,L	$q_{HFOL,AGING}$ *($X_{HFO,L}$+$X_{HFO,L,P}$)
Fast binding of P on active HFO,H	$q_{P,HFO,P,COPREC}$*$X_{HFO,H}$*$Msat_{SPO4,KP,HFO,BIND}$
Slow binding of P on active HFO,L	$q_{P,HFO,P,BIND}$*$X_{HFO,L}$*$Msat_{SPO4,KP,HFO,BIND}$
Desorption of P from $X_{HFO,H,P}$	$q_{HFOH,DESORP}$*$X_{HFO,H,P}$*$Minh_{SPO4,KiP,HFO,DESORP}$
Desorption of P from $X_{HFO,L,P}$	$q_{HFOL,DESORP}$*$X_{HFO,L,P}$*$Minh_{SPO4,KiP,HFO,DESORP}$
Dissolution of P from $X_{HFO,H,P,old}$ and $X_{HFO,L,P,old}$	$q_{HFO,DISS}$*($X_{HFO,H,P,old}$+$X_{HFO,L,P,old}$)*$Loginh_{SPO4,KiP,HFO,DISS}$

Table 6 Kinetic rate expressions for HFO processes

Symbol	Name	Default	Unit
$ASF_{HFO,H}$	Active site factor for HFO,H	1.2	mol P.mol Fe^{-1}
$ASF_{HFO,L}$	Active site factor for HFO,L	0.2	mol P.mol Fe^{-1}

Table 7 HFO stoichiometric parameters

Symbol	Name	Default	Unit
$q_{HFOH,AGING}$	Rate of $X_{HFO,H}$ aging	250	d^{-1}
$q_{HFOL,AGING}$	Rate of $X_{HFO,L}$ aging	1.00	d^{-1}
$q_{P,HFO,P,COPREC}$	Rate of P binding and coprecipitation on $X_{HFO,H}$	150	d^{-1}
$q_{P,HFO,P,BIND}$	Rate of P binding on $X_{HFO,L}$	1.00	d^{-1}
$q_{HFOH,DESORP}$	Rate of $X_{HFO,H,P}$ desorption	100	d^{-1}
$q_{HFOL,DESORP}$	Rate of $X_{HFO,L,P}$ desorption	10	d^{-1}
$q_{HFO,DISS}$	Rate of $X_{HFO,H,P,old}$ and $X_{HFO,L,P,old}$ redissolution	100	d^{-1}
$K_{P,HFO,BIND}$	Half-saturation of PO_4 for binding on HFO	0.10	g $P.m^{-3}$
$Ki_{P,HFO,DISS}$	Half-inhibition of PO_4 in HFO redissolution	0.01	g $P.m^{-3}$
$Ki_{P,HFO,DESORP}$	Half-inhibition of PO_4 in HFO desorption	0.100	g $P.m^{-3}$

Table 8 HFO kinetic parameters

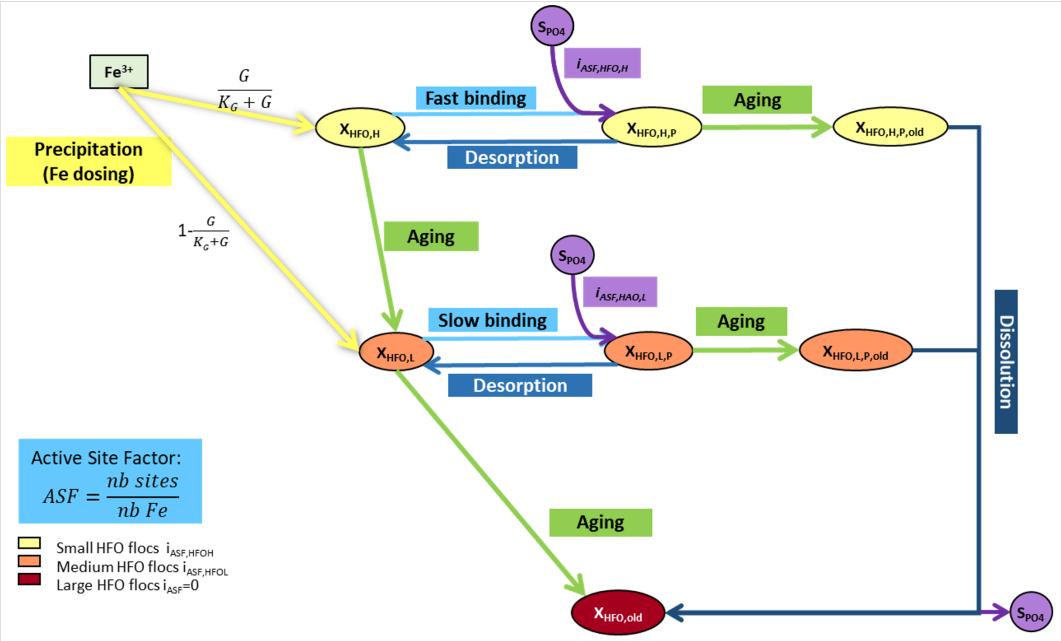


Figure 2.3 Chemical phosphorus removal modelling concept in Sumo

Hauduc, H., Takács, I., Smith, S., Szabo, A., Murthy, S., Daigger, G.T., Spérandio, M., 2015. A dynamic physicochemical model for chemical phosphorus removal. Water Res. 73, 157–170. https://doi.org/10.1016/j.watres.2014.12.053

Hiemstra, T., VanRiemsdijk, W.H., 1996. A surface structural approach to ion adsorption: The charge distribution (CD) model. J. Colloid Interface Sci. 179, 488–508. https://doi.org/10.1006/jcis.1996.0242

Smith, S., Gray, H., Neethling, J.B., 2011. Surface Complexation Modelling and Aluminum Mediated Phosphorus White Paper | IWA Publishing [WWW Document]. URL https://www.iwapublishing.com/books/9781780406848/surface-complexation-modelling-and-aluminum-mediated-phosphorus-%13-white-paper *(accessed 2.26.19).*

Smith, S., Takács, I., Murthy, S., Daigger, G.T., Szabo, A., 2008. Phosphate complexation model and its implications for chemical phosphorus removal. Water Environ. Res. 80, 428–438.

Szabo, A., Takács, I., Murthy, S., Daigger, G.T., Licsko, I., Smith, S., 2008. Significance of design and operational variables in chemical phosphorus removal. Water Environ. Res. 80, 407–416. https://doi.org/10.2175/106143008X268498

Chemical precipitation reactions

Six precipitates are implemented in Sumo models (Iron sulfide only available in Sumo2S).

Symbol	Name	Formula
X_{CaCO3}	Calcium carbonate ($CaCO_3$)	$CaCO_3$
X_{STR}	Struvite (STR)	$MgNH_4PO_4 * 6H_2O$
X_{BSH}	Brushite	$CaHPO_4 * 2H_2O$
X_{ACP}	Amorphous calcium phosphate (ACP)	$Ca_3(PO_4)_2 * 4H_2O$
X_{Vivi}	Vivianite (Vivi)	$Fe_3(PO_4)_2 * 8H_2O$
X_{FeS}	Iron sulfide (FeS) (only in Sumo2S)	FeS

To predict precipitation, the kinetic rate expression from Musvoto *et al.* (2000) is used: it depends on a kinetic parameter q_{PREC} and on a driving force that characterizes the deviation from the thermodynamic equilibrium. Mathematically, the driving force is the difference between the ionic product and the solubility constant. The solubility constant is corrected in Sumo for ionic activity, thus the ionic strength effect is modelled.

$$DrivingForce = \underbrace{\left[Mg^{2+}\right]^{\frac{1}{3}} \times \left[{PO_4}^{3-}\right]^{\frac{1}{3}} \times \left[{NH_4}^{+}\right]^{\frac{1}{3}}}_{\text{ionic product}} - \underbrace{{K_{sp,STR}}^{\frac{1}{3}}}_{\text{solubility constant}}$$

Musvoto, E., Wentzel, M., Loewenthal, R., Ekama, G., 2000. Integrated chemical-physical processes modelling - I. Development of a kinetic-based model for mixed weak acid/base systems. Water Res. 34, 1857e1867. http://dx.doi.org/10.1016/S0043-1354(99)00334-6 .

Influent characterization

You find answers to the question: How to translate influent measurement into model fractions?

Introduction

Understanding the influent composition of a wastewater treatment plant is one of the most important tasks for an engineer. This directly impacts the design of a treatment plant and ability to simulate a plant performance using an activated sludge model. The characterization of wastewater is done by either measuring and/or identifying the carbonaceous, nitrogen containing components, and phosphorus containing components in soluble, colloidal, and particulate fractions and their biodegradable and unbiodegradable portions. Distinguishing influent content based on biodegradable and unbiodegradable COD is important to know the mass flow of biodegradable material to a plant which can be essential in calculating carbonaceous oxygen demand at a given sludge retention time.

Model options

There are three influent types model selection options, concentration, mass flow, and state variable. The concentration and mass based have an option of selecting a COD-based, or BOD-based input. Except for state variable based all other rely on specifying the fractions as an input.

Model inputs

Fraction of VSS/TSS

Calculates the inert inorganic solids in the wastewater. Changing this directly impacts the mixed liquor concentration.

Fraction of filtered COD (SCCOD, 1.5 µm, incl. colloids) in total COD

Calculates the filtered COD of wastewater. This contains a sum of colloidal and soluble organics.

Fraction of flocculated filtered (SCOD, without colloids) COD in total COD

This fraction contains only soluble COD, after colloidal material is removed, both biodegradable and unbiodegradable. This fraction is always equal to or smaller than the Fraction of filtered COD. The difference between the two fractions calculates the colloidal organics present in wastewater.

Fraction of VFA in filtered COD (SCCOD, 1.5 µm, incl. colloids)

Calculates the amount of VFA in the influent. Important for designing and predicting and biological P removal plants.

Fraction of soluble unbiodegradable organics (S_U) in filtered COD (SCCOD, 1.5 µm, incl. colloids)

Calculates the soluble organics COD from the filtered COD. This fraction is not impacted by biological processes and the mass entering leaves a process at steady state conditions. This COD leaves with the effluent discharge. This number is typically identified after performing a filtered COD measurement on the effluent of a plant with minimum of 3 days of SRT.

Fraction of particulate unbiodegradable organics (X_U) in total COD

Calculates the unbiodegradable particulates from the total COD. This fraction is not impacted by biological processes and the mass entering leaves a process at steady state conditions. This COD gets enmeshed in the sludge and accumulates in the system until a process reaches steady state and then the mass of XU leaving the system is the mass of XU entering the system. A major portion of XU leave the plant through solids wasting or sludge disposal. This value will control MLSS concentration (more so when the SRT is high, so MLSS is more sensitive to XU fraction as the SRT increases) in the aeration tanks and digester performance. The XU can be calculated by subtracting SU and all the biodegradable COD from the influent total COD measurement. Measuring XU is more difficult – a 6-week SBR test is recommended.

Fraction of heterotrophs (X_{OHO}) in total COD

This fraction of biomass associated with Total COD and is essential when simulating processes with sludge retention time of less than 3 days. Also, when simulating primary fermentation, it is important to estimate or measure this fraction accurately.

Fraction of endogenous products (X_E) of OHOs

This is the decay product of OHOs in the influent and have minimal impact on the performance of the process – it mostly behaves as unbiodegradable material and will show up in the sludge wastage.

Fraction of colloidal unbiodegradable organics (C_U) in colloidal COD

This fraction calculates the colloidal unbiodegradable COD from the difference between SCCOD and SCOD.

Fraction of NHx in total Kjeldahl nitrogen (TKN)

Calculates ammonia concentration, ammonia is important for growth of biomass, and it is converted to nitrite and/or nitrate.

Fraction of PO4 in total phosphorus (T_P)

Calculates the orthophosphate (OP) concentration of wastewater, very essential for growth of biomass.

Fraction of N in readily biodegradable substrate (S_B)

Calculated the soluble organic nitrogen that will undergo ammonification to release ammonia. Ammonification usually completes when the SRT is more than 3 days.

Fraction of N in particulate unbiodegradable substrate (X_U)

The unbiodegradable portion of particulate organic nitrogen remains unchanged in the system and leaves a plant with sludge disposal

Fraction of P in readily biodegradable substrate (S_B)

Portion of P that is bound to the soluble organics, these organics release OP during the treatment process.

Fraction of P in particulate unbiodegradable substrate (X_U)

Portion of P bound to the unbiodegradable organics and remain unchanged in the system, they leave with the sludge disposal or wasting.

Important variables that are calculated from the inputs

Using the above inputs, the influent PU model calculates the following important state variables:

Soluble biodegradable organics (S_B)

This variable is metabolized at an extremely fast rate and contribute to high oxygen uptake rate; it represents the non-VFA organics. The is an important variable to know for getting oxygen uptake rate, denitrification, and biological P performance correctly.

Particulate biodegradable organics (X_B)

This variable is first hydrolysed or broken down by extracellular enzymes into SB and then metabolized. This means that the oxygen uptake rate or rate of metabolization of XB is limited by the rate of hydrolysis, which is much slower than the rate of SB metabolism. Under long SRTs (longer than 3 days), the XB fraction compared to MLSS is small in the treatment system.

Particulate biodegradable organic nitrogen ($X_{N,B}$)

This variable undergoes hydrolysis to form soluble biodegradable organic nitrogen and then ammonification to release ammonia. When designing for complete nitrification and estimating the alkalinity demand it is important to take biodegradable TKN which is a sum of ammonia, and the particulate and soluble biodegradable organic nitrogen, into consideration. This variable is essential in simulating ammonia release in the anaerobic digesters.

Particulate biodegradable organic phosphorus ($X_{P,B}$)

This variable undergoes hydrolysis to for soluble biodegradable organic phosphorus and then releases P. When designing for P removal, it is essential to take biodegradable TP which is a sum of ortho-P, and the particulate and soluble biodegradable organic phosphorus, into consideration. This variable is essential in simulating phosphorus release in the anaerobic digesters and certain precipitate formation.

Colloidal biodegradable organics (C_B)

This variable is first flocculated to particulate X_B, then hydrolysed into SB and then metabolized. These are important when simulating primary clarifier performance or a process with SRT of less than 3 days.

Other influent characterization parameters

The maximum specific growth rate constant of nitrifying organisms and/ammonia oxidizing organisms can vary greatly with different municipal wastewater especially when a portion of wastewater contains industrial flow. This is true especially for systems with one stage BOD-nitrification process, in such systems the growth rate of nitrifiers must be considered. Correctly knowing the nitrification rate can be significant in design and operation optimization. A high nitrification rate can mean shorter SRTs meaning saving on aeration and tank volume.

How to estimate the fractions for model input?

These fractions or variables are not directly measured on regular basis at a plant. Certain plants might dive into specific measurements, such as VFA measurement might be necessary, and done more occasionally by plants doing biological P removal. Most of the plants will measure TSS, VSS, BOD, TCOD, SCOD, Ammonia, OP, TKN, and TP in their influent and may be some in the effluent as well. Sumo provides a tool that can be used to estimate the fractions to the influent model using these measured data.

How to fractionate?
Checks to matching your influent measurement and calibration

Check 1: How to screen for bad data?

The following states conditions always has to be kept:

- NH_x can never be more TKN
- OP can never be more than TP
- Filtered COD can never be more than TCOD
- Filtered flocculated COD can never be more than filtered COD
- VSS can never be more than TSS
- VFA can never be more than Filtered COD

- COD/BOD, NH_3/TKN, VSS/TSS and other fractions, although can vary, should show some consistency in a large dataset.

Check 2: What to use if you have a lot of data?

Are you using monthly or yearly average measurements for inputs?

- NH_x to TKN fraction or OP to TP or VFA concentration can change from season to season.
- Divide data into reasonable period to simulate, winter and summer

Comparing my data to usual values in US are different, why?

- Look at trends of past data and compare certain ratios, is there an outlier?
- For example, typically COD/BOD ratio 2.2, for my plant its 1.5, historical trend shows 2 to 2.5. Look to see if BOD or COD is incorrect and eliminate the outlier.

Check 3: Avoid negative balances

Negative balance means that TKN or TP is not enough to be distributed between ammonia or OP and other organics. Could be measurement issue (adjust the ammonia/TKN or OP/TP concentration based on historic data), or highly soluble wastewater. Reduce N and P fractions to balance N and P if the NHx and OP measurement is deemed reliable.

- Fraction of N in readily biodegradable substrate (S_B)
- Fraction of N in particulate unbiodegradable substrate (X_U)
- Fraction of P in readily biodegradable substrate (S_B)
- Fraction of P in particulate unbiodegradable substrate (X_U)

Check 4: Reproduce VSS and BOD based on Influent tool

This can be done by adjusting X_{OHO}, X_U, and C_U fractions:

- Increase X_U to decrease BOD and reduce VSS
- If BOD matches but not the VSS, adjust X_{OHO} fraction.
- Decrease C_U fraction to increase BOD, this will have a small impact on VSS. In wastewaters where VSS and BOD cannot be reproduced, changing the colloidal fraction is recommended.

Check 5: Adjust the particulate substrate (X_B) COD/VSS ratio to match VSS

This fraction can change based on the composition of the influent for instance:

Carbohydrates: 1.07 g COD/g VSS

Proteins: 1.53 g COD/g VSS

Lipids: 2.92 g COD/g VSS

Other fractions are relatively constant, do not change, such as:

Biomass: 1.42 g COD/g VSS

Influent model calibration

This is done by performing preliminary simulations of the plant.

Calibrating nitrogen content of unbiodegradable organics to predict effluent TKN

Typically, a completely nitrifying plant especially a BNR plant will have very low effluent ammonia concentration. So, majority of effluent TKN is particulate and soluble organic nitrogen. The concentration of particulate organic nitrogen is decided by the removal efficiency of the secondary clarifier by matching the total suspended solids. However, in most cases soluble organic nitrogen associated with the unbiodegradable portion of COD contributes significantly to the TKN measurement. Here we take into consideration **the N content of the soluble unbiodegradable COD**. This parameter can be adjusted to match effluent TKN.

Calibrating organic nitrogen either as soluble or particulate to predict nitrate concentration in effluent

Nutrient load to a plant dictates its performance, when a plant has primary clarification then the primary effluent load to its biological treatment must be well reproduced. Apart from getting the primary effluent ammonia and TSS correct, it is important to match the TKN concentration and the composition. As the biodegradable particulate organic nitrogen get captured in the primary, they will not show up as nitrate in your effluent, because particulate get waste through sludge. So, it is important to look at the composition of the organic nitrogen, more biodegradable soluble organic nitrogen will mean high nitrate.

Industrial wastewater characterization

The activated sludge models are mechanistically sound for application on industrial wastewater treatment and provide a good basis for evaluation of certain industrial wastewaters, especially food processing.

- Industrial inputs can contain P precipitating chemicals, resulting in a higher inorganically bound P content.
- For municipal wastewater effluent, colloidal concentration is almost negligible if a plant's SRT is > 3 days. However, industrial wastewater effluent might contain high colloidal concentration that might not be easily absorbed during the treatment. It becomes essential to measure filtered and flocculated filtered COD to estimate the correct fraction.
- Due to high strength of the industrial wastewater there might be a much higher effluent unbiodegradable soluble COD compared to municipal wastewater.
- Physico-chemical evaluation of industrial wastewater in some cases might not be possible due to highly soluble nature of the wastewater and the soluble portion may contain many compounds with distinctive microbial degradation rates. In such cases, OUR tests, anoxic batch testing, and SBR based tests can be especially useful.

- Industrial inputs can be toxic or inhibitory to nitrifying organisms. Toxic – when the decay rate is impacted and needs to be increased, inhibitory – when the growth rate is more impacted and needs to be decreased. So, evaluating the inhibition of influent on nitrifying sludge can be especially useful. See nitrification denitrification document.
- Wastewater from meat industry can contain a high concentration of nitrogen containing colloidal material both biodegradable and unbiodegradable.
- Wastewater from dairy industry is highly biodegradable and input influent fractions can differ from municipal wastewater especially, the readily biodegradable COD can be more than double the fraction found in municipal wastewater, lower unbiodegradable soluble fraction, and a high fraction of ortho-phosphate.

Process units in Sumo

List of available process units in Sumo with a short description

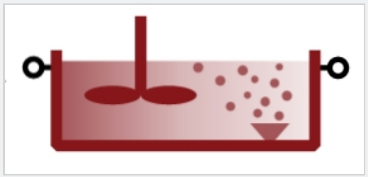
Introduction

The following page gives list of the available process units in Sumo with a short description of their features.

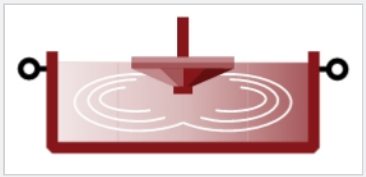
Process units

Bioreactors

CSTR



diffused aeration



mechanical aeration

Continuously Stirred Tank Reactor with constant volume and ideally mixed concentration.

Sumo offers two types of CSTRs: *mainstream* (with kinetic parameters preset for the liquid train) and *sidestream* (adapted to suit better for sludge train applications). The CSTR can also be switched to be non-reactive for specific modeling purposes. There are further options available regarding the aeration process:

Aeration options:

- *diffused* (with various built-in diffuser system specifications)
- *mechanical*

Dissolved oxygen handling:

- *input DO* (air flow requirement is calculated based on proper gas transfer)
- *calculated DO* (DO is calculated based on input air flow and proper gas transfer description)

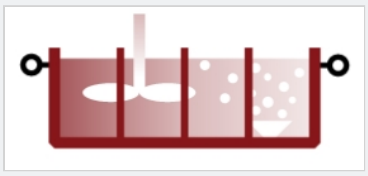
Alpha factor options:

- *predicted alpha* (based on a correlation with TSS, therefore dynamically changing)

- *input alpha* (user-provided fixed value)

A simplified CSTR model is available for Museum models.

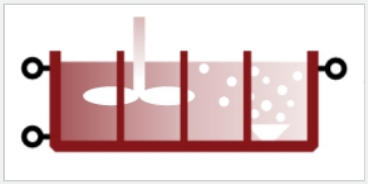
PFR segment



Plug Flow Reactor with constant volume and ideally mixed concentration in the individual segments.

This type of bioreactor is available for *mainstream* applications and can be used to simplify the layout by representing a number of CSTRs connected in series. The aeration related options are the same as for CSTRs (except for mechanical aeration, which is not available). Influent or RAS split, as well as internal recirculation between the segments is not available in this model (for such applications, use the PFR process unit instead).

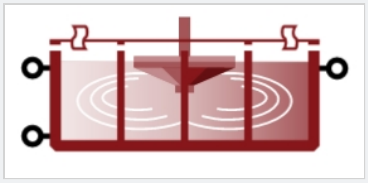
PFR



Plug Flow Reactor with constant volume and ideally mixed concentration in the individual segments, with influent/RAS split and internal recycle.

This type of bioreactor is available for both *mainstream* and *sidestream* applications and can be used to simplify the layout by representing a number of CSTRs connected in series. In addition to the basic PFR segment model, this bioreactor can be configured for step feed (influent split), multiple internal recirculation pathways, as well as RAS split from the individual segments. The aeration related options are the same as for CSTRs (except for mechanical aeration, which is not available).

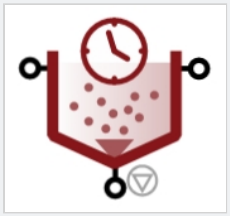
HPO



Plug Flow Reactor aerated using high purity oxygen, with step feed option.

This model represents a series of closed *mainstream* CSTRs mechanically aerated with high purity oxygen. Influent split is available for modeling step feed, RAS split and internal recycling are not offered. Aeration related options regarding DO handling and alpha factor are alike to CSTRs.

SBR



Sequencing Batch Reactor with various setup possibilities regarding the cycle of timed phases and tank structure for settling.

The SBR reactor is available for both *mainstream* and *sidestream* applications and can be set up to represent different configurations, such as:

Typical SBR cycle:

Featuring a fixed order of timed phases such as reaction, settling, decanting and wasting (idle phase is available as well). The tank is considered ideally mixed in the reaction phase. Decanting and sludge wasted is calculated with TSS concentration as setpoint.

- with *calculated DO*: DO is calculated based on input air flow and proper gas transfer
- with *input DO*: DO is set and input air flow requirement is calculated based on proper gas transfer description

Flexible SBR cycle:

Featuring a flexible order of timed phases such as reaction, settling, decanting and wasting; based on user setup. The tank is considered ideally mixed in the reaction phase. Decanting and sludge wasted is calculated with TSS concentration as setpoint.

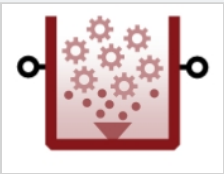
- with *calculated DO*: DO is calculated based on input air flow and proper gas transfer
- With *input DO*: DO is set and input air flow requirement is calculated based on proper gas transfer description

Layered SBR with calculated DO:

Multiple layered tanks where mixing, settling and aeration is calculated according to the phase of the cycle. The settling model is identical to the 1D layered clarifier model. Available for *typical* and *flexible* cycle configurations as well but restricted to *calculated DO* handling.

For more details, please refer to the Process unit descriptions page.

MBBR



Moving Bed BioReactor with ideally mixed bulk phase and conservative media using the SumoBioFilm model with fixed film thickness.

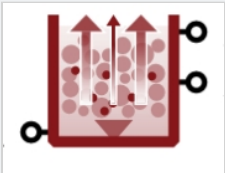
The media is described with its specific surface and volume fill ratio, specified by the type of the media used in the system. The biofilm is distributed into layers and diffusion, internal solid transfer, displacement, attachment, and detachment is calculated as transport processes between the layers and between the outer layer and the bulk phase. The latter is considered ideally mixed (alike to a CSTR). Aeration is restricted to diffuser systems, alpha factor can be *predicted* or *input*, identically to the CSTR model.

DO control options:

- *Calculated DO* (DO is calculated based on input air flow by proper gas transfer description)
- *DO controlled in bulk* (DO is set and input air flow requirement is calculated based on proper gas transfer description)

A simplified MBBR model is available for Museum models (in this case, DO is set in bulk phase, as aeration is not modeled).

BAF



Upflow Biological Aerated Filter using the SumoBioFilm model with fixed film thickness.

This bioreactor is an upflow biological filter with two vertical biofilm reactor zones, aerated either in the bottom (resulting in a fully aerated configuration) or at mid height (denitrifying configuration). Aeration is diffused, alpha factor can be *predicted* or *input*, identically to the CSTR model.

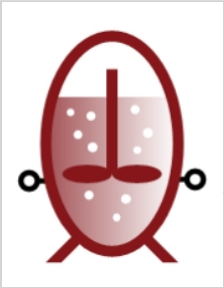
DO control options:

- *Calculated DO* (DO is calculated based on input air flow by proper gas transfer description)
- *DO controlled in bulk* (DO is set and input air flow requirement is calculated based on proper gas transfer description)

Backwash is simulated as a continuous process flow.

For more details, please refer to the Process unit descriptions page.

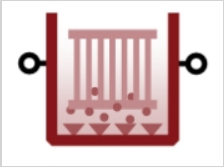
Digester



Ideally mixed closed tank with fixed gas volume above the sludge and proper gas transfer calculations.

This unaerated bioreactor can be used for modeling anaerobic sludge stabilization or fermentation processes.

MABR



Membrane Aerated Biofilm Reactor using the SumoBioFilm model with fixed film thickness.

The membrane aerated biofilm reactor model offers three options for oxygen transfer through the membrane:

- variable O_2 transfer
- fixed O_2 transfer
- fixed air flow transfer

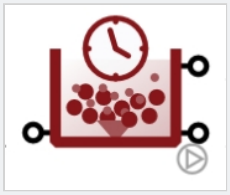
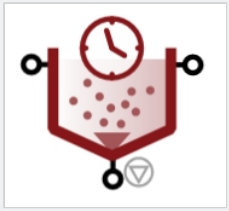
The biofilm is distributed into layers and diffusion, internal solid transfer, displacement, attachment and detachment is calculated as transport processes between the layers and between the outer layer and the bulk phase.

Diffused aeration is available in the bulk phase, with the following DO control options:

- *Calculated DO* (DO is calculated based on input air flow by proper gas transfer description)
- *DO controlled in bulk* (DO is set and input air flow requirement is calculated based on proper gas transfer description)

The alpha factor can be *predicted* or *input*, identically to the CSTR model.

Granular SBR

Sequencing batch reactor with ideally mixed bulk phase and granular biofilm extension (fixed film thickness).

The biofilm on the surface of the granules is distributed into layers and diffusion, internal solid transfer, displacement, attachment and detachment is calculated as transport processes between the layers and between the outer layer and the bulk phase.

Two modes of SBR operation are offered:

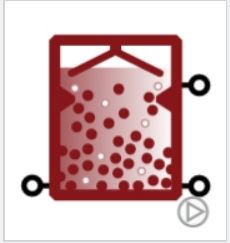
- *Conventional SBR* (feeding into the mixed tank during reaction phase)
- *Aerobic Granular Sludge reactor* (feeding to the bottom during decanting phase)

Diffused aeration is available in the bulk phase, with the following DO control options:

- *Calculated DO* (DO is calculated based on input air flow by proper gas transfer description)
- *DO controlled in bulk* (DO is set and input air flow requirement is calculated based on proper gas transfer description)

The alpha factor can be *predicted* or *input*, identically to the CSTR model.

UASB



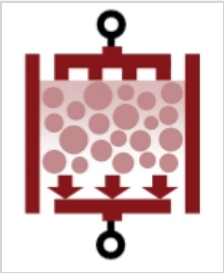
Upflow Anaerobic Sludge Blanket reactor (built upon the anaerobic digester model).

The UASB model in Sumo was developed in two versions with different complexity levels:

- Simple (completely mixed approach)
- Three compartment (for modeling stratification)

For more details, please refer to the Process unit descriptions page.

Trickling filter



Trickling filter using SumoBioFilm with fixed film thickness and controlled DO transfer.

Trickling filter is a complex process unit. The whole volume is divided the filter into top, middle and bottom sections and using the effluent of the top as influent of the lower units. The media is described with the specific surface and volume fill ratio specified by the type of the media used in the system.

The biofilm is distributed into layers whereas diffusion, internal solid transfer, displacement, attachment and detachment is calculated as transport processes between the layers and between the outer layer and the bulk phase. The bulk phase volume is negligible from the biological activity point of view.

MBR

Membrane BioReactor with fixed or variable volume and ideally mixed concentration.

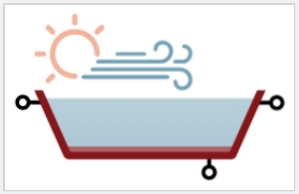
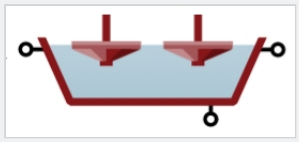
The membrane bioreactor model consists of a constant or variable volume aerated reactor (with coarse diffuse aeration system) and an ideal point separator with user-specified effluent solids concentration.

Dissolved oxygen handling:

- *input DO* (air flow requirement is calculated based on proper gas transfer)
- *calculated DO* (DO is calculated based on input air flow and proper gas transfer description)

For variable reactor volume, only the *calculated DO* option is available. The alpha factor can be *predicted* or *input*, just like in the CSTR model.

Pond

 Gen3 model	 Gen2 model / diffused aeration	 Gen2 model / mechanical aeration	**Pond/lagoon with variable volume sludge and water subcompartments.**

The pond/lagoon model is available in two levels of complexity. The Gen2 model can be aerated mechanically or with a diffuser system and does not consider heat balance or algae growth. The Gen3 model considers the latter two and features mechanical aeration. Detailed description of these models can be found in the Process unit descriptions chapter.

Flow elements

Influent

The influent represents the incoming sewage flow to the plant. In this process unit we define the composition of the incoming wastewater based on COD (preferred method, as mass balance can be performed on this basis) or BOD. Three types of influent specification are offered by Sumo:

- *Concentration based* (specify concentrations of a few key components combined with influent fractions)
- *Mass flow based* (specify mass flows of a few key components combined with influent fractions)
- *State variable based* (specify the concentration of every state variable)

Most often the *concentration based* option is used (also being the default choice). For this type of influent, a handy **Influent tool** is provided as guidance on setting the proper influent fractions, based on available lab data and common values in the US. The *mass flow based* option might be better suited for specific applications, while the *state variable based* option comes handy e.g. when simulation results from one modeled plant are to be transferred to another plant model.

If pH is considered for the modeling, the pH specification can be done by following approaches:

- Input pH and alkalinity
- Input cations and CO_2

Primary effluent

Similar to the influent process unit, but representing effluent from primary settlers. The specification options are identical to the influent and a dedicated **Primary effleunt tool** is also available.

Carbon dose

The carbon unit can be used to dose three types of carbon sources:

- Methanol
- Volatile fatty acids (VFA)
- Readily biodegradable substrate (non-VFA)

The dosage type can be concentration or mass flow.

Metal dose

The metal unit can be used to dose the following metal salts:

- $AlCl_3$
- $Al_2(SO_4)_3$
- $FeCl_2$
- $FeCl_3$
- $FeSO_4$
- $Fe_2(SO_4)_3$

The metal dose inputs can be provided based on the following options:

- concentration based (flow rate is input, m^3/d)
- mass flow based (mass flow is input, kg/d)

For the above options the concentration of the chemical is an input. The following choices are available

- Concentration of dosed element (g element/m^3)
- Concentration of salt (g component/m^3)
- % by mass of salt and liquid density (% by mass and kg/m^3 of solution)

Any combination of the above can be used.

An empirical metal dosage option is available for the ASM2D Museum model.

Chemicals

The chemicals unit can be used to dose the following chemicals:

- Caustic
- Ammonium bicarbonate
- Calcium chloride
- Calcium hydroxide
- Magnesium chloride
- Magnesium hydroxide
- Nitric acid
- Phosphoric acid
- Potassium nitrate
- Potassium nitrite
- Sodium bicarbonate
- Sodium carbonate
- Sulfuric acid

The chemical dose inputs can be provided based on the following options:

- concentration based (flow rate is input, m^3/d)
- mass flow based (mass flow is input, kg/d)

For the above options the concentration of the chemical is an input. The following choices are available

- Concentration of dosed element (g element/m^3)
- Concentration of salt (g component/m^3)
- % by mass of salt and liquid density (% by mass and kg/m^3 of solution)

Any combination of the above can be used.

Water

Specific process unit to represent clean washwater inputs on the drawing board. State variables are set to non-detect values, while the alpha factor is set to 1. Component concentrations can be customized, nevertheless.

Effluent

Specific process unit to represent effluent flow leaving the plant. There are no specifications for this unit as it is used solely for reporting results.

Sludge

Specific process unit to represent sludge flow leaving the plant. Four types of sludges can be specified, the choice will only have effect on the operational cost estimations (via disposal fees):

- Screening
- Grit
- Grease
- Sludge

Product

Specific process unit to represent marketable product flow (i.e. from P recovery) leaving the plant. There are no specifications for this unit as it is used solely for reporting results.

Sludge feed

Specific process unit to represent sludge input flows when only the sludge treatment is the aim of the modeling. Four types of sludge can be specified:

- Thickened primary
- Thickened waste activated sludge
- Food waste
- Thickened primary and waste activated sludge

In the case of *food waste*, five additional types can be specified:

- Organic fraction of municipal
- Meat-rich
- Dairy-rich
- Fruit and sugar rich
- Vegetable rich

Typical concentrations and influent fractions are preconfigured according to the choices made.

Dividers

In most cases, the plant layout employs flow dividers. Sumo offers two geometric variants for these, with the same underlying model:

- Side flow divider
- T flow divider

The flow split between the two outgoing pipes can be specified as:

- *pumped*: a fixed pumped flow is routed to one pipe (denoted by pump sign), while the remaining (if any) is routed to the other pipe (denoted by grey arrow)
- *proportional*: a fixed fraction of the incoming flow is routed to one pipe (denoted by pump sign and red arrow), while the remaining is routed to the other pipe (denoted by grey arrow)

The operation of the dividers can be specified as:

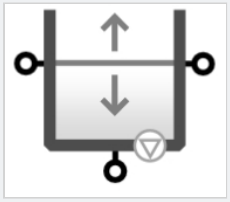
- continuous (*pump cycling Off*)
- cyclic (*pump cycling On*)

Combiners

In most cases, the plant layout employs flow combiners. Sumo offers three geometric variants for these, with the same underlying model:

- Side flow combiner (adjoining two incoming flows arriving from prependicular pipes)
- T flow combiner (adjoining two incoming flows arriving from two pipes facing each other)
- Multi flow combiner (adjoining three incoming flows)

Equalization basin

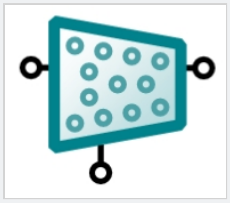


Variable volume tank with ideally mixed concentration, featuring pumped output and overflow for flow balancing.

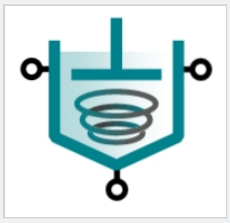
This process unit can be set up to be *reactive* or *non-reactive* (note that the latter is the default setting). In most aspects it behaves - and can be configured - just like a CSTR, apart from the DO handling (which is always calculated) and the flow dynamics (the EQ tank has a fixed pumped output flow and overflows if the predefined volume is exceeded).

Separators

Screen

	**Mass balance based volumeless point separator model with specified percent solids removal and underflow solids concentration.**

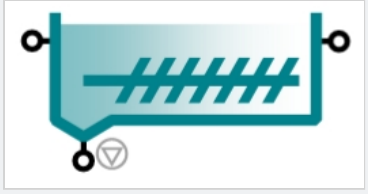
Grit chamber

	**Mass balance based volumeless point separator model (vortex grit chamber) with specified input VSS increment or removed grit mass.**

Grease trap

	**Mass balance based volumeless point separator model with specified percent FOG (fat, oil and grease) removal and removed FOG flow fraction.**

Primary

	**Primary settler model with options for three levels of complexity (volumeless point separator, three-compartment model and 1D layered flux model).**

Volumeless units employ mass balance based algebraic models with various input parameter combinations:

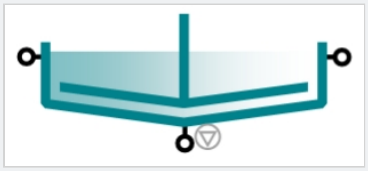
- fixed sludge flow and effluent solids concentration
- fixed sludge flow with percent solids and colloidal removal
- fixed sludge flow with specified solids percent removal and VSS/TSS ratio increase in effluent
- fixed sludge solids concentration with specified solids percent removal and VSS/TSS ratio increase in effluent

Three-compartment units consist of a feed well, a clear water compartment and a sludge blanket (offering reactive volumes for each), interconnected with volumeless point separator models (more details on this can be found in the Process unit specific models chapter). In the feed well, polymer can be added. An elutriation flow allows natural or forced circulation of flow from sludge blanket to clear liquid to account for the diffusion of soluble components. Sumo offers three-compartment primary models with the following input parameter combinations:

- fixed sludge solids concentration with solids percent removal and VSS/TSS ratio increase in effluent
- fixed sludge flow with specified solids percent removal and VSS/TSS ratio increase in effluent

The 1D layered model employs a triple exponential settling velocity model that handles the solid flux exchanges among the various layers of the settler volume (the number of layers is customizable) and predict effluent solids concentration (more details on this can be found in the Process unit specific models chapter). The volume is non-reactive by default but can be set to reactive as well. The positioning (depth) of the feed and the sludge flow are to be specified by the user. Settling parameters can be derived from zone settling lab tests (for this purpose a **Vesilind settling parameters tool** is provided).

Clarifier



Clarifier model with options for three levels of complexity (volumeless point separator, three-compartment model and 1D layered flux model).

Volumeless units employ mass balance based algebraic models with various input parameter combinations:

- fixed sludge flow with specified effluent solids
- fixed effluent solids with specified sludge concentration
- fixed sludge flow with specified solids percent removal efficiency

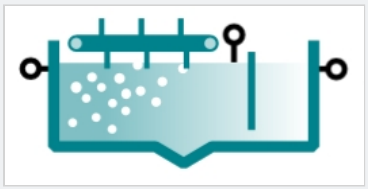
Three-compartment units consist of a feed well, a clear water compartment and a sludge blanket (offering reactive volumes for each, except for the clear phase of the conventional clarifiers), connected with volumeless point separators (more details on this can be found in the Process unit specific models chapter). In the feed well, polymer can be added. Sumo offers three-compartment models for conventional and A-stage clarifiers with the following input parameter combinations:

- A-stage with specified sludge concentration and fixed solids removal efficiency
- A-stage with specified sludge flow and fixed solids removal efficiency
- conventional with fixed effluent solids and specified sludge flow
- conventional with fixed effluent solids and fixed sludge concentration
- conventional with fixed solids removal efficiency and specified sludge flow

In the A-stage clarifiers, an elutriation flow allows natural or forced circulation of flow from sludge blanket to clear liquid to account for the diffusion of soluble components.

The 1D layered model employs a triple exponential settling velocity model that handles the solid flux exchanges among the various layers of the settler volume (the number of layers is customizable) and predict effluent solids concentration (more details on this can be found in the Process unit specific models chapter). The volume is non-reactive by default but can be set to reactive as well. The positioning (depth) of the feed and the sludge flow are to be specified by the user. Settling parameters can be estimated from SVI or derived from zone settling lab tests (for this purpose a **Vesilind settling parameters tool** is provided).

DAF



Mass balance based volumeless model of Dissolved Air Flotation for simultaneous solids and FOG (fat, oil and grease) removal.

The mass balance based algebraic DAF models offer the following input parameter combinations:

- fixed effluent solids concentration and sludge flow with specified FOG removal efficiency
- fixed solids removal efficiency and sludge flow with specified FOG removal efficiency
- fixed solids removal efficiency and sludge concentration with specified FOG removal efficiency

Thickener

Thickener model with options for three levels of complexity (volumeless point separator, three-compartment model and 1D layered flux model).

Volumeless units employ mass balance based algebraic models with various input parameter combinations:

- fixed effluent solids with specified thickened sludge flow
- fixed solids percent removal efficiency with specified thickened sludge concentration
- fixed solids percent removal efficiency with specified thickened sludge flow

Three-compartment units consist of a feed well, a clear water compartment and a sludge blanket (offering reactive volumes for each, except for the clear phase), interconnected with volumeless point separators (more details on this can be found in the Process unit specific models chapter). In the feed well, polymer can be added. An elutriation flow allows natural or forced circulation of flow from sludge blanket to clear liquid to account for the diffusion of soluble components. Sumo offers three-compartment thickener models with the following input parameter combinations:

- fixed solids percent removal efficiency with specified thickened sludge concentration
- fixed solids percent removal efficiency with specified thickened sludge flow

The 1D layered model employs a triple exponential settling velocity model that handles the solid flux exchanges among the various layers of the settler volume (the number of layers is customizable) and predict effluent solids concentration (more details on this can be found in the Process unit specific models chapter). The volume is non-reactive by default but can be set to reactive as well. The positioning (depth) of the feed and the sludge flow are to be specified by the user. Settling parameters can be derived from zone settling lab tests (for this purpose a **Vesilind settling parameters tool** is provided).

Dewatering

General and predictive volumeless models for describing sludge dewatering processes.

The two general volumeless units employ mass balance based algebraic models with the following input parameter combinations:

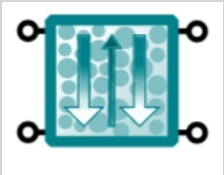
- fixed solids percent removal efficiency with specified dewatered cake solids concentration
- fixed solids percent removal efficiency with specified sludge flow

The two advanced volumeless units employ a mechanistic modelling approach to simulate and predict sludge bound water content and dewaterability for various types of dewatering units:

- Centrifuge
- Beltfilter press
- Screw press

- Crown press

Sand filter



Mass balance based volumeless point separator model with backwash flow.

The mass balance based algebraic model considers the net result of filter operation (no intermittent stages), offering the following input parameter combinations:

- fixed effluent solids concentration and colloids removal efficiency
- fixed solids and colloids removal efficiency

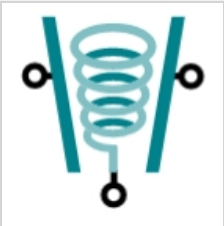
Disc filter

Mass balance based volumeless point separator model with internal backwash flow.

The mass balance based algebraic model considers the net result of filter operation (no intermittent stages), offering the following input parameter combinations:

- fixed effluent solids and backwash flow
- fixed solids removal efficiency and backwash flow

Cyclone

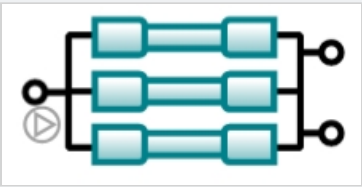


Mass balance based volumeless point separator model with specified underflow fraction and state variable separation.

This mass balance based algebraic model offers two options:

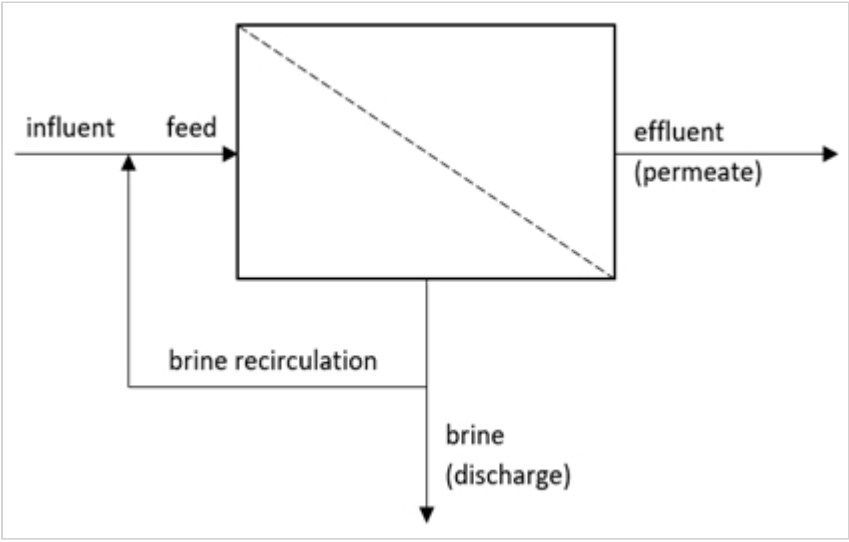
- general *state variable separator* (specify fixed removal efficiency for any SV as input)
- *anammox cyclone* (with specified inorganic solids and annamox removal efficiency as inputs)

RO



Simplified volumeless membrane separator model without surface area, designed for modelling RO mass balance and scaling risk.

Sumo offers a simple mass balance based RO model with the internal structure and specification options outlined below. The model can deal with multiple parallel trains of RO regarding pumps.



Recovery options	Brine recirculation options
▸ Recovery ratio (permeate flow fraction)	▸ Not recirculated

Recovery options	Brine recirculation options
▸ Permeate flow	▸ Specified fraction of brine recirculated ▸ Specified flow of brine recirculated

Point separator

Ideal, mass balance based volumeless solids separator unit with various specification options available, as listed out below.

- perfect separator with specified recycle flow
- fixed effluent solids
- fixed effluent solids and proportional underflow
- fixed solids removal efficiency
- fixed solids removal efficiency and proportional underflow

Special units

AS design

Activated sludge design example to demonstrate the algebraic model capabilities of Sumo. Simple AS design to calculate reactor volume and sludge production from design load, SRT and MLSS.

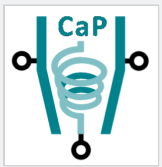
AOP

	**Advanced oxidation process to convert soluble unbiodegradable organic material into biodegradable fractions.**

Deflocculator

	**Deflocculator is a process unit to mimic the impact of pumping on sludge: it break the structure of flocs and increases the colloidal fraction in the wastewater.**

P recovery

		**Dedicated process unit for phosphorus recovery technology producing struvite of calcium phosphate.**

Two phosphorus recovery units have been developed to be able to simulate several commercialized processes:

- the first process unit uses magnesium dosage (magnesium chloride and magnesium hydroxide),
- the second one uses calcium dosage (Calcium chloride and calcium hydroxide).

In both, aeration to strip bicarbonate for pH increase and a caustic dosage are available.

The following dosage options are available:

- With $Mg(OH)_2$ and $MgCl_2$
- With $Ca(OH)_2$ and $CaCl_2$

The chemical dose inputs can be provided based on the following options:

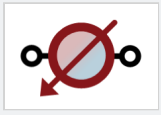
- concentration based (flow rate is input, m^3/d)
- mass flow based (mass flow is input, kg/d)

For the above options the concentration of the chemical is an input. The following choices are available

- Concentration of cation (Mg or Ca as element)
- Concentration of salt ($Mg(OH)_2$, $MgCl_2$, $Ca(OH)_2$ and $CaCl_2$)
- % by mass of salt and liquid density

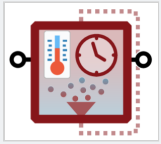
Any combination of the above can be used.

Temperature adjustment



The temperature adjustment unit is prepared to calculate the energy demand of increasing the temperature of a liquid stream.

THP



The THP, alias thermal hydrolysis unit describes the physical processing of sludge. An algebraic calculation is used to model impact on particulate material solubilization under technology specific thermal and pressure conditions. The particulate matter is converted into soluble components.

Catchments and rivers

The catchments and rivers extension in Sumo enables the user to handle sewers, plant and river within the same configuration. This feature employs two simplified process models (one for urban sewer system and another for river system) integrated into the process units, which can be connected to the standard full-plant Sumo models using model connectors.

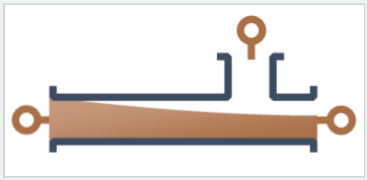
Urban catchment

Simple urban catchment with empirical infiltration model and dry weather flow plus runoff generation involving depression storage, evaporation and catchment hydrology (represented by runoff tank). Collection system is represented as on-line volume.

River catchment

Simple river catchment (natural watershed) with empirical infiltration and base flow model plus runoff generation involving depression storage, evaporation and catchment hydrology (represented by runoff tank).

Circular pipe

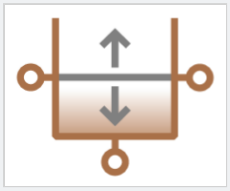


Circular pipe with overflow and backwater effect for urban sewer system with solids sedimentation and mixing.

Pipe tank

Rectangular pipe with overflow and backwater effect for urban sewer system with solids sedimentation and mixing.

Off-line tank



Variable volume off-line tank model with overflow and simple screen for urban sewer system.

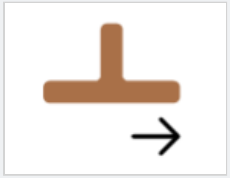
Influent sewer

State variable based simple influent process unit customized for urban sewer system.

River stretch

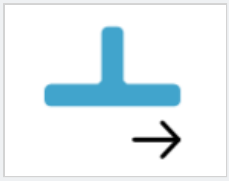
River stretch with simple biokinetics (nitrification and BOD reactions, reaeration, photosynthesis/respiration), BOD sedimentation and hydraulics modeled as channel flow, featuring a dedicated port for sewage/WRRF effluent input (discharge).

Sewer combiner



Simple flow combiner process unit to be used with urban sewer system elements.

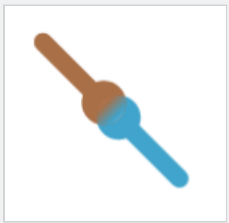
River combiner

	**Simple flow combiner process unit to be used with river system elements.**

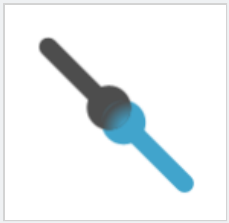
Sewer_WRRF connector

	**Connector process unit for interfacing between urban sewer system and Sumo models (handling state variable conversions).**

Sewer_River connector

	**Connector process unit for interfacing between urban sewer system and river models (handling state variable conversions).**

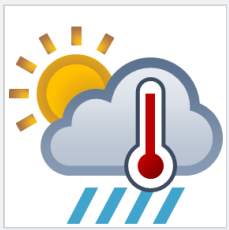
WRRF_River connector

	**Connector process unit for interfacing between Sumo and river models (handling state variable conversions).**

Influent generator dynamic

	**Intrinsic model for synthetising dynamic flow and pollutant mass flows from daily averages using dilution, replenishment and resuspension caused by large, medium and small events.**

Meteo box

	**Special unit for meteorological parameters that can be used for collective weather parameter mapping.**

Energy units

Aeration units

Blower energy calculator

			**Blower energy calculator unit to calculate the power demand of the process required airflow.**
Empirical	**Positive displacement**	**Turbo**	

The unit is called Blower energy calculator as it is using the process model calculated input air flow and defines the blower operation point to calculate the power demand and energy consumption. Undersized blower will not impact the performance of the process model but will indicate the fact of undersized blower.

Three type of energy calculation option is available based on:

- empirical model (considering input efficiency model for pneumatic power demand)
- positive displacement blower (detailed blower curves to calculate blower efficiency and power demand)
- turbo blower (detailed blower curves to calculate blower efficiency and power demand)

Production units

CHP

	**Combined heat and power generation unit using input efficiency or calculated efficiency model to estimate the electric power and heat generation capability of the facility.**

The generated power and heat is calculated based on methane mass flow from the process model. The efficiency is defined as input parameter or can be calculated based on performance curve of the CHP unit.

Efficiency calculation options:

- Input efficiency
- Calculated efficiency

Gastank

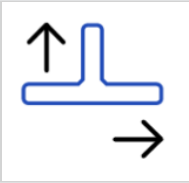
Biogastank with integrated gas composition model using input gas flow parameter and allowing overflow biogas to flare.

Flare

Simple flare unit to indicate if any gas is burned outside the CHP unit. Uses input methane gas mass flow and participates in greenhouse gas emission calculation.

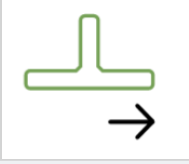
Connectors

Air connector



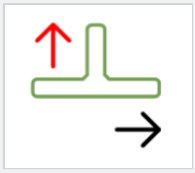
Airflow connector to allow to supply multiple aerated tanks from a single blower group.

Biogas flow combiner



Biogas flow combiner to allow the connection of multiple digesters or UASB units to a single biogas tank or CHP unit.

Biogas flow divider



Biogas flow divider to allow the supply of different biogas tanks or CHP units from a single digester/UASB unit.

Flow split options are:

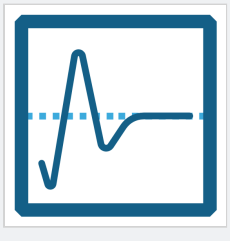
- Flow based ("pumped" biogas flow is the input parameter)
- Proportional (fraction of input flow is the input parameter)

Plantwide units

The goal of plantwide units is to allow the user to set up calculation between different units in the same project. Typical usecases are controllers where the control variable may be at different location as the manipulated variable.

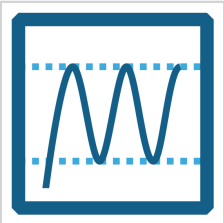
Controllers

Continuous P controller



The continuous P controller is using the proportional part of the discrete PID controller. It is continuous as the manipulated variable is handled as state variables: it is recalculated every integration step.

Deadband controller



Deadband controller can be configured to switch the manipulated variable between a lower and higher value based on the value of the control variable compared to a control range.

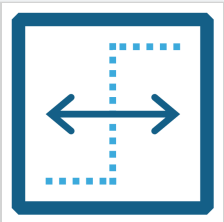
PID controller

Discrete PID controller, velocity form. The manipulated variable is recalculated at every predefined time step. Proportional, integral and derivative gains are input parameters.

Ratio controller

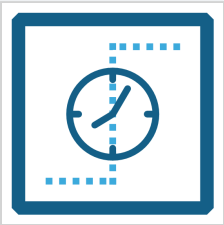
Ratio controller is a continuous controller where the manipulated variable value and the control variable ratio is fixed through a user defined parameter value.

Switch controller



Switch controller continuously changes the manipulated variable between two values depending on the control variable value compared to a threshold.

Time based on-off controller

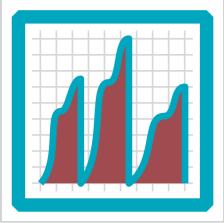


Time based on/off controller changes the manipulated variable between two values based on user defined cycles.

Statistics

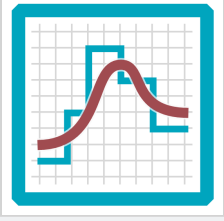
Statistical units are helpful tools to generate results from the simulation in the form they are needed for comparison with measurements.

Cycle based totalizer



Cycle based totalizer integrates a variable for the cycle time set up by the user. It can provide the total daily flow from an hourly based dynamic input table of influent flow.

Moving average

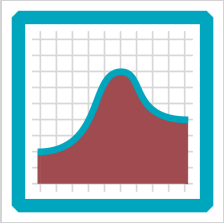


Moving average unit is a discrete value sampling unit which every given timestep stores the variable value and provides the average for the user defined average time period.

Noise

	**Noise unit places measurement noise upon a variable. The noise can be white or Gaussian.**

Totalizer

	**Totalizer unit integrates a selected variable for the simulation time.**

Process unit specific models

Detailed descriptions of specific models developed for process units.

Gas transfer model

Please cite as: *Bencsik D., Wadhawan T., Házi F., Karches T. (2024). Plant-Wide Models for Optimizing the Operation and Maintenance of BTEX-Contaminated Wastewater Treatment and Reuse. Environments 11(5), 88. DOI: 10.3390/environments11050088*

The equilibrium between the vapor and liquid phases for gases soluble in water is simulated using Fick's two-film theory, with gas transfer processes described in our biokinetic models to simulate absorption and desorption. The impact of equilibrium processes on state variables is described within the process model's Gujer matrix. We note that, within the gas transfer equations, standard conditions regarding gases are interpreted as 101,325 Pa for pressure (p_{NTP}) and 293.15 K for temperature ($T_{NTP,K}$).

The internal gas phase components are simulated in units of mass per liquid volume. This makes mass and component balancing substantially simpler (compared to using the gas volume as the basis). Equation (1) describes the component balance for gas i.

$$\frac{dG_i}{dt} = \frac{F_{G_{i,air,inp}} - F_{G_{i,air,outp}} + rateF_{G_i}}{V_r}, \quad (1)$$

$F_{Gi,air,inp}$ denotes the mass flow of gas *i* from the air supply and is calculated based on the composition of the input gas and the air flow based on the ideal gas law, as shown by Equation (2). The equivalent molar mass $MM_{EQ,i}$ of gaseous components is expressed according to the unit mass of the model state variable, e.g. derived from the theoretical oxygen demand in case of CH4.

$$F_{G_{i,air,inp}} = \frac{G_{i,air,inp}/100 \cdot p_{NTP} \cdot Q_{air,NTP} \cdot MM_{EQ,i}}{R \cdot T_{NTP,K}}, \quad (2)$$

For gas phase mass balancing, the output gas mass flow $F_{Gi,air,outp}$ is calculated by Equation (3), where the concentrations expressed per liquid volume must be converted per volume of gas.

$$F_{G_{i,air,outp}} = G_i \cdot \frac{V_r}{V_{gas,NTP}} \cdot Q_{gas,outp,NTP}, \quad (3)$$

The volume of the gas phase in the reactors is estimated based on the gas hold-up fraction ε_{gas}. The gas hold-up is an input parameter, for which this paper uses a value of 0.01 m^3_{gas} m^{-3} in case of aerated conditions and

0.001 m^3_{gas} m^{-3} regarding non-aerated conditions (Herrmann-Heber et al., 2019). The gas volumes at field conditions and standard conditions (V_{gas} and $V_{gas,NTP}$, respectively) are calculated by Equations (4) and (5).

$$V_{gas} = \frac{V_r}{\frac{1}{\varepsilon_{gas}} - 1}, \quad (4)$$

$$V_{gas,NTP} = \frac{V_{gas} \cdot p_{gas} \cdot T_{NTP,K}}{p_{NTP} \cdot T_{air,K}}, \quad (5)$$

The gas phase pressure p_{gas} is determined by Equation (6) in accordance with EPA guidelines on dissolved oxygen saturation calculations (U.S. Environmental Protection Agency – USEPA, 1989a).

$$p_{gas} = \left(p_{air} + h_{sat,eff} \cdot \rho_{H_2O} \cdot g - p_{v,T}\right) \cdot \frac{p_{NTP}}{p_{NTP} - p_{v,T}}, \quad (6)$$

The vapor pressure $p_{v,T}$ is calculated by Equation (7) based on the water temperature and Antoine-coefficients, where a multiplication factor is used for unit conversion from mmHg to Pa.

$$p_{v,T} = 10^{\left(A_{H_2O} - B_{H_2O}/\left(T + C_{H_2O}\right)\right)} \cdot 133.322, \quad (7)$$

The air pressure p_{air} is calculated by the barometric Equation (8), considering the elevation of the facility above sea level h_{sea} (the molar mass of air MM_{air} is converted from the unit g mol^{-1} to kg mol^{-1}). The parameter L_{air} for the temperature lapse rate applies a value of 0.0065 K m^{-1} (Sincero et al., 2002).

$$p_{air} = p_{NTP} \cdot \left(1 - \frac{L_{air} \cdot h_{sea}}{T_{air,K}}\right)^{\frac{g \cdot MM_{air}/1000}{R \cdot L_{air}}}, \quad (8)$$

The calculation of the effective saturation depth depends on whether the tank is aerated, in which case $h_{sat,eff}$ is calculated by Equation (9), and in case there is no aeration, the diffuser submergence h_{diff} is replaced by the total side water depth (h_r). The saturation depth fraction $f_{h,sat,eff}$ may be assigned according to various approaches; the mid-depth concept provides reasonable accuracy in diffused aeration (Stenstrom et al., 2006).

$$h_{sat,eff} = h_{diff} \cdot f_{h,sat,eff}, \quad (9)$$

For the diffuser depth calculation, the diffuser mounting height is subtracted from the liquid height, according to Equation (10).

$$h_{diff} = h_r - h_{diff,floor} \quad (10)$$

Unlike liquid phase hydraulic balancing, where the effluent flow is assumed to be equal to the influent, gas phase volumetric balancing needs to take into account the input air flow, as well as the gas transfer activity in the volumetric unit. Equation (11) determines the outgoing gas volumetric flow, $Q_{gas,outp,NTP}$, which, physically, cannot be negative; this is reflected in the model code (using a maximum function).

$$Q_{gas,outp,NTP} = Q_{air,NTP} + Q_{gas,transfer,NTP}, \quad (11)$$

The volumetric flow of the gas transfer $Q_{gas,transfer,NTP}$ is derived from the summation of the individual gas component transfer molar flows, calculated by Equation (12).

$$Q_{gas,transfer,NTP} = \sum_i \frac{rateF_{G_i}}{MM_{EQ,i}} \cdot \frac{R \cdot T_{NTP,K}}{p_{NTP}}, \quad (12)$$

Two gas transfer routes are modelled: between the atmosphere and water surface and between the bulk-of-the liquid and bubbles. According to Fick's first law, the process rate involving the transfer of gas i between the atmosphere and water surface is described by Equation (13), with the driving force of either dissolution or stripping is determined by the difference in the saturation concentration and the liquid phase concentration. The transfer rate of exchange at the gas bubble interface is fundamentally analogous, described by Equation (14).

$$r_j = k_L a_{i,bub} \cdot (S_{i,bub,sat} - L_i), \quad (13)$$

$$r_j = k_L a_{i,sur} \cdot (S_{i,sur,sat} - L_i), \quad (14)$$

Regarding gas transfer through bubbles, the volumetric liquid-side mass transfer coefficients $k_L a_{i,bub,st,cw}$—in clean water for a standard 20 °C temperature—and $k_L a_{i,bub}$—in wastewater at the field temperature—are calculated by Equations (15) and (16).

$$k_L a_{i,bub,st,cw} = k_{L,i,bub,st,cw} \cdot a_{bub}, \quad (15)$$

$$k_L a_{i,bub} = k_L a_{i,bub,st,cw} \cdot \alpha \cdot \theta^{(T-20)}, \quad (16)$$

The interfacial transfer area a_{bub} is calculated by Equation (17) on a geometrical basis. Based on the literature review, in this study, the bubble Sauter mean diameter d_{bub} is input as 0.003 m for aerated conditions and as 0.01 m under non-aerated conditions (Herrmann-Heber et al., 2019; DelSontro et al., 2015; Jensen et al., 2018).

$$a_{bub} = \frac{6 \cdot \frac{V_{gas}}{V_r}}{d_{bub}}, \quad (17)$$

It shall be noted that in cases of fully covered tanks, atmospheric gas transfer is not modelled; the specific surface area a_{bub} is extended with the specific contact area between the water surface and the headspace, as shown by Equation (18).

$$a_{bub} = \frac{6 \cdot \frac{V_{gas}}{V_r}}{d_{bub}} + \frac{A_r \cdot f_{wave}}{V_r} \quad (18)$$

On the basis of the Higbie penetration theory, values of the liquid-side mass transfer coefficient $k_{L,i,bub,st,cw}$ are calculated using the respective diffusivities of volatile and soluble gas components by Equation (19) (Roberts et al., 1984), relying on $k_{L,O2,bub,st,cw}$ as a model parameter with the input value of 0.54 m h^{-1} (Khalil et al., 2021). The parameter for the fraction in the liquid side $f_{kL,i}$ equals 1 for all gases in this study, as they diffuse slowly through the liquid film, with the exception of 0.05 in the case of ammonia, due to its very high solubility (Batstone and Flores-Alsina, 2022).

$$k_{L,i,bub,st,cw} = f_{k_{L,i}} \cdot \sqrt{\frac{D_{i,25}}{D_{O_2,25}}} \cdot k_{L,O_2,bub,st,cw} \quad (19)$$

Throughout aerated compartments, the α correction factor is modelled dynamically from process variables representative of wastewater characteristics and loads, explained in the chapter ‘Predictive alpha model’. The θ compensation factor for simulating Arrhenius-type temperature sensitivity in mass transfer is taken as 1.024, following standard procedures in wastewater treatment design (U.S. Environmental Protection Agency – USEPA, 1989a).

For aerated conditions, regarding oxygen, $k_La_{O2,bub}$ is calculated by Equation (20), incorporating a further correction factor for diffuser fouling, an input parameter of aerated unit processes (U.S. Environmental Protection Agency – USEPA, 1989b), which, in practice, is best adjusted knowing the diffuser age and the time of the last cleaning procedure (Jiang et al., 2020). For non-aerated conditions (and regarding coarse bubbles), the correction factor for fouling is not interpreted (equal to one).

$$k_La_{O_2,bub} = k_La_{O_2,bub,St,cw} \cdot \alpha \cdot F \cdot \theta^{(T-20)} \quad (20)$$

Regarding oxygen, under aerated conditions, $k_La_{O2,bub,st,cw}$ directly relates to the clean water performance of diffusers; thus, it is derived—according to Equation (21)—from the standard oxygen transfer rate involving air bubbles, $SOTR_{bub}$.

$$k_L a_{O2,bub,st,cw} = \frac{SOTR_{bub}}{S_{O_2,bub,sat,st,cw} \cdot V_r}, \quad (21)$$

$SOTR_{bub}$ is derived from the specific standard oxygen transfer efficiency *SSOTE*, which describes the diffused aerator characteristics in clean water, as Equation (22) shows.

$$SOTR_{bub} = SSOTE/100 \cdot h_{diff} \cdot F_{G_{O_2},air,inp}, \quad (22)$$

The prediction of *SSOTE* is explained in the chapter 'SSOTE estimation model'.

At the atmospheric interface, calculating the volumetric liquid-side mass transfer coefficients involves the specific mass transfer coefficients (k_L) estimated for the liquid surface. The clean water $k_L a_{i,sur,st,cw}$ at standard conditions and the process water $k_L a_{i,sur}$ for field conditions are calculated by Equations (23) and (24), respectively.

$$k_L a_{i,sur,st,cw} = k_{L,i,sur,st,cw} \cdot a_{sur}, \quad (23)$$

$$k_L a_{i,sur} = k_L a_{i,sur,st,cw} \cdot \alpha \cdot \theta^{(T-20)} \quad (24)$$

The liquid-side mass transfer coefficient regarding the water surface $k_{L,i,sur}$ is determined by Equation (25) using the same principle as for the gas bubble interface, as previously shown by Equation (19).

$$k_{L,i,sur} = f_{k_{L,i}} \cdot \sqrt{\frac{D_{i,25}}{D_{O_2,25}}} \cdot k_{L,O_2,sur} \quad (25)$$

The specific surface area of the liquid a_{sur} is calculated by Equation (26), incorporating the multiplication factors f_{cover} for reactor coverage and f_{wave} for turbulence (waviness). The model inputs of 0.54 m h^{-1} for $k_{L,O2,sur}$ and 1.9 for f_{wave} in this study are adjusted based on the typical measured values of $k_L a_{O2,sur}$ found in the relevant literature (Plósz et al., 2003).

$$a_{sur} = \frac{A_r \cdot (1 - f_{cover}) \cdot f_{wave}}{V_r}, \quad (26)$$

The water surface area A_r is defined by basin geometry, according to Equation (27).

$$A_r = V_r / h_r, \quad (27)$$

According to Fick's law, as illustrated previously by Equations (13) and (14), the saturation concentration of a component determines whether the gas–liquid transfer process is driven towards dissolution or stripping. They are calculated by Henry's law based on the partial pressure of a component, with temperature dependency correction implemented using the van't Hoff equation (Sander, 2015). The saturation concentrations of gases attributed to the liquid–gas bubble interface $S_{i,bub,sat,st,cw}$, standardized at 20 °C for clean water (thus requiring temperature conversion from 25 °C, used as the basis of Henry's law), are modelled based on Equation (28). The variable for process water at field conditions, $S_{i,bub,sat,st}$, is expressed by Equation (29).

$$S_{i,bub,sat,st,cw} = p_{partial,i,bub,st} \cdot Henry_{i,25} \cdot e^{Henry_{i,dt} \cdot \left((1/T_{NTP,K}) - (1/T_{SATP,K})\right)} \cdot MM_{EQ,i}, \quad (28)$$

$$S_{i,bub,sat} = \beta \cdot p_{partial,i,bub} \cdot Henry_{i,25} \cdot e^{Henry_{i,dt} \cdot \left((1/T_{K}) - (1/T_{SATP,K})\right)} \cdot MM_{EQ,i}, \quad (29)$$

The β correction factor for impurities in process water uses an input parameter value of 0.95, which is typical of municipal wastewater (U.S. Environmental Protection Agency – USEPA, 1989a).

With regard to the bubble–water interface, partial pressures for standard conditions, $p_{partial,i,bub,st}$, and for process conditions, $p_{partial,i,bub}$, are calculated by Equations (30) and (31), respectively.

$$p_{partial,i,bub,st} = \frac{G_i / MM_{EQ,i}}{n_{gas,bub}} \cdot p_{st,h,sat,eff}, \quad (30)$$

$$p_{partial,i,bub} = \frac{G_i / MM_{EQ,i}}{n_{gas,bub}} \cdot p_{gas} \quad (31)$$

Equation (32) calculates the molar quantity of gas bubbles per unit liquid volume, $n_{gas,bub}$.

$$n_{gas,bub} = \frac{V_{gas,NTP} \cdot p_{NTP}}{V_r \cdot R \cdot T_{NTP,K}}, \quad (32)$$

As explained by Equation (33), the pressure at standard conditions, $p_{st,h,sat,eff}$, is also compensated for the effective saturation depth, as diffuser testing in clean water involves the design submergence (Water Environment Federation – WEF, 2009).

$$p_{st,h,sat,eff} = \left(p_{NTP} + h_{sat,eff} \cdot \rho_{H_2O} \cdot g - p_{v,T}\right) \cdot \frac{p_{NTP}}{p_{NTP} - p_{v,T}} \quad (33)$$

The off-gas composition in molar or volume percent units (interchangeable according to Avogadro's law) may be calculated using Equation (34), expressing $G_{i,percent}$, derived from the individual gas component molar concentrations and their sum.

$$G_{i,percent} = \frac{G_i / MM_{EQ,i}}{\sum_i G_i / MM_{EQ,i}} \cdot 100, \quad (34)$$

The saturation concentrations for the atmosphere–liquid interface, $S_{i,sur,sat,st,cw}$ in the case of clean water and $S_{i,sur,sat}$ regarding process water, are calculated by Equations (45) and (46).

$$S_{i,sur,sat,st,cw} = p_{partial,i,sur,st} \cdot Henry_{i,25} \cdot e^{Henry_{i,dt} \cdot \left((1/T_{NTP,K}) - (1/T_{SATP,K})\right)} \cdot MM_{EQ,i}, \quad (45)$$

$$S_{i,sur,sat} = \beta \cdot p_{partial,i,sur} \cdot Henry_{i,25} \cdot e^{Henry_{i,dt} \cdot \left((1/T_K) - (1/T_{SATP,K})\right)} \cdot MM_{EQ,i}, \quad (46)$$

For the atmospheric saturation concentration calculations, the composition of the atmosphere around the water surface is required. The compositional figures $G_{i,atm}$ are defined as model constants, measured in volumetric percentages. Equations (47) and (48) quantify the partial pressure of gases in the atmosphere, $p_{partial,i,sur,st}$ for standardized conditions and $p_{partial,i,sur}$ for field conditions.

$$p_{partial,i,sur,st} = G_{i,atm}/100 \cdot p_{NTP}, \quad (47)$$

$$p_{partial,i,sur} = G_{i,atm}/100 \cdot p_{air}, \quad (48)$$

To sum up, the gas phase composition and the amount of gas dissolving or stripping are dependent on individual gas state variables that impact one another, according to the laws of mass balance. In accordance, the sufficient injection of air or nitrogen gas production will result in other gaseous components (e.g. CO2) stripping out of the liquid.

Nomenclature:

α	alpha (wastewater/clean water) correction factor for mass transfer coefficient
a_{bub}	specific contact area between the gas bubble surface and liquid phase [$m^2\ m^{-3}$]
a_{sur}	specific contact area between the surface gas and liquid phase [$m^2\ m^{-3}$]
$A_{diff,sp}$	area per diffuser [m^2]
A_r	liquid surface [m^2]
β	beta (wastewater/clean water) correction factor for the saturation concentration
$coeff_{lead,h,diff}$	leading coefficient in a diffuser submergence correction term [m^{-1}]

$coeff_{lin,h,diff}$	linear coefficient in a diffuser submergence correction term [m^{-1}]
d_{bub}	bubble Sauter mean diameter [m]
d_{diff}	diffuser density [m^2 m^{-2}]
$D_{i,25}$	diffusion coefficient of gas state variable i in water [m^2 d^{-1}]
$div_{d,diff}$	divisor value in a diffuser density correction term [m^2 m^{-2}]
ε	gas hold-up [m^3_{gas} m^{-3}]
exp_{SSOTE}	exponent in SSOTE correlation [d m^{-3}_{gas}]
F	diffuser fouling factor
f_{cover}	covered fraction of the reactor surface
F_{Gi}	mass flow of gas phase state variable i [g d^{-1}]
$f_{h,sat,eff}$	effective saturation depth fraction
$f_{kL,i}$	fraction in the liquid side for the mass transfer of gas state variable i
F_{Li}	mass flow of liquid phase state variable i [g d^{-1}]
f_{wave}	waviness factor
G_i	concentration of gas phase state variable i in off-gas, per liquid volume [g m^{-3}]
$G_{i,air,inp}$	concentration of gas phase state variable i in the air input [%V V^{-1}]
$G_{i,atm}$	concentration of gas phase state variable i in the atmosphere [%V V^{-1}]
$G_{i,percent}$	concentration of gas phase state variable i in off-gas, percentage [%V V^{-1}]
h_{diff}	diffuser submergence [m]
$h_{diff,floor}$	diffuser height from floor [m]
$Henry_{i,dt}$	temperature dependency factor for Henry coefficient of gas i [K]
$Henry_{i,SATP}$	Henry coefficient of gas i, standard (SATP) temperature (25 °C) [mol m^{-3} Pa^{-1}]
h_r	reactor depth [m]
$h_{sat,eff}$	effective saturation depth [m]
h_{sea}	elevation above sea level [m]

$k_{L,i,bub,st,cw}$	liquid-side mass transfer coefficient for gas bubbles, standard conditions [m d^{-1}]
$k_{L,i,sur,st,cw}$	liquid-side mass transfer coefficient for liquid surface, standard conditions [m d^{-1}]
$k_L a_{i,bub}$	volumetric mass transfer coefficient for gas bubbles, field conditions [d^{-1}]
$k_L a_{i,bub,st,cw}$	volumetric mass transfer coefficient for gas bubbles, standard conditions [d^{-1}]
$k_L a_{i,sur}$	volumetric mass transfer coefficient for liquid surface, field conditions [d^{-1}]
$k_L a_{i,sur,st,cw}$	volumetric mass transfer coefficient for liquid surface, standard conditions [d^{-1}]
L_{air}	temperature lapse rate for air pressure calculation [K m^{-1}]
L_i	concentration of liquid phase state variable i [g m^{-3}]
MM_{air}	molar mass of air [g mol^{-1}]
$MM_{EQ,i}$	equivalent molar mass of gas phase state variable i [g mol^{-1}]
n_{diff}	number of diffusers
$n_{gas,bub}$	molar quantity of gas bubbles per unit liquid volume [mol m^{-3}]
p_{air}	air pressure at field elevation [Pa]
p_{gas}	gas phase pressure [Pa]
p_{NTP}	pressure at standard (NTP) conditions (101,325 Pa) [Pa]
$pow_{d,diff}$	power value in a diffuser density correction term
$pow_{h,diff}$	power value in a diffuser submergence correction term
$p_{partial,i,bub}$	partial pressure of gas state variable i in the gas phase [Pa]
$p_{partial,i,bub,st}$	partial pressure of gas state variable i in the gas phase, standard conditions [Pa]
$p_{partial,i,sur}$	partial pressure of gas state variable i in the atmosphere [Pa]
$p_{partial,i,sur,st}$	partial pressure of gas state variable i in the atmosphere, standard conditions [Pa]
$p_{st,h,sat,eff}$	pressure at standard conditions and effective saturation depth [Pa]

$p_{v,T}$	saturated vapor pressure of water at temperature T [Pa]
θ	Arrhenius temperature correction factor for the mass transfer coefficient
Q	volumetric flow of wastewater [$m^3\ d^{-1}$]
$Q_{air,NTP}$	air flow at standard (NTP) conditions [$m^3_{gas}\ d^{-1}$]
$Q_{air,NTP,sp}$	air flow per diffuser at standard (NTP) conditions [$m^3_{gas}\ d^{-1}$]
$Q_{gas,transfer,NTP}$	gas transfer flow at standard (NTP) conditions [$m^3_{gas}\ d^{-1}$]
$Q_{gas,outp,NTP}$	off-gas flow at standard (NTP) conditions [$m^3_{gas}\ d^{-1}$]
$rateF_i$	mass rate of state variable i [$g\ d^{-1}$]
$rate_i$	reaction rate for the state variable [$g\ m^{-3}\ d^{-1}$]
r_j	process rate regarding process j (from Gujer matrix) [$g\ m^{-3}\ d^{-1}$]
$S_{i,bub,sat}$	saturation concentration at the gas bubble interface [$g\ m^{-3}$]
$S_{i,bub,sat,st,cw}$	saturation concentration at the gas bubble interface, standard conditions [$g\ m^{-3}$]
$S_{i,sur,sat}$	saturation concentration at the atmospheric interface [$g\ m^{-3}$]
$S_{i,sur,sat,st,cw}$	saturation concentration at the atmospheric interface, standard conditions [$g\ m^{-3}$]
S_{O2}	dissolved oxygen concentration [$g_{O2}\ m^{-3}$]
$SOTR_{bub}$	standard oxygen transfer rate from bubbles [$g\ d^{-1}$]
SSOTE	specific standard oxygen transfer efficiency [$\%\ m^{-1}$]
$SSOTE_0$	intercept in SSOTE correlation [$\%\ m^{-1}$]
$SSOTE_{asym}$	asymptote in SSOTE correlation [$\%\ m^{-1}$]
T	liquid temperature [°C]
$T_{air,K}$	field air temperature [K]
T_K	liquid temperature in an SI unit [K]
$T_{NTP,K}$	temperature at standard (NTP) conditions (20 °C) [K]
$T_{SATP,K}$	temperature at standard (SATP) conditions (25 °C) [K]
V_{gas}	gas phase volume [m^3_{gas}]

$V_{gas,NTP}$	gas phase volume at standard (NTP) conditions [m^3_{gas}]
$\nu_{j,i}$	stoichiometric coefficient of state variable i in process j
V_r	reactive volume [m^3]

References:

Batstone D., Flores-Alsina X. (2022). Generalised Physicochemical Model (PCM) for Wastewater Processes, IWA Publishing: London, UK. ISBN: 978-1-78040-982-5

DelSontro T., McGinnis D., Wehrli B., Ostrovsky I. (2015). Size Does Matter: Importance of Large Bubbles and Small-Scale Hot Spots for Methane Transport. Environmental Science & Technology 49, pp. 1268–1276. DOI: 10.1021/es5054286

Herrmann-Heber R., Reinecke S. F., Hampel U. (2019). Dynamic Aeration for Improved Oxygen Mass Transfer in the Wastewater Treatment Process. Chemical Engineering Journal 386, 122068. DOI: 10.1016/j.cej.2019.122068

Jensen M. B., Kofoed M. V. W., Fischer K., Voigt N. V, Agneessens, L.M.; Batstone, D.J.; Ottosen, L.D.M. (2018). Venturi-Type Injection System as a Potential H2 Mass Transfer Technology for Full-Scale in Situ Biomethanation. Applied Energy 222, pp. 840–846. DOI: 10.1016/j.apenergy.2018.04.034

Jiang L.-M., Chen L., Zhou Z., Sun D., Li Y., Zhang M., Liu Y., Du S., Chen G., Yao J. (2020). Fouling Characterization and Aeration Performance Recovery of Fine-Pore Diffusers Operated for 10 Years in a Full-Scale Wastewater Treatment Plant. Bioresource Technology 307, 123197. DOI: 10.1016/j.biortech.2020.123197

Khalil A., Rosso D., DeGroot C.T. (2021). Effects of Flow Velocity and Bubble Size Distribution on Oxygen Mass Transfer in Bubble Column Reactors—A Critical Evaluation of the Computational Fluid Dynamics-Population Balance Model. Water Environment Research 93, pp. 2274–2297. DOI: 10.1002/wer.1604

Plósz B. G., Jobbágy A., Grady, C. P. L. (2003). Factors Influencing Deterioration of Denitrification by Oxygen Entering an Anoxic Reactor through the Surface. Water Research 37, pp. 853–863. DOI: 10.1016/S0043-1354(02)00445-1

Roberts P. V., Munz C., Dändliker P. (1984). Modeling Volatile Organic Solute Removal by Surface and Bubble Aeration. Journal of Water Pollution Control Federation 56, pp. 157–163.

Sander R. (2015). Compilation of Henry's Law Constants (Version 4.0) for Water as Solvent. Atmospheric Chemistry and Physics 15, pp. 4399–4981. DOI: 10.5194/acp-15-4399-2015

Sincero, A. P., Sincero, G. A. (2002). Physical-Chemical Treatment of Water and Wastewater, 1st ed., CRC Press: Boca Raton, FL, USA, 2002. ISBN: 978-1-58716-124-7

Stenstrom M. K., Leu S.-Y., Jiang P. (2006). Theory to Practice: Oxygen Transfer and the New ASCE Standard. In: Proceedings of the Water Environment Federation 2006, 7, pp. 4838–4852.

U.S. Environmental Protection Agency (1989a). Design Manual: Fine Pore Aeration Systems, EPA/625/1-89/023, U.S. Environmental Protection Agency: Cincinnati, OH, USA.

U.S. Environmental Protection Agency (1989b). Summary Report: Fine Pore (Fine Bubble) Aeration Systems, EPA/625/8-85/010; U.S. Environmental Protection Agency: Cincinnati, OH, USA.

Water Environment Federation (2009). Design of Municipal Wastewater Treatment Plants MOP 8, 5th ed., McGraw-Hill Education: Alexandria, VA, USA. ISBN: 978-0-07-166358-8.

SSOTE estimation model

Aeration is one of the most energy-intensive processes at water resource recovery facilities, therefore it is essential to apply a model representative of wide air flow ranges and various aerator configurations, for quantifying the efficiency of diffusers.

The main purpose of modelling aeration efficiency is to be able to properly evaluate oxygen transfer that depends on several physical dimensions within a treatment plant, and varying air flow requirements due to changes in loading – essential for process design involving diurnal influent flow patterns and optimization of treatment plants using dynamic simulation.

Numerous empirical correlations have been developed to describe aerator performance in the field of municipal wastewater treatment, with regression parameters specific to types and manufacturers. Standard oxygen transfer efficiency (SOTE) is a function of the mass transfer coefficient k_La, and research on bubble columns has shown that k_La may be correlated using a power function with superficial gas velocity that is the product of air flow and the reactor area (Shah et al., 1982).

Models have been implemented for calculating SOTE directly in function of air flow and other operational parameters. One approach is applying a polynomial regression equation, relating SOTE to air flow rate per diffuser (air flux), and the depth and density of diffusers (Hur, 1994). This equation has later been modified by the addition of a natural log function to provide a better correlation between SOTE and air flux. (Frank et al., 2009).

Efforts have also been made to apply correlations for the diffuser depth-related aeration efficiency, or specific standard oxygen transfer efficiency (SSOTE) by dimensional analysis (Gillot et al., 2005).

Regarding previously developed correlations, air flux is limited within the ranges used for model calibration and they shall not be extrapolated outside of them. And using logical functions to set strict threshold levels for variables may lead to potential numerical issues when utilized in a dynamic wastewater simulator.

This chapter presents a novel empirical model for estimating SSOTE based on an exponential formula, with the aim of bounding SSOTE between equipment-specific limits; ensuring that it is applicable for virtually any setting of air flux. Correction factors are used to account for diffuser submergence and density.

Methodological Approach

The proposed model was designed to reflect the behavior of fine and coarse bubbles considering previous studies on diffused aeration systems.

Concerning fine bubble aerators, SSOTE is known to drop significantly with increased air flow rate (Morgan et al., 1960). With increasing air flow, size of the air bubbles increases – reducing their specific contact surface and retention time; along with the greater interference of rising bubbles (Ippen et al., 1954; Ellise et al., 1980; Stenstrom et al., 1981).

On the other hand, coarse bubble diffusers show an increasing trend of SSOTE with increasing air flow, as the superficial contact area increases due to bubbles breaking up as a result of higher turbulence (Eckenfelder, 1959).

The general expression selected to model SSOTE in function of air flux is shown below:

$$\mathrm{SSOTE} = \left(\mathrm{SSOTE_0} - \mathrm{SSOTE_{asym}}\right) \cdot \mathrm{e}^{-\mathrm{exp_{SSOTE}} \cdot \mathrm{Q_{air,NTP,sp}}} + \mathrm{SSOTE_{asym}}$$

Where, $SSOTE_0$: Intercept in SSOTE correlation (%/m)

$SSOTE_{asym}$: Asymptote in SSOTE correlation (%/m)

exp_{SSOTE}: Exponent (absolute value) in SSOTE correlation (-)

$Q_{air,NTP,sp}$: Normalized air flow per diffuser (m^3/d at NTP)

The novelty of this proposed formula is that with any air flux input, the calculated SSOTE will always be capped between the values of the intercept and the asymptote. In case of fine bubbles, the asymptote (value of SSOTE achieved with an infinitely large air flux) is lower than the intercept (SSOTE value with zero air flux). When modelling coarse bubbles, the asymptote is higher than the intercept, as they show the opposite trend of SSOTE in function of air flux. The diffuser-specific air flux $Q_{air,NTP,sp}$ quantifies air flow per number of diffusers:

$$\mathrm{Q_{air,NTP,sp}} = \frac{\mathrm{Q_{air,NTP}}}{\mathrm{n_{diff}}}$$

Where, $Q_{air,NTP}$: air flow at standard (NTP) conditions (m^3/d at NTP)

n_{diff}: number of diffusers

Further paper research was conducted to integrate the influence of commonly available diffuser characteristics into the model. The absolute transfer efficiency, SOTE increases with diffuser depth, because of the longer contact time of bubbles, and the increased driving force due to the greater partial pressure of oxygen (Mavinic et al., 1974). It is also known that SOTE does not increase linearly with depth, especially in tanks deeper than 8 meters (Pöpel et al., 1994), therefore the proposed SSOTE correlation was extended by a correction term for diffuser submergence:

$$\mathrm{SSOTE} = \frac{\left(\mathrm{SSOTE_0} - \mathrm{SSOTE_{asym}}\right) \cdot \mathrm{e}^{-\mathrm{exp_{SSOTE}} \cdot \mathrm{Q_{air,NTP,sp}}} + \mathrm{SSOTE_{asym}}}{\mathrm{corr_{h,diff}}}$$

$$\mathrm{corr_{h,diff}} = \mathrm{coeff_{lead,h,diff}} \cdot \mathrm{h_{diff}}^{\mathrm{pow_{h,diff}}} + \mathrm{coeff_{lin,h,diff}} \cdot \mathrm{h_{diff}} + 1$$

Where, h_{diff}: Diffuser submergence (m)

$coeff_{lead,h,diff}$: Leading coefficient (1/m)

$pow_{h,diff}$: Power value (-)

$coeff_{lin,h,diff}$: Linear coefficient (1/m)

It has been investigated that in fine bubble aeration, increasing the diffuser floor coverage raises SSOTE (Wagner et al., 1998), as the residence time of bubbles increases with a more evenly distributed mixing profile. A correction term for diffuser density is also applied to the presented correlation, only for modelling fine bubble diffusers:

$$SSOTE = \frac{\left(SSOTE_0 - SSOTE_{asym}\right) \cdot e^{-exp_{SSOTE} \cdot Q_{air,NTP,sp}} + SSOTE_{asym}}{corr_{h,diff}} \cdot corr_{d,diff}$$

$$corr_{d,diff} = \frac{d_{diff}}{div_{d,diff}}^{pow_{d,diff}}$$

Where, d_{diff}: Diffuser floor density (m^2 diffuser/m^2 tank)

$div_{d,diff}$: Divisor value (m^2 tank/m^2 diffuser)

$pow_{d,diff}$: Power value (-)

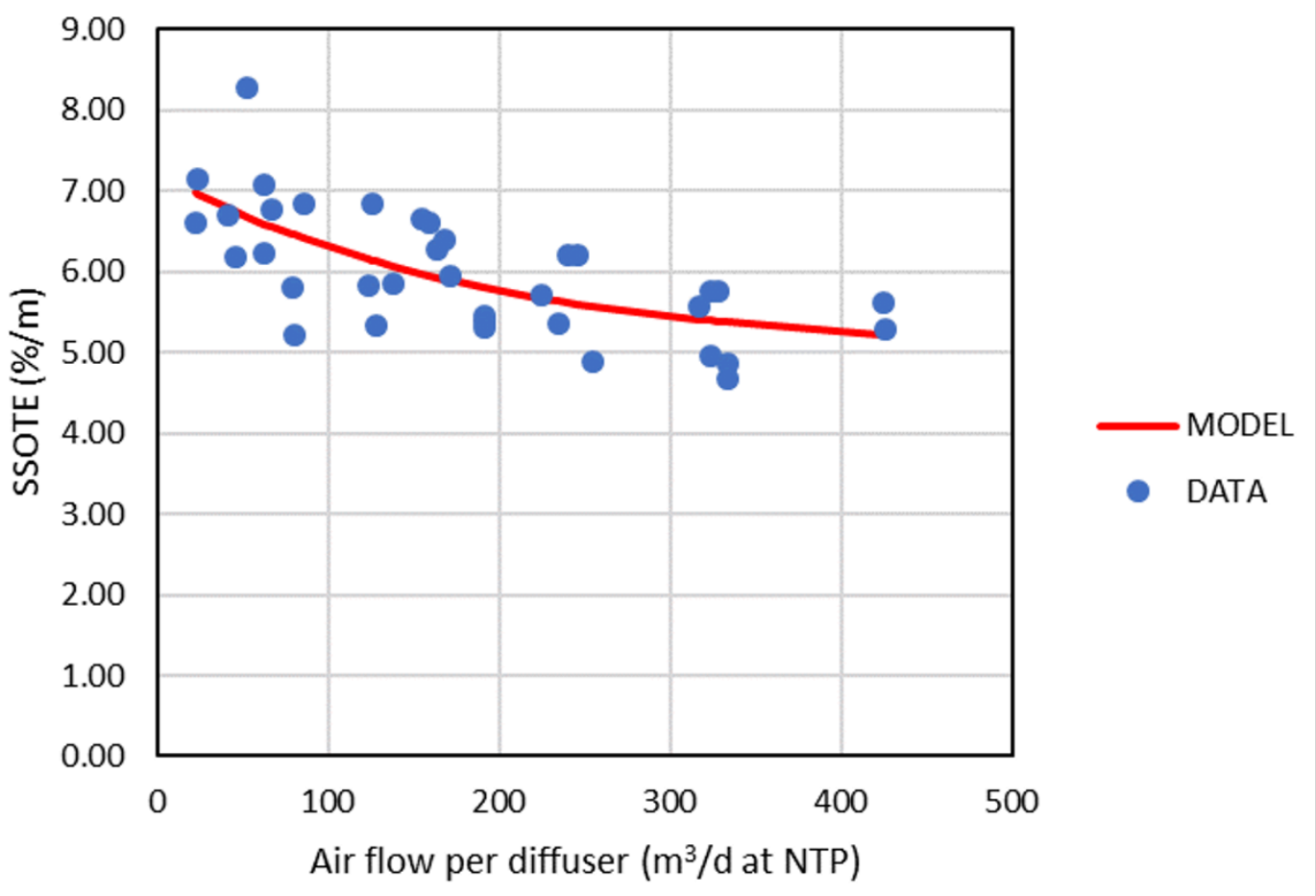
The diffuser floor density d_{diff} is the ratio of the total diffuser area to the tank surface:

$$d_{diff} = \frac{n_{diff} \cdot A_{diff,sp}}{A_r}$$

Where, $A_{diff,sp}$: area per diffuser (m^2)

A_r: liquid surface (m^2)

Following model development, a generalized model calibration was carried out based upon data collected from extensive aeration literature review, regarding a type of coarse bubble, and five different types of fine pore diffuser applications (Fig. 1). The Solver add-in from Microsoft Excel was utilized for curve fitting, with the target of minimizing the sum of errors squared, between the measured and correlated SSOTE.



GTM Figure 1 - Illustration of model fitting for membrane disc type diffusers.

Model validation was performed comparing air flow measurements from two water resource recovery facilities, with the commercial simulation package Sumo 19.3, with dissolved oxygen, diffuser configuration and alpha factor as model inputs.

A Microsoft Excel-based tool was prepared to provide an interface for automated re-estimation of correlation parameters based on diffuser manufacturer specification sheets or plant measurement campaigns, developed using the Visual Basic for Application programming language. For details see Tools in Sumo.

References:

Eckenfelder W. W. (1959). Factors affecting the aeration efficiency of sewage and industrial wastes. Sewage and Industrial Wastes 31(1), pp. 60–70.

Ellise S., Stanbury, R. (1980). The Scale-up of Aerators. In: Symposium on The Profitable Aeration of Waste Waters, 3, BHRA Fluid Engineering Report, Cranfield, Bedford, England.

Frank K., Davies G., Shirodkar N., Sauvageau A. (2009). Aerating a high rate low SRT activated sludge reactor: coarse or fine bubble aeration – how about a hybrid? In: Proceedings of the Water Environment Federation 2009, 8, pp. 7215–7224. DOI: 10.2175/193864709793957382

Gillot S., Capela-Marsal S., Roustan M., Héduit A. (2005): Predicting oxygen transfer of fine bubble diffused aeration systems – model issued from dimensional analysis. Water Research 39(7), 1379–1387. DOI: 10.1016/j.watres.2005.01.008

Hur D. S. (1994). A computer program for optimal aeration system design for activated sludge treatment plants. M.S. Thesis, University of California, Los Angeles.

Ippen A. T., Carver C. E., Dobbins W. E. (1954). Basic factors of oxygen transfer in aeration systems. Sewage and Industrial Wastes 26(7), pp. 813–829.

Mavinic D. S., Bewtra J. K. (1974). Bubble size and contact time in diffused aeration systems. Journal of Water Pollution Control Federation 46, pp. 2129–2137.

Morgan P. F., Bewtra J.K. (1960). Air diffuser efficiencies, Journal of Water Pollution Control Federation 32, pp. 1047–1059.

Pöpel H. J., Wagner M. (1994). Modelling of Oxygen Transfer in Deep Diffused-Aeration Tanks and Comparison with Full-Scale Plant Data. Water Science and Technology, 30(4), pp. 71-80. DOI: 10.2166/wst.1994.0161

Shah Y. T., Kelkar B. G., Godbole S. P., Deckwer W. D. (1982). Design Parameters Estimation for Bubble Column Reactor, AIChE Journal, 28(3).

Stenstrom M. K, Gilbert, R. G., (1981). Effects of Alpha, Beta and Theta Factor upon the Design, Specification and Operation of Aeration Systems. Water Research 15, pp. 643-654.

Wagner M., Pöpel H. J. (1998). Oxygen transfer and aeration efficiency – influence of diffuser submergence, diffuser density, and blower type. Water Science and Technology 38(3), DOI: 10.1016/S0273-1223(98)00445-4

Predictive alpha model

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The performance of aeration – one of the costliest processes at water resource recovery facilities – is heavily impacted by actual wastewater characteristics and diffuser usage, that are commonly taken into account using the α and F factors, respectively. The α factor changes depending on loading – meaning both in time and spatially (e.g., along plug flow reactors). In standard design practice it is often considered as a fixed number, or at best, a predefined time series. There is a need to more accurately predict α for the design and operation of WRRFs. The objective of this study is to propose such a method by the use of process modelling, adjusting to diurnal and seasonal variations in hydraulic and organic loading.

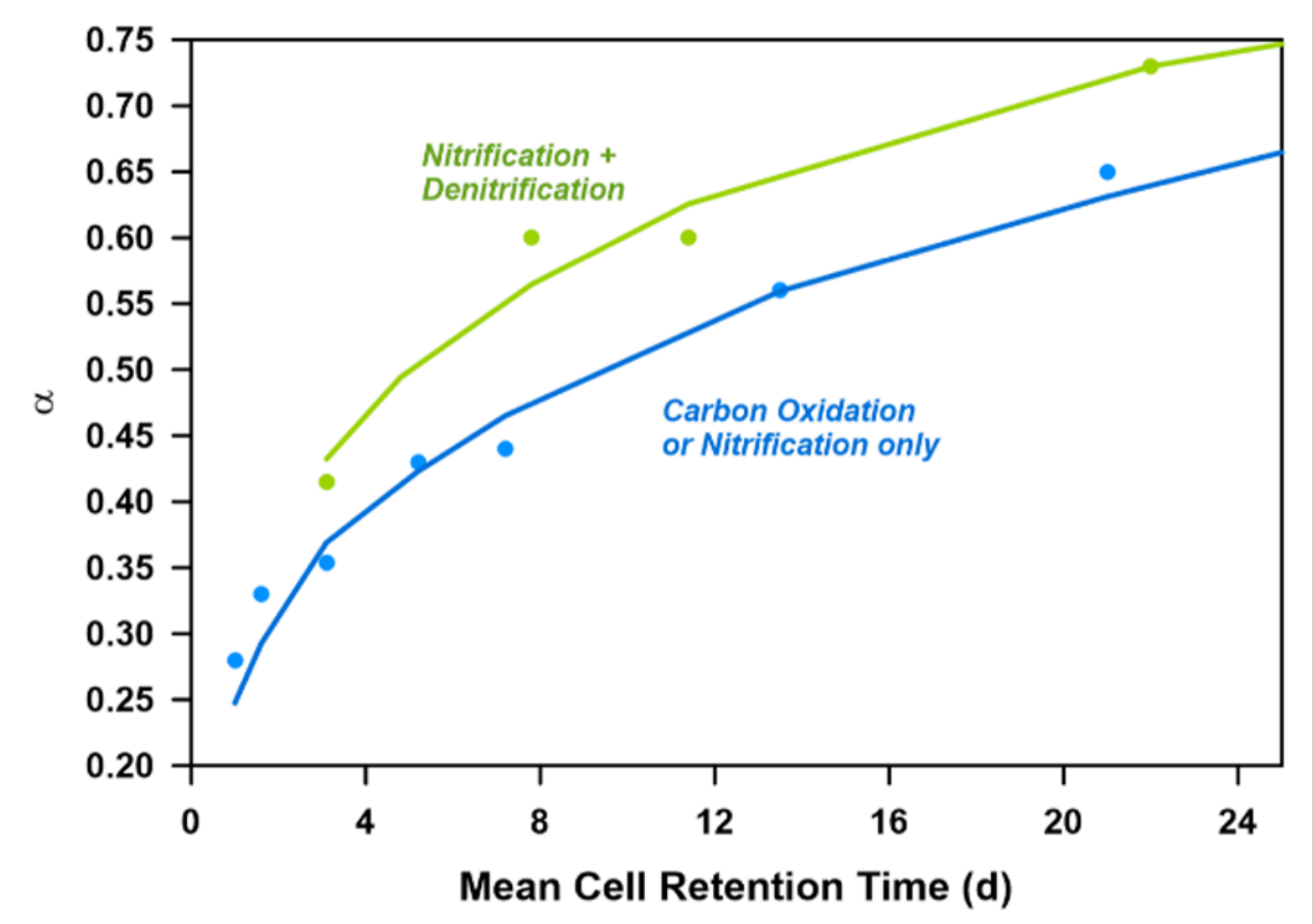
Methodological Approach

The concept of dynamic prediction of the α factor is based on a “typical” or “average” degradable component. As this component sorbs to flocs and degrades kinetically in the system, α increases towards the clean water value. This novel concept was selected because change of the α value in space and time cannot be directly linked to any of the state variables (readily biodegradable substrate, ammonia etc.) that models typically deal with. The model developed by the authors takes into account the dependence of α on sludge retention time in the form of degradation kinetics, the effect of organic loading (influent filtered COD), the presence or absence of anoxic zones and the effect of high MLSS found in certain, e.g., MBR technologies.

Data was collected from results of off-gas measurement campaigns, clean water and process water tests; while also relying on aeration literature review (Rosso et al., 2008; Leu et al., 2009; Baquero-Rodríguez et al., 2018). Reconciliation of data was carried out according to IWA Good Modelling Practice Guidelines (Rieger et

al., 2013). The model was then first fitted to averaged α factor measurements from facilities applying newly commissioned fine pore diffusers – with and without non-aerated selectors – in function of the given plant MCRT values (Figure 1). Suspended solids-related correction in the model was fine-tuned based upon α factor batch tests without loading. The modelled behaviour of α in terms of influent filtered COD was adjusted based on diurnal continuous off-gas testing.

A variant of the BSM1 test configuration (Alex et al., 2008) was set up in Sumo21© and used to evaluate potential CAPEX and OPEX (energy and effluent fines) savings due to using the proposed predictive α model (and the resulting more correct blower sizes and control) instead of fixed overly cautious or too optimistic design values.



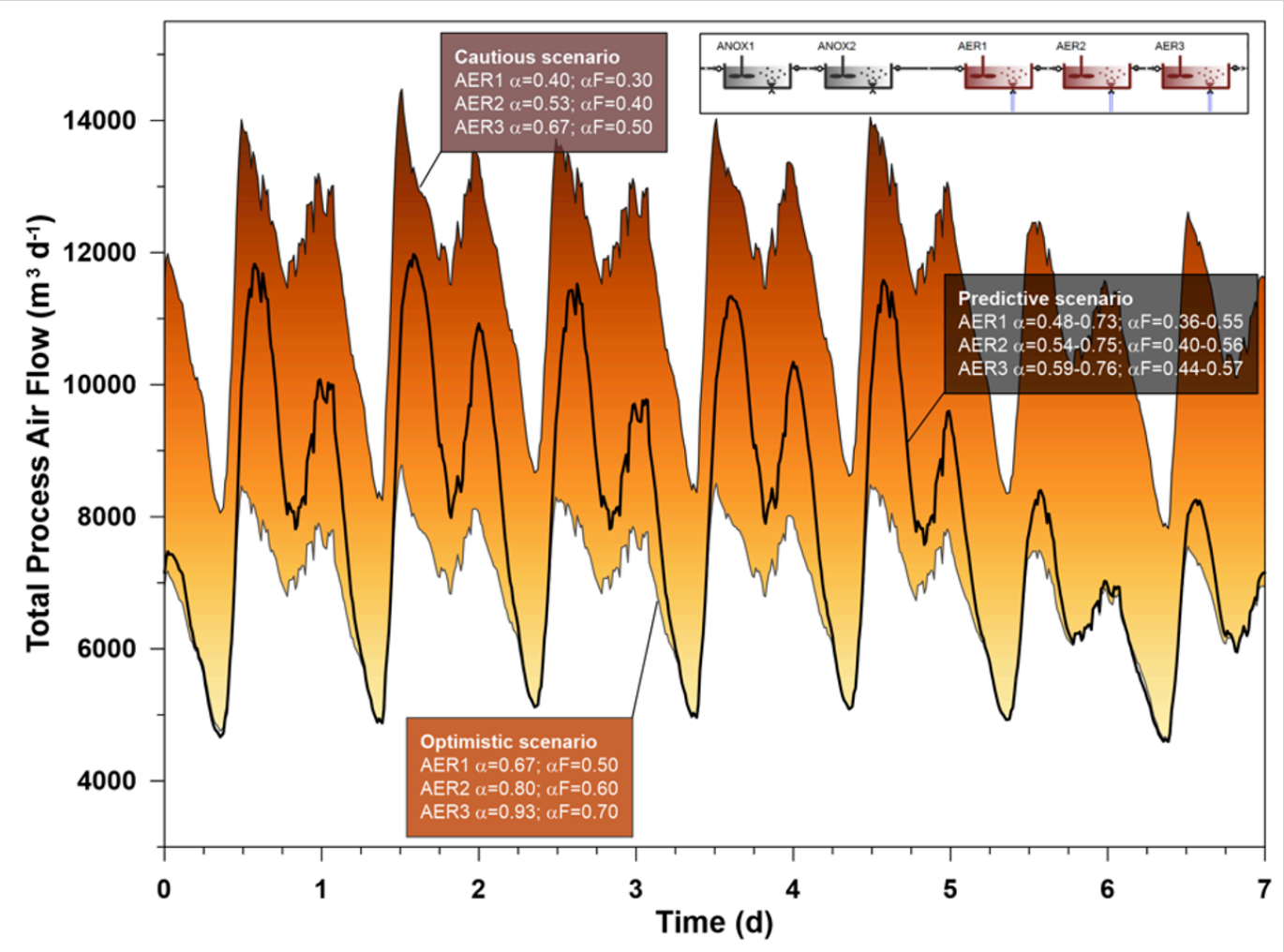
GT Figure 2 - Model fitting results regarding α factor versus MCRT

Mini_Sumo was selected as a biokinetic model – in favor of an up-to-date gas transfer concept, extended by Sumo's blower and pump models to assess energy and associated costs. Throughout model simulation, α factor for aged diffusers (αF, including fouling factor) was used for results interpretation – assigning a fixed value of 0.75 for F.

Results and Discussion

In the authors' first study the model was run to dry weather steady-state using Sumo's combined global and local solvers, followed by 5 weeks of repeated dry weather diurnal weeks (GT Figure 3). Three runs were performed in order to obtain the required blower sizes for the following different design methods:

1. Kinetic-based model prediction (space and time varying αF):
   average calculated αF at 0.48, 0.5 and 0.53 in AER1, AER2 and AER3
2. Cautious design:
   αF set to 0.3, 0.4 and 0.5 in AER1, AER2 and AER3
3. Optimistic design:
   αF set to 0.5, 0.6 and 0.7 in AER1, AER2 and AER3



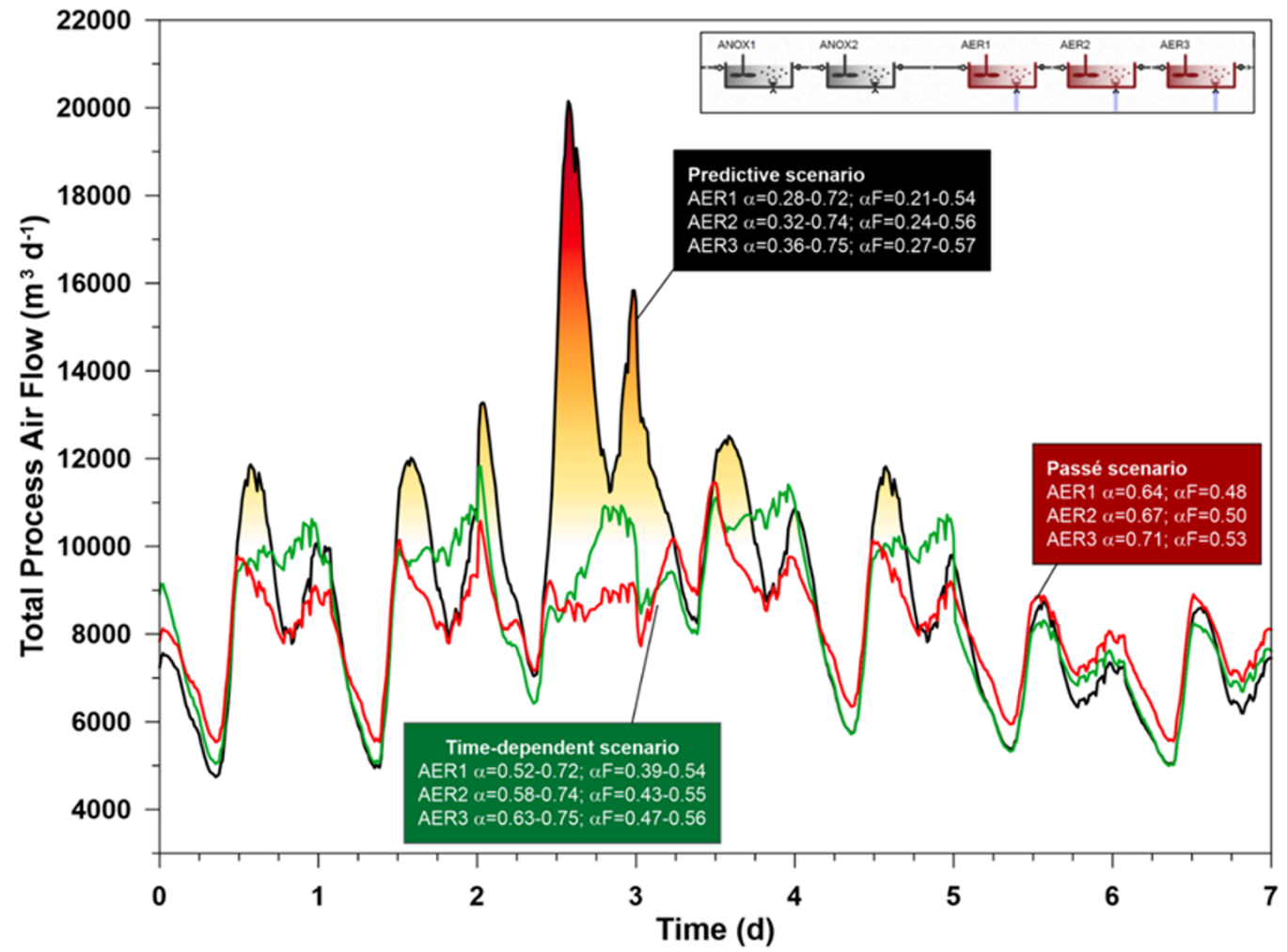
gt Figure 3 - Air flow comparison between constant and model-predicted αF-based design scenarios

Compared to the cautious design example that estimates an accumulated blower energy consumption of 45,846 kWh, the time and location-specific αF prediction use case determines only 34,765 kWh, suggesting 24% savings on operational costs. Although the weekend air demand estimated by the optimistic design approach shows good agreement with the predictive method, it only assumes 31,362 kWh of required blower energy; and it would potentially lead to insufficient air supply during most of the week.

In another experimental study, model-predicted αF was compared to best sinusoidal approximation. A sinusoidal approximation for αF in each reactor was created using a cos() function. The sinusoidal αF variation was based on the dynamically predicted model results, by matching the average and the timing and value of the highest αF peak in each reactor separately for weekdays and weekend days.

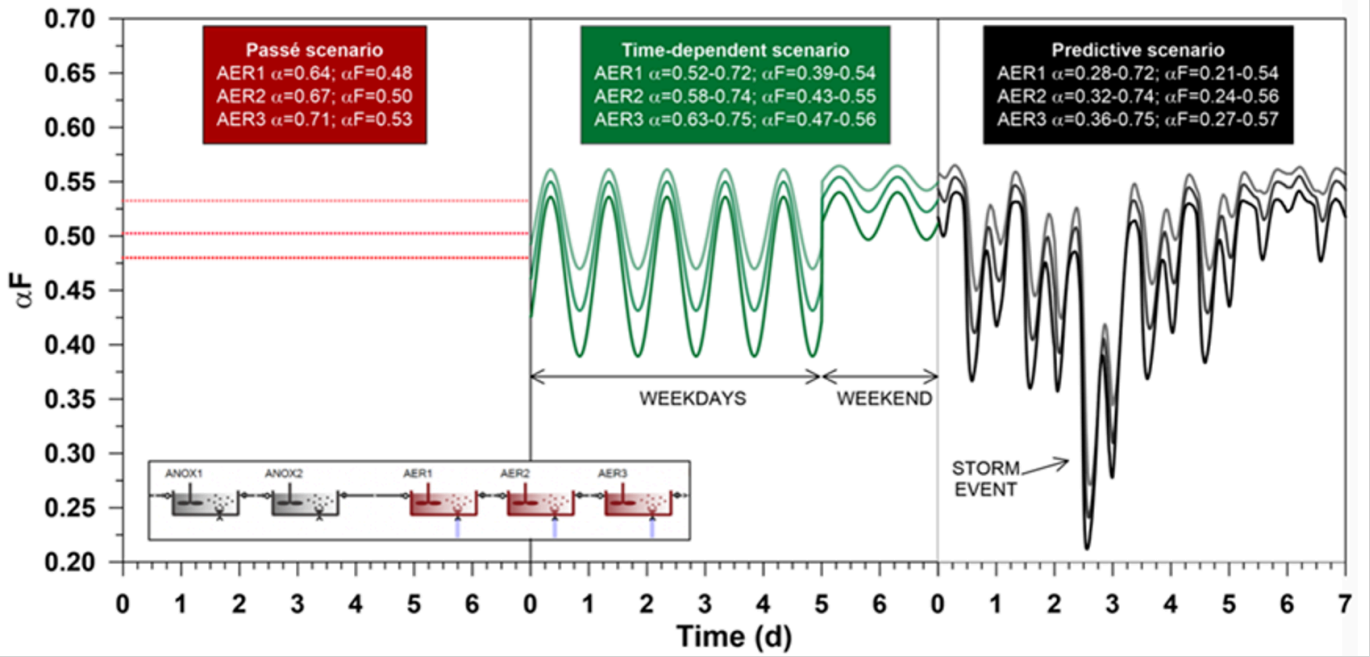
After steady-state and 5 weeks of dry weather loading, a 6th week was simulated where the flow (and therefore the load) on Wednesday was doubled. The sinusoidal αF prediction was not changed during the overload

period. The blower used was the best design (12,000 m^3/h). The air flow requirement for this run can be compared to the response of the dynamic prediction run for the same week (GT Figure 4).



GT Figure 4 - Air flow comparison between constant, sinusoidal, and predicted αF scenarios; with overload

If the load increase is considered, it turns out that 12,000 m^3/h blower capacity would in fact not be enough, while the sinusoidal αF design suggests it will suffice. Blower size was not restricted in this run. The predictive approach evaluates (properly) lower αF, and consequently, higher air flow associated with it. The sinusoidal and constant scenarios calculate slightly reduced air flow – they do not account for αF reduction by the sudden load variation (Figure 4), and due to the high hydraulic load ammonia is washed out to a peak of 27 mg N/L in all three scenarios. DO setpoints are maintained in all three scenarios, but in reality, only the dynamic αF case would be able to maintain them, the other two αF presumptions are flawed and consequently the air flow is wrong.



GT Figure 5 - Illustration of αF factor profile by constant, sinusoidal, and model-predicted use cases

References:

Alex J., Benedetti L., Copp J., Gernaey K., Jeppsson U., Nopens I., Pons M.-N., Rieger L., Rosén C., Steyer J.P., Vanrolleghem P.A., Winkler S. (2008). Benchmark Simulation Model no. 1 (BSM1). In: Report by the IWA Task Group on Benchmarking of Control Strategies for WWTPs, pp. 19–20.

Baquero-Rodríguez G.A., Lara-Borrero J.A., Nolasco D., Rosso D. (2018). A Critical Review of the Factors Affecting Modeling Oxygen Transfer by Fine-Pore Diffusers in Activated Sludge. Water Environment Research 90(5). DOI: 10.2175/106143017x15131012152988

Bencsik D., Takács I., Budai P., Rosso D. (2021). The last barrier to accurate aeration design: The alpha factor – How to predict in time and along the reactor, In: WRRmod2021 conference proceedings, International Water Association (IWA), pp. 130-134.

Leu S.-Y., Rosso D., Larson L.E., Stenstrom M.K. (2009). Real-time aeration efficiency monitoring in the activated sludge process and methods to reduce energy consumption and operating costs. Water Environment Research 81(12), pp. 2471-81. DOI: 10.2175/106143009X425906

Rieger L., Gillot S., Langergraber G., Ohtsuki T., Shaw A., Takács I., Winkler S. (2013). Guidelines for using activated sludge models. IWA, Scientific and Technical Report No. 22.

SumoBioFilm model

The SumoBioFilm model is used in the following process units:

- BAF
- MBBR

- MABR
- Trickling filter
- Granular SBR

Model implementation

The biofilm model of Sumo (called SumoBioFilm) is developed by Dynamita to provide a reasonable simplified description of biofilm systems for wastewater process modelling. The first modelled technology was the Moving bed bioreactor solution, called MBBR.

The simplifications are the following:

1. Fixed biofilm thickness with n layers:
   The model uses an average biofilm thickness, thus layer thickness via the layer number as input parameter. Inside the biofilm layers the biofilm is ideally mixed, similar to the CSTR (Continuously Stirred Tank Reactor).
2. 1D model
   The model has 1D extension with the homogeneous biofilm layers. In the basic reactor unit biofilm composition is uniform.
3. Active media surface model
   Input parameters are required to provide information about the active surface of the media used in the technology. The specific surface, the media fill ration and the media water displacement parameters define the biofilm amount with the biofilm thickness.
4. Biofilm specific mass
   The biofilm specific mass describes the TSS content of the biofilm growing on the active surface of the media as g TSS/m^2 active media surface. This parameter defines the biofilm dry matter content which is kept during the simulation with a built in TSS controller.
5. Detailed mass transfer description for the biofilm
   The model uses 4 different transport mechanism to describe the mass transfer inside the biofilm:
6. Diffusion of components and convection for enthalpy:
   - between bulk and biofilm,
   - between biofilm layers
7. Active solids transfer between biofilm layers
8. Attachment from the bulk phase to biofilm
9. Detachment from the biofilm to the bulk phase

Biofilm characterization

The biofilm can be characterized via the following parameters at the input setup:

	Biofilm and biofilm carrier parameters		
Symbol	**Name**	**Default**	**Unit**
n	Number of biofilm layers	3	-
z_F	Biofilm thickness	300	micron

z_{BL}	Boundary layer thickness	30	micron
$X_{TSS,spec}$	Biofilm specific mass	10	g TSS.m^{-2} biofilm
$A_{sp.carrier}$	Specific surface of biofilm carrier	500	m^2 biofilm.m^{-3} loose media
$i_{carrier}$	Ratio of reactor volume filled by carriers	0.5000	m^3 loose media.m^{-3} reactor
$V_{sp.carrier}$	Water displaced by carrier	0.1800	m^3 loose media.m^{-3} reactor

From the advanced view the biofilm density can be set:

	Biofilm density		
Symbol	**Name**	**Default**	**Unit**
ρ_F	Biofilm density	1020	kg.m^{-3}

The active media/carrier surface (considered as biofilm surface) and volume is calculated as follows:

	Biofilm carrier parameters		
Symbol	**Name**	**Default**	**Unit**
$A_{carrier}$	Total biofilm carrier surface*	$i_{carrier}$*$A_{sp.carrier}$*L.V**	m^2 media/biofilm surface
$V_{carrier}$	Volume displaced by the carrier	$i_{carrier}$*$V_{sp.carrier}$*L.V	m^3
* Equals to biofilm surface. ** L.V is the reactor total volume - including liquid phase, media/carrier volume and biofilm volume. Input parameter, technically it is the depth x tank surface.			

Biofilm volume is calculated based on the above calculated biofilm surface:

	Biofilm properties		
Symbol	**Name**	**Expression**	**Unit**
A_F	Total biofilm surface	$A_{carrier}$	m^2 biofilm
z_L	Biofilm layer thickness	z_F/n	m
	Biofilm volume		
Symbol	**Name**	**Expression**	**Unit**
V_F	Biofilm volume	A_F*z_L*	m^3 biofilm
* With additional sum for each biofilm layer (can be expressed as: n * A_F * z_L)			

The biofilm dry matter (TSS) content is defined as follows:

	Biofilm properties		
Symbol	**Name**	**Expression**	**Unit**
$X_{TSS,target}$	Target TSS concentration in biofilm	$X_{TSS,spec}$ * A_F/V_F * (ρ_F * $c_{g,kg}$)/ρ_{H2O}	g TSS.m^{-3} biofilm
$X_{TSS,F}$	Dry matter content of biofilm	M,$X_{TSS,film,total}$/(V_F*ρ_F)	g.kg^{-1}
* $c_{g,kg}$ is the unit conversion between kg and g ** ρ_{H2O} is the density of water *** M,$X_{TSS,film,total}$ is the total TSS mass stored in the the biofilm (ideally as $X_{TSS,target}$ * V_F)			

Example based on default parameters

Based on the default parameters in 1 m^3 reactor volume there is 250 m^2 active carrier surface with 300-micron biofilm thickness providing a total 0.075 m^3 biofilm. The total TSS in the biofilm is 2500 g TSS, thus the

XTSS,target is 33333 g/m^3 biofilm, which is 3.26 g/kg dry matter content (based on the 1020 kg/m^3 biofilm density).

Mass transfer

The mass transfer processes are differentiated between the different components based on the specification of the component in the models. The components can be soluble, colloidal or particulate based on their characteristic. The following processes are considered in the SumoBioFilm model for each component type for the 2 main transfer surfaces:

Processes	On the surface between bulk and biofilm			Inside biofilm (surface between biofilm layers)		
	Soluble components	Colloidal components	Particulate components	Soluble components	Colloidal components	Particulate components
Diffusion	X	X		X	X	
Solids transfer			X			X
Attachment of solids			X			
Detachment of solids			X			
TSS controller						X

In general, the mass transfer processes specified above are described based on the driving force as concentration difference on the two sides of the transfer surface multiplied by a specific transfer coefficient.

Separation models

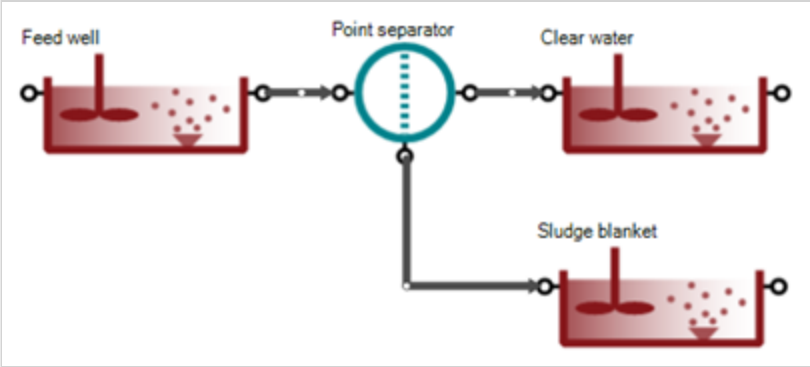
Volumeless separation model

Mass balance based algebraic models with various input parameter combinations.

Three compartment separation model

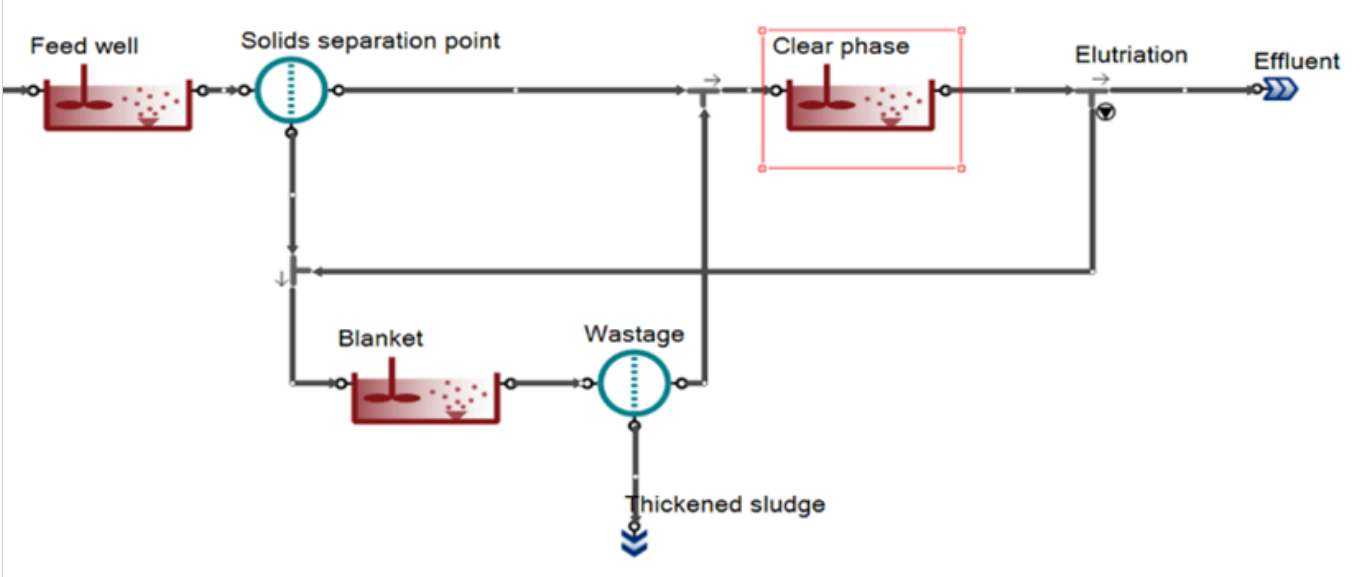
The models are valid for Sumo1, Sumo2, Sumo2C and Sumo2S models.

This is a complex unit composed with a feed well, a point separator, a clear water compartment and a sludge blanket (SM Figure 1). These three compartments are CSTR with diffused aeration and input DO units. Feedwell and Sludge blanket are reactive for model reactions. In the feed well, polymer can be added.



SM Figure 1 - Model layout of three compartment units

In sludge flow or sludge concentration specified models an elutriation flow allow natural or forced circulation of flow from sludge blanket to clear liquid to account for the diffusion of soluble components.



SM Figure 2 - Complex model layout of three compartment units with elutriation

Input parameters

Settings parameters are:

- Total volume
- Feed well volume
- Sludge blanket volume
- Sludge solids concentration or Sludge flow
- Effluent solids concentration or Percent solids solids removal (with and without polymer)

Polymer addition parameters are:

- Polymer concentration
- Rate of precipitation with polymer
- Half-saturation of polymers in flocculation

- Half-saturation of colloidal substrate in flocculation with polymers
- Half-saturation of polymers for solid percent removal improvement

Other parameters are:

- Surface of clarifier
- Elutriation rate:
  - 0: no elutriation;
  - Few % - natural elutriation
  - 1: forced elutriation to wash out VFA

Polymer addition concepts

The polymer addition in this process unit impacts the solid removal in two ways:

The colloidal substrate flocculation

The flocculation of colloidal substrates with polymer processes rates are calculated in the code sheet.

$rate_{FLOC,CB,polymer} = q_{FLOC,polymer} * Msat_{FLOC,polymer} * Msat_{CB,KFLOC,polymer} * X_{polymer}$

$rate_{FLOC,CU,polymer} = q_{FLOC,polymer} * Msat_{FLOC,polymer} * Msat_{CU,KFLOC,polymer} * X_{polymer}$

The rates are first order to polymer concentration and have a Monod saturation function on the colloidal substrate and on the polymer concentration.

The half saturation of polymers in flocculation is the half of the optimal dose to reach the maximum flocculation rate.

The removal efficiency of solids

The removal efficiency will be adjusted between the Solids percent removal without polymer and Solids percent removal with polymer values given by the user

The adjustment between the two values uses a Monod function with the half-saturation of polymers for solid percent removal improvement parameter

Triple exponential settling model

Parameter estimation

The 1-D layered settling models used in various separator process units in Sumo employ parameters that are based on Vesilind zone settling velocity lab tests. Following the release of Sumo21, continued effort was made to facilitate the use of this approach. Users are more familiar with the sludge volume index (SVI) which is also a routine lab test. Despite its shortcomings form the modeling aspect, it is a widely available data, as opposed to zone settling velocity tests.

On one hand, empirical correlation functions from literature had been evaluated and three of them (Ozinsky and Ekama, 1995; Härtel and Pöpel, 1992 – DOI:10.2166/wst.1992.0128; Daigger, 1995 – DOI:10.2175/106143095X131231) were chosen to be included as an option to estimate Vesilind settling parameters from SVI values, if the user opts to do so, instead of entering Vesilind parameters directly.

On the other hand, an Excel tool has been developed to ease the processing of the Vesilind lab test data. The key part of this task is to identify the linear section of the individual settling curves and fit a line to this part in order to derive the settling velocity for the specific MLSS concentration (the lab test is executed for a range of MLSS). The tool is capable of automatically performing this fit, after the user enters/imports the test data. The applied algorithm uses first and second differentials (akin to first and second derivatives of continuous functions) in various resolutions and a ranking mechanism based on the goodness of the fits and the range of the data used for the fits. Manual refining is also an available option. Once this task is done for all the available settling tests, the tool collects the corresponding MLSS and settling velocity data pairs and makes a fit to come up with the maximum Vesilind settling velocity and the hindered settling parameter.

Dewaterability model

A mechanistic modelling approach is identified and developed to simulate and predict sludge bound water content and dewaterability in the context of whole plant simulation. Currently, whole plant simulators do not predict bound water content and use a simplified solid-phase separation unit to model mechanical dewatering. The model unit requires cake solids concentration and solids capture percentage as inputs. This limits the use of the model to only one operational scenario unless these inputs were changed accordingly to reflect the impact of operation or new technologies in dewatering performance. The composition of wastewater and the biological, chemical and physical transformational forces applied to it play a role in how bound water content of the sludge and its dewaterability changes. We successfully applied a model to predict the bound water content and dewaterability in terms of cake solids at a large wastewater treatment plant, Virginia Initiative Plant operated by Hampton Roads Sanitary District, Virginia, USA.

Process unit descriptions

Detailed descriptions of process units available in Sumo

Introduction

This page contains the detailed description of the process units available in Sumo. Or eventually will contain. We update this content continuously.

Bioreactors

SBR (Sequencing Batch Reactor)

General description

The SBR process unit implements sequencing batch reactors in Sumo.

Port specification

The SBR process unit has 3 ports as detailed in Table 3.1.

Port name	Description
Inp	The input port of the SBR is used for feeding water into the SBR tank. Currently there is no automatic mechanism in Sumo for having feed only in certain cycle phases; the user must provide the respective feeding pattern synchronized with the SBR cycle structure manually (e.g. via input files).
Decant	The flow on the decantation port is controlled according to the SBR cycle organization – decanting from the SBR takes place through this port. The decantation port flow can be controlled manually as well; in this case the water quality appearing on this port is the bulk quality if the reactor is in mixed phase, and is equal to the supernatant quality if the reactor is not mixed.

Port name	Description
Uflow	The flow of the underflow port is controlled according to the SBR cycle organization – sludge wasting from the SBR takes place through this port. The underflow can be controlled manually as well; in this case, if the reactor is mixed, the bulk water quality is available, and the settled fraction of the reactor is available if no mixing takes place.

Table 3.1 - Port specification of the SBR

Parameters available for the user

Table 3.2, Table 3.3 and Table 3.4 provide the full parameter list available for the user. All these parameters are covered in the sections introducing the SBR operation in Sumo.

Symbol	Name	Default	Unit
A_{tank}	Surface	1000.0	m^2
$h_{tank,max}$	Depth when tank is full	5.00	m
h_{decant}	Decant to this level	3.50	m

Table 3.2 - SBR physical parameters

Symbol	Name	Default	Unit
t_{cycle}	Cycle length	6	h
t_{react}	React phase length	4	h
t_{settle}	Settle phase length	1	h
t_{decant}	Decant phase length	0.9	h
t_{waste}	Wasting phase length	0.1	h
t_{idle}	Idle phase length	0	h
t_{offset}	Cycle offset	0	h
SRT_{target}	Target SRT	10	d
$X_{TSS,decant,target}$	Effluent solids concentration	20	$g.m^{-3}$

Symbol	Name	Default	Unit
$X_{TSS,sludge,target}$	Sludge concentration	10000	$g.m^{-3}$

Table 3.3 - SBR operational parameters

Symbol	Name	Default	Unit
$S_{O2,input}$	Dissolved oxygen (O2) setpoint input	2	$g\ O_2/m^3$
α	Alpha (clean water/wastewater) factor	0.7	-
h_{sea}	Elevation above sea level	200	m
$h_{diff,floor}$	Diffuser distance from tank bottom	0.2	m
d_{diff}	Diffuser floor density (diffuser area/tank area)	0.1	m^2/m^2
A_{diff}	Area per diffuser	0.0373	m^2

Table 3.4 - SBR aeration settings

SBR cycle organization

The SBR operation is organized into cycles that are built from phases according to Table 3.5. The length of the cycles can be given in parameter *tcycle* in hours. Table 3.5 contains a short summary of the cycle phases. The phases are detailed in the sections below.

Phase name	Reactive	Mixed
reaction phase	yes	yes
settling phase	no	no
decanting phase	no	no
idling phase	no	no

Table 3.5 - SBR cycle organization as implemented in Sumo

According to the current implementation, biological reactions occur only in the reaction phase, where the reactor content is completely stirred.

Reaction phase

As it can be seen in Table 3.5 there is no separate feeding phase. Instead of a dedicated feeding phase a certain part of the reaction phase can be used for feeding the reactor. Currently there is no automatic feeding mechanism in Sumo for having feed only at certain reaction phases; the user must provide the respective feeding pattern synchronized with the SBR cycle structure, manually (e.g. via input files).

During the reaction phase all the biological reaction equations according to the user-determined biological model are calculated and the respective state and calculated variables are available through the general interfaces described in the user manual.

Settling phase

The settling method implemented currently in Sumo is quite simple: The settling efficiency is determined by the user by providing the desired effluent TSS value at the overflow and pumped ports (i.e. TSS in the settler supernatant) as well as the desired TSS concentration in the settled sludge.

The settling itself occurs instantaneously as the reactor enters the settling phase. There is no mixing and no biological reactions take place during the settling phase. The supernatant water is available via the overflow and pumped ports, whereas the settled sludge is available via the underflow port.

The length of the settling phase is determined by the parameter t_{settle} (in hours).

Decanting phase

Sumo currently works with fixed volume decanting. During the decanting there is no mixing in the reactor so there's two phases available via the respective ports. The length of the decanting phase is determined by the parameter t_{decant}, whereas the volume to be decanted is determined by the actual volume minus the surface multiplied by the decant target level(in m^3).

Sludge wasting also occurs in the last minutes of the decanting phase. The wasting phase duration is determined by the parameter t_{waste} (h). The wasted sludge amount (g/d) in one wasting phase is also determined by the user from the actual TSS mass divided by the target SRT and the number of cycles. The waste sludge volume and flow rate is determined using the sludge mass to be wasted, the settled sludge suspended solids concentration and the duration of the wasting period.

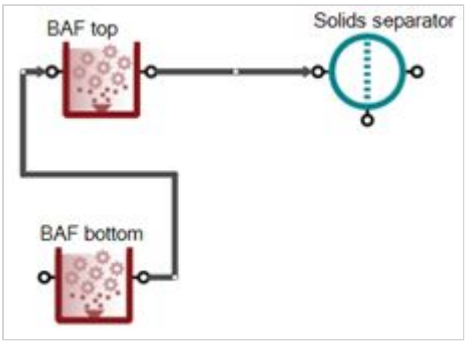
Idle phase

The length of the idling phase is the difference between the total cycle length and the sum of the reaction, settling and decanting phase duration. Neither mixing nor biological reactions take place during the idling phase.

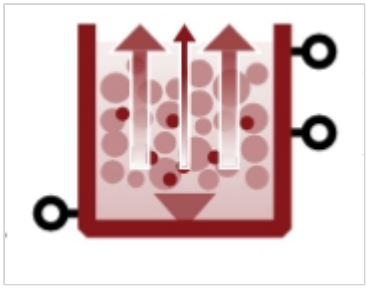
BAF (Biologically Aerated Filters)

Key points

- Upflow 2 vertical zone BAF complex unit with aeration either in bottom or top
- 1D layered heterogenous biofilm model with n layers
- Fixed film thickness as gTSS/m2 and Film thickness input
- Works with any biological model in Sumo format



This figure shows the compartmentalized version of BAF unit



This is the unit image in Sumo

Model description

This complex unit is an upflow biological filter with 2 vertical biofilm reactor zones, with aeration either in the bottom or mid height. Backwash is simulated as a continuous process flow.

The volume and the corresponding depth of the bottom reactor compartment are determined by the user input fraction of the total volume. As for the top compartment, the remaining fraction will take up the rest of the specified total volume and depth.

BAF media characteristics typically differ from those used in the underlying biofilm subunits and are mapped there from the main unit's input parameters. The media is assumed to be flooded in this type of process unit, therefore the carrier filling degree is hardcoded to be 1 m^3/m^3, with the height of water above the media depending on the water displaced by carrier.

BAF units with bottom air supply location are of a fully aerated configuration – the aeration gas composition is defined for the bottom, and the input gas composition of the top compartment is the same as that of the off-gas from the bottom.

With air supply from the middle, a BAF unit is in a denitrifying configuration – there is no air introduced to the bottom, the aeration gas composition is defined for the top compartment.

Complex units with a vertically layered gas phase inside underlying subunits require balance equation extensions for any compartment other than the bottom: For fully aerated BAF units, air is introduced at the bottom; thus

- input gas mass flows to the top have to take into account the output gas from the bottom,

- the output gas volumetric flow must include not only the top's gas transfer in volumetric unit but the off-gas flow from the bottom as well.

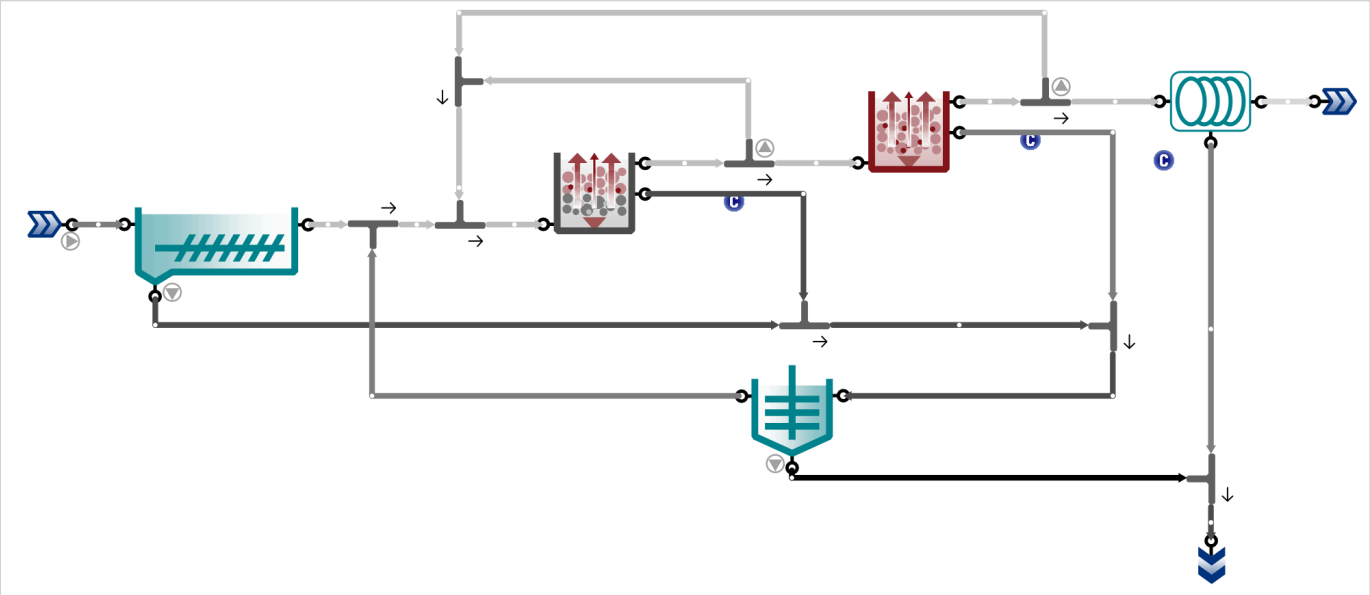
For BAF units with denitrifying configuration, air is introduced at the top; so

- along with the off-gas from the bottom, the aeration gas mass flow must also be added for the top input gas,
- apart from the gas transfer in volumetric unit from the top, the outgoing volumetric flow accounts for the air flow from the top, as well as the off-gas from the bottom.

A vertically staged gas phase within subunits of a complex unit requires saturation depth correction for any compartment other than the top: the hydrostatic pressure increases with liquid depth, so the entire height of the water column above a given compartment must be added to the effective saturation depth of its own section (by default half of the compartment depth).

Example file

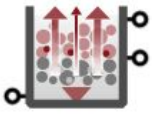
Below is the configuration setup used as an example (it can be found in the home page – BAF plant.sumo). Here two BAF units are designed in series to treat settled wastewater.



Example configuration for BAF

Input tab

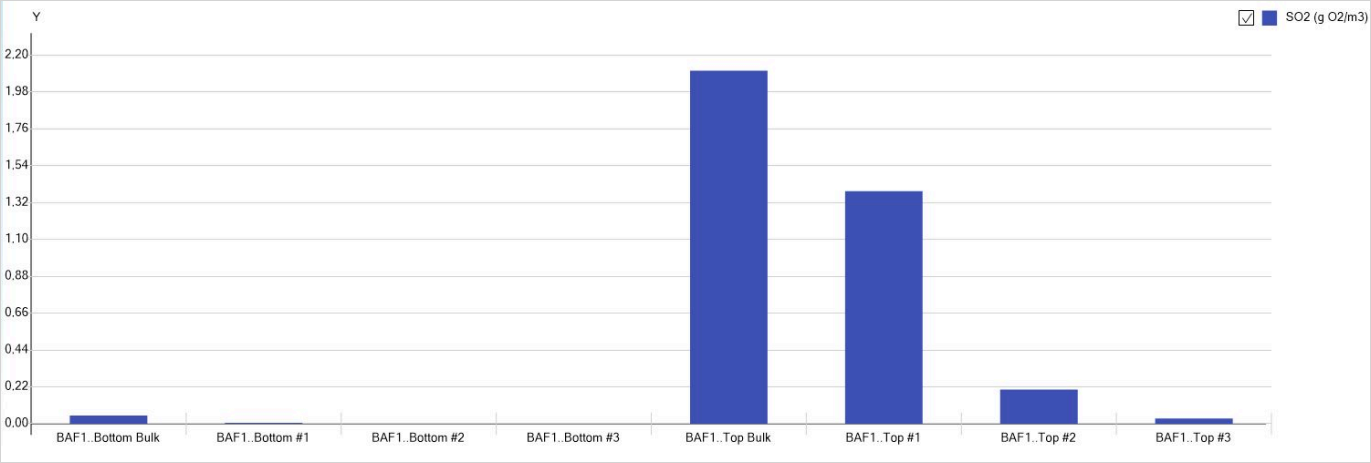
BAF1



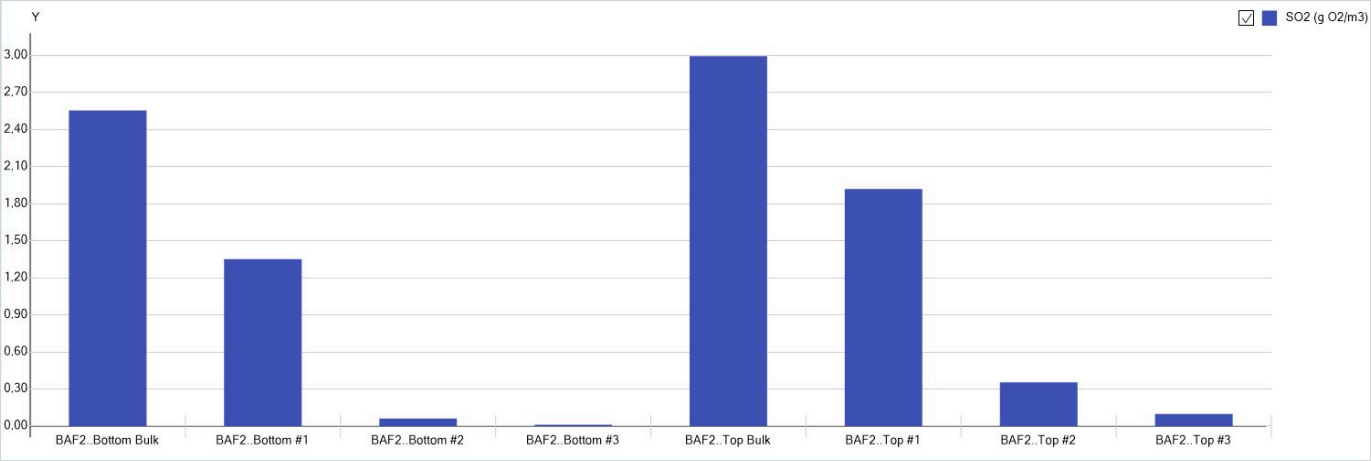
Name	Default	Value	Unit
Number of trains	1	1	
Liquid volume per train	1000.0	**1500.0**	m3
Tank depth	5.00	5.00	m
Fraction of bottom compartment to total volume	50.0	50.0	%
Solids percent removal	60.0	**80.0**	%
Backwash flow	1000.0	**1600.0**	m3/d

Reactor input information for BAF1

Results



DO profile for BAF1



DO profile for BAF2

Name	Influent	Primary Sludge	Internal recirculation	BAF1 Backwash	BAF2 Backwash	Disc filter Sludge	Effluent	Unit
Flow rate	24000	532	38400	1600	570	720	23142	m3/d
Total chemical oxygen demand mass flow	10080	3577	2410	4222	313	329	855	kg COD/d
Total suspended solids (TSS) mass flow	4434	2659	482	3224	235	244	27	kg TSS/d
Volatile suspended solids (VSS) mass flow	3763	2187	420	2811	204	212	24	kg VSS/d
Total biochemical oxygen demand (5 days) mass flow	4396	1289	791	1443	103	108	216	kg O2/d
Total nitrogen mass flow	826	120	580	201	22	25	307	kg N/d
Nitrate and nitrite (NOx) mass flow	Non-detect	Non-detect	121	2.1	6.3	8.0	256	kg N/d
Total ammonia (NHx) mass flow	576	13	376	19	0.48	0.61	20	kg N/d
Total phosphorus mass flow	103	18	78	46	4.9	5.3	41	kg P/d
Orthophosphate (PO4) mass flow	60	1.3	67	2.8	0.94	1.2	38	kg P/d

Table with mass flow information for frequently measured variables

UASB (Upflow anaerobic sludge blanket reactor)

The UASB model in Sumo was developed in two versions with different complexity levels.

a) Completely mixed approach

This is a complex unit of completely mixed reactor with suspended growth, a settling function and a wastage pump. In this type of unit, the TSS concentration in the reactor is assumed to be homogeneous, and it is controlled empirically to the user-defined target by adjusting the solids percent removal of the settling function, that may not capture the specified non-settleable fraction of the reactor TSS. The sludge underflow of the settling function is back-mixed according to the user-input flow fraction. The volumetric flow of the wastage pump is determined by the user-specified sludge mass flow target, based on the TSS concentration in the completely mixed process unit model.

b) Three compartment approach

This is a three vertical compartment-based complex unit with suspended growth, settling functions and a wastage pump. The volume and the corresponding depth of the sludge bed and sludge blanket reactor compartments are determined by the user input fraction of the total volume. As for the settling zone compartment, the remaining fraction will take up the rest of the specified total volume and depth. In this type of unit the distribution in TSS concentration between the sludge bed, sludge blanket and settling zone is estimated by a logistic function, and the average TSS is targeted by manipulating the solids percent removal of each compartment's settling function, according to the distribution curve. TSS in the sludge bed is driven by the targeted average TSS, but regulated using a function striving to ensure that the input non-settleable solids fraction is not captured. TSS in the sludge blanket and settling zone is adjusted based upon the actual average TSS concentration, to keep a reasonable sludge distribution even if the sludge bed TSS falls short of the target range.

In this three-compartment concept, user-determined volumetric flow portions of the influent are assumed to short-circuit to the sludge blanket and settling zone directly. The sludge underflow of the settling function is back-mixed at each compartment according to the user-input flow fraction. The volumetric flow of the wastage pump is determined by the user-specified sludge mass flow target, based on the TSS concentration in the sludge bed (wasted from the lowermost compartment). Complex units with a vertically layered gas phase inside underlying subunits require balance equation extensions for any compartment other than the bottom: as for UASB with a compartmented model concept, the gas moves through the sludge blanket and the settling zone; thus:

- input gas mass flows to the sludge blanket and settling zone have to take into account the output gas from the sludge bed and sludge blanket, respectively,
- the off-gas volumetric flow sludge blanket and settling zone must include not only their own respective gas transfer in volumetric unit, but the off-gas flow from the sludge bed and sludge blanket, respectively, as well.

A vertically staged gas phase within subunits of a complex unit requires saturation depth correction for any

compartment other than the top: the hydrostatic pressure increases with liquid depth, so the entire height of the water column above a given compartment must be added to the effective saturation depth of its own section (by default half of the compartment depth).

Pond and Lagoon modeling - Gen2 vs Gen3

Gen2 and Gen3 describe two different modeling concepts applied to Pond and Lagoon systems. The Gen2 model was originally developed to simulated aerated facultative lagoons whereas the Gen3 model was developed for algal systems. ***The Gen3 Pond model should be used in most cases for both Ponds and Lagoons as it is a more advanced and powerful model.*** For example, unlike the Gen2 model, the Gen3 model includes algal photosynthesis and heat exchanges/temperature modeling. The Gen2 model remains available for legacy users of this modeling approach.

a) Gen2: Flow-based pond layer exchanges

General description

The Gen2 pond/lagoon model is a “complex unit” utilizing two variable volume bioreactors (EQ tanks) to represent (1) the Water Column and (2) the Sediments or Sludge layer. As shown in the Figure below, the model includes a number of pipe connections (P1 through P18) to represent exchanges between the Water Column and the Sediment layer. Exchanges between layers are modeled using piped flows and this is different from the 3rd generation pond model which models exchanges between layers explicitly as “fluxes”. To illustrate, settling of solids from the Water Column to the Sediment layer is modeled without any bulk movement of liquid volume (flow) in the Gen3 model but does require flow in the Gen2 model through pipes P6 and P7. The Gen3 pond model is described in the next section.

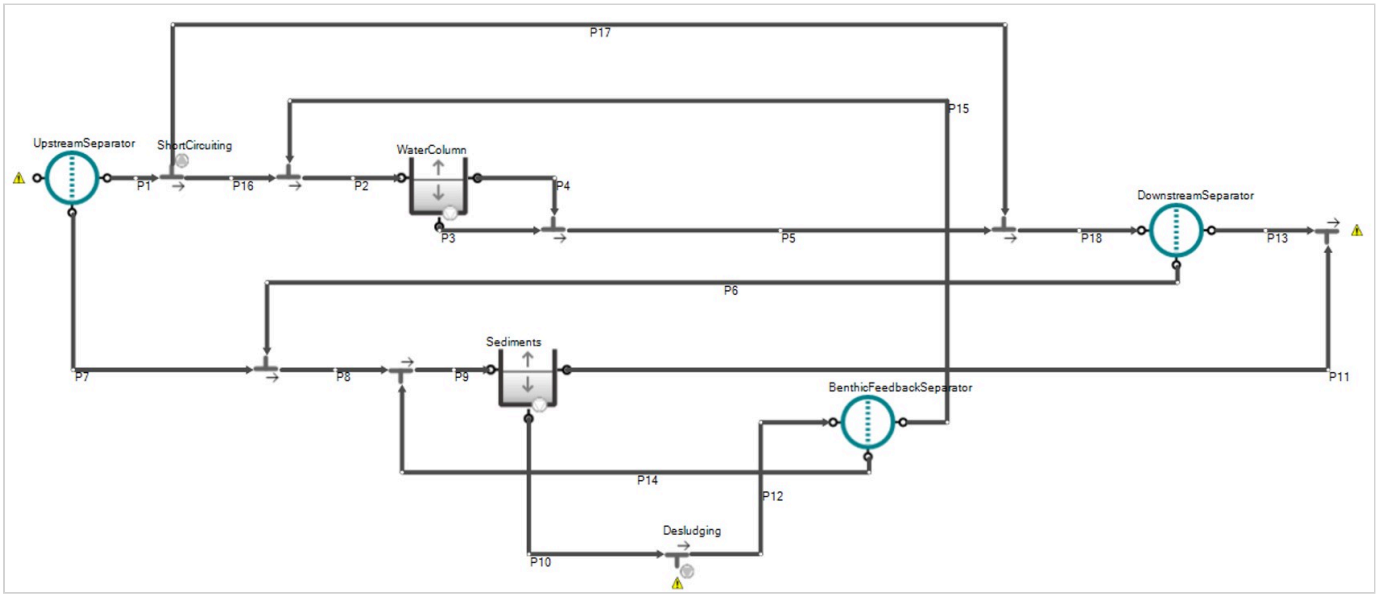


Figure: Complex flow schematic for the Gen2 Pond with flow-based layer exchanges

Model transport processes

Settling of solids from the Water Column to the Sediment layer:

In the default model configuration, Pond TSS removal is modeled downstream of the Water Column in P6. Solids capture through P7 is set to zero but can be changed in the underlying PU file. This is an advanced user feature. Pond TSS removal is specified by the user in the “Treatment Performance / Sludge Blanket Management” input form shown in the Figure below.

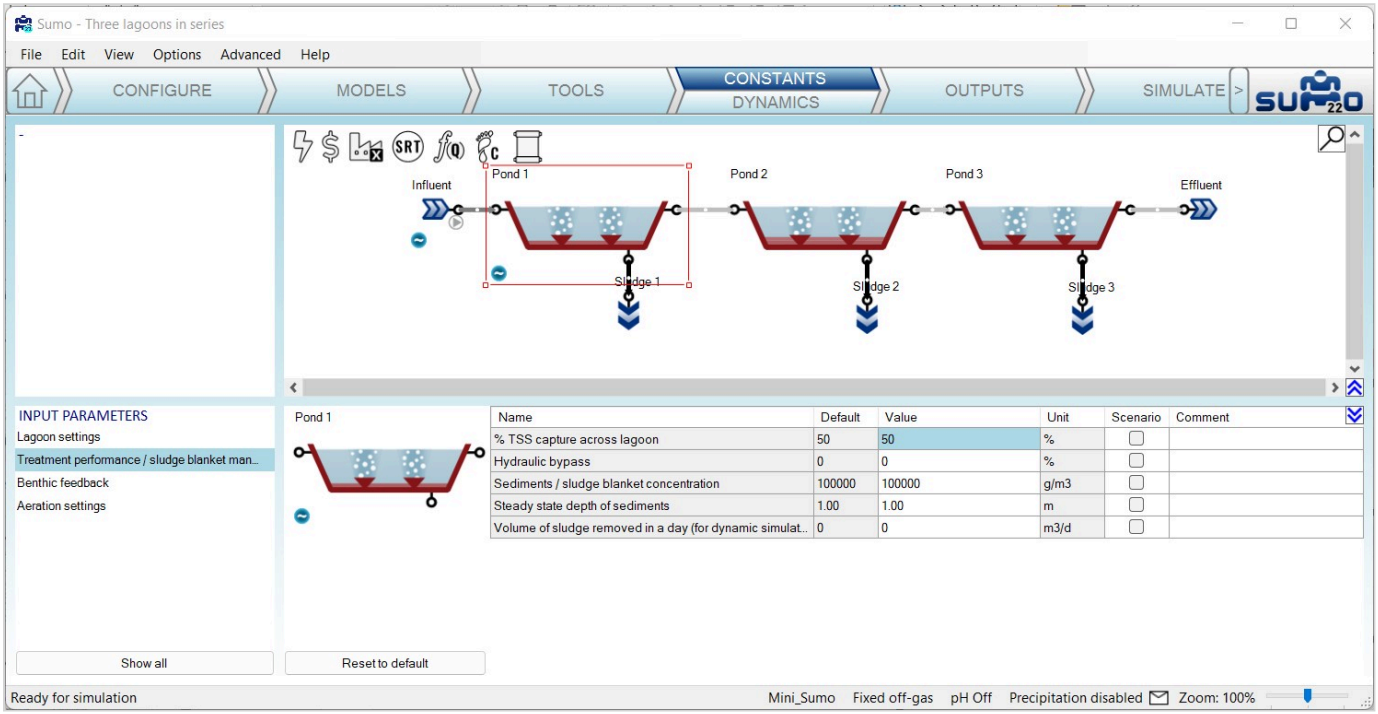


Figure: % TSS capture input form for the Gen2 pond/lagoon model

Short-circuiting or bypass:

Flow around the Water Column is modeled in P17. This flow percentage is specified in the “Treatment Performance / Sludge Blanket Management” input form shown in the above Figure.

Variable depth of Water Column and Sediments:

As Sediments accumulate at the bottom of the Pond, the decrease in Water Column depth and volume is modelled by pumping flow through P3. Pumping of flow from Sediments through P10 is modeled to achieve target sediments solids concentration as specified in “Treatment Performance / Sludge Blanket Management” input form shown in Figure 2. The default value for this parameter is 100,000 mg/L (10% solids) but this may vary based on site specific factors.

Benthic feedback from Sediments to Water Column:

Soluble components including ammonia, phosphate and volatile fatty acids (VFA) are carried from the Sediments to the Water Column in P15. Note that, in the default model configuration, only soluble components are returned and there is complete retention of particulate material in the Sediment layer in the “BenthicFeedbackSeparator”. The rate of benthic feedback from Sediments to the Water Column is specified as the rate of “Rate of benthic exchange” in the “Benthic Feedback” input form shown in the Figure below. Note that at higher rates of benthic exchange you should observe a decrease in ammonia and phosphate concentrations in the Sediments zone.

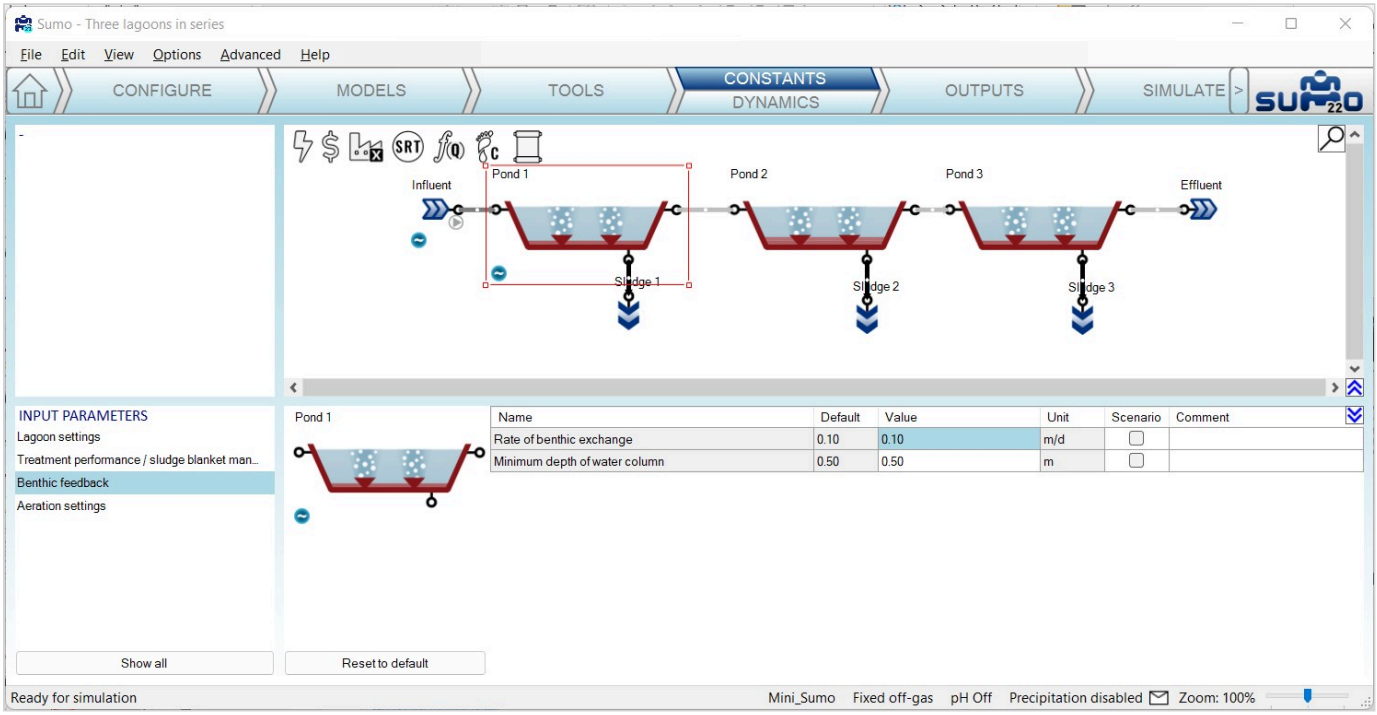


Figure: Rate of benthic exchange input form for the Gen2 pond/lagoon model

Scouring of the Sediments:

In cases where the Sediment layer has reached its maximum allowable depth, scouring of Sediments returns both particulate and soluble material to the Pond effluent through P11 and the % TSS capture specified by the user will likely not be achieved. The maximum allowable depth of the Sediment layer is defined with respect to the Minimum depth of Water Column defined in the “Benthic Feedback” input form shown in the above Figure.

Desludging:

The “Desludging” flow splitter connected to P10 can be used to simulate manual removal of sludge from the Sediment layer. In “Steady state”, the model will calculate the desludging flow required to achieve the target “Steady state depth of sediments” specified in the “Treatment Performance / Sludge Blanket Management”. In dynamic simulations, the user must specify the “Volume of sludge removed in a day” which by default is zero. This value can be specified dynamically to simulate desludging after several years of operation as demonstrated in the example file “Three lagoons in series” and shown in the Figure below.

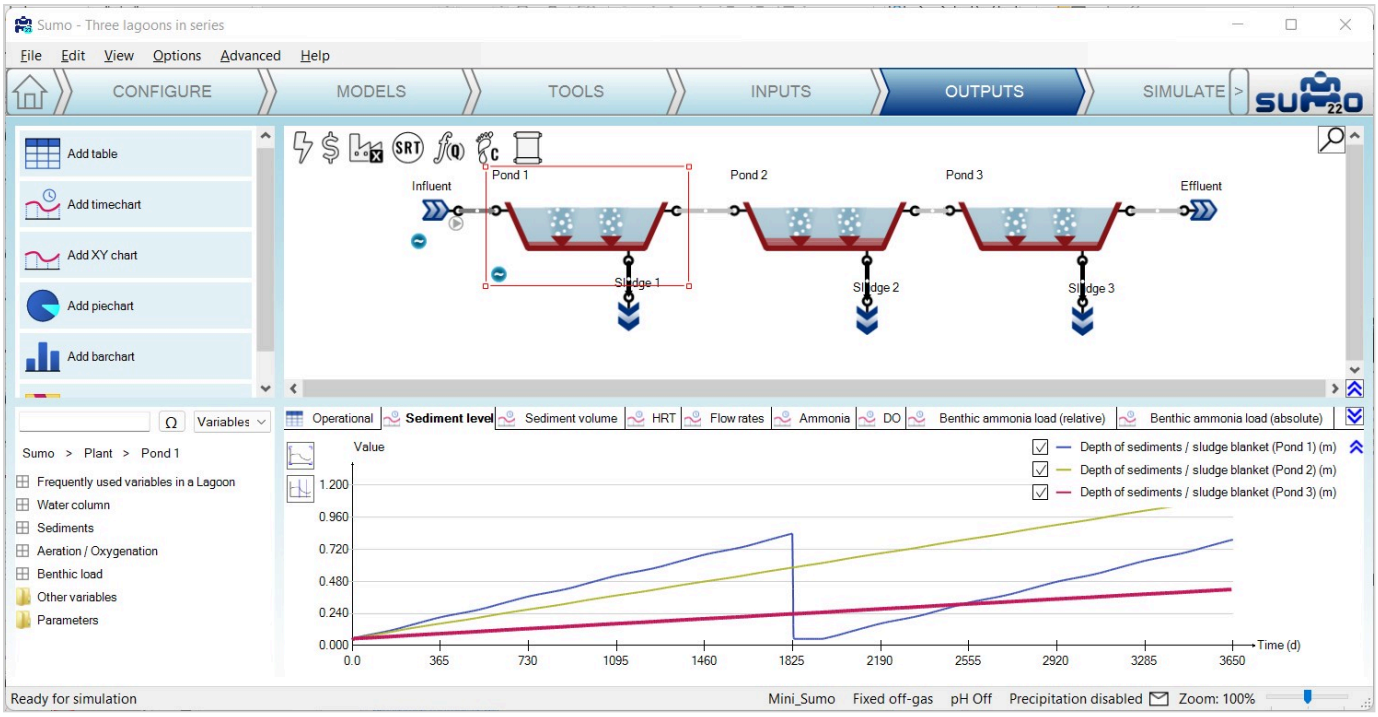


Figure: Simulation of pond sediment depth accumulation with desludging event after 5 years

Pond Reactive Model:

The Water Column and the Sediments are compatible with all of the standard Sumo model libraries though Mini_Sumo is recommended for fastest simulation times. The difference in reactions modeled in the Water Column and Sediment layer relate only to the availability of oxygen, hydraulic and solids residence times and solids concentrations. In most cases the Sediment layer will generate methane and the Water Column may be aerobic or anaerobic based on the ratio of BOD loading to Pond surface area and mechanical aeration.

Pond Aeration:

Oxygen transfer is modeled into the Water Column through a combination of natural surface transfer, mechanical surface aeration or subsurface diffused aeration. The default diffused aeration model is “Coarse bubble” though this can be modified in the “Configure” step of the SUMO model setup. The airflow rate or mechanical aeration energy input may be changed in the “Aeration settings” input form.

b) Gen3: Flux-based pond layer exchanges

General description

The default depth (1.5 m) and aeration intensity (0.5 W/m^3) of the Gen3 model is representative of a facultative pond in which algal photosynthesis and natural surface aeration are the primary drivers for oxygenation. However, these defaults can be user specified to simulate a wide range of waste stabilization pond designs including anaerobic ponds and lagoons with higher mechanical aeration intensities.

The Gen3 pond/lagoon model in SUMO22 explicitly models settling of particulate material from the Water Column to the Sediments as a flux and thus is a simpler and more powerful modeling approach than the Gen2 model. Unlike the Gen2 model, it includes algal photosynthesis and heat exchanges for dynamic simulation of temperatures.

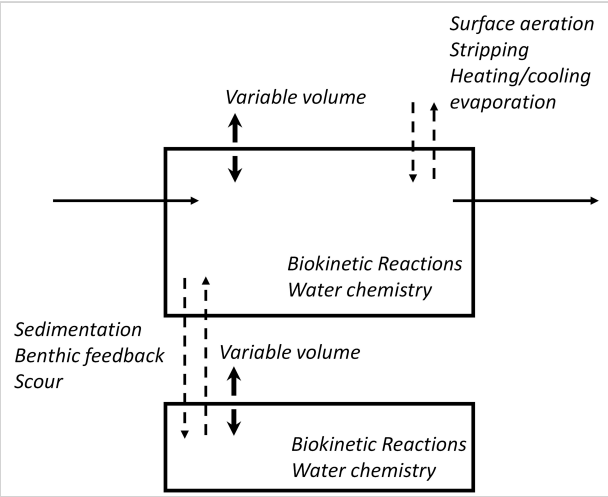


Figure: Gen3 pond model schematic illustrating explicit modeling of exchanges of particulate and soluble material between Water Column and Sediments and surface exchanges including Heating and Cooling

Transport model

The model input parameters from the SUMO “INPUT” tab are presented in the following tables. Note that the “Heat transfer parameters” only appear if the option “Calculate heat loss and gain” is selected in the “CONFIGURE” tab.

Volumes and hydraulics

The physical input parameters for the Gen3 pond model are presented in the Table below:

Name	Default	Units	Comments
Initial liquid volume	96,000	m^3	Liquid volume at simulation start.
Maximum liquid volume	96,000	m^3	Default volume set to provide 4 days of hydraulic retention time with the default influent flow of 24,000 m^3/d. Change to represent site conditions.
Maximum liquid depth	1.5	m	Surface area is calculated based on volume and this depth.

Name	Default	Units	Comments
Initial volume of sediments	6,400	m3	Volume of sediments at simulation start.

Settling rates

The model parameters which govern settling processes in the Gen3 model are presented in the Table below:

Name	Default	Units	Comments
Settling rate of particulates	0.5	d^{-1}	First-order settling rate of all particulate material except heterotrophs, nitrifiers and algae.
Settling rate of ordinary heterotrophs	0.5	d^{-1}	First-order settling rate of heterotrophs.
Settling rate of nitrifiers	0.05	d^{-1}	First-order settling rate of nitrifiers.
Settling rate of algae	0.05	d^{-1}	First-order settling rate of algae.
Non settleable TSS	15	$g.m^{-3}$	As Water Column TSS concentration approaches this value, all particulate material settling rates are switched to zero. By raising this parameter value, the Water Column TSS concentration can be calibrated to a desired value.
Sediment layer fraction for scouring process	0.8	unitless	As the ratio of Sediment volume to total liquid volume approaches this value, release of particulate material from the Sediment layer to the Water Column (scouring) is switched on.

Sediments or sludge layer

The model parameters which govern settling processes in the Gen3 model are presented in the Table below:

Name	Default	Units	Comments
Concentration of total solids or dry matter (XDM) in	0.1	-	The volume of the sediments will be calculated based on the mass of solids in the layer divided by

Name	Default	Units	Comments
sediments			this value. The default value of 0.1, or 10% dry solids, corresponds to an equivalent concentration of 100,000 g/m^3.
Volume of sediments removed per day by desludging	0	$m^3.d^{-1}$	The volume of solids removed through desludging per day. This parameter is only used in dynamic simulations and is best simulated as a dynamic input.
Steady state depth of sediments	0.1	m	During steady state simulations, the model will calculate the equivalent average daily sludge removal required to achieve this sediment depth.

Benthic release

The model parameters which govern benthic release in the Gen3 model are presented in the Table below. Benthic release refers to the exchange of soluble material from the Sediments to the Water Column.

Name	Default	Units	Comments
Diffusion constant for solubles in sludge blanket	1.00E-04	$m^2.d^{-1}$	Governs the rate of diffusion of soluble components from the Sediments to the Water Column.
Mass transfer resistance layer at interface of sediments and water column	0.01	m	Used in calculating the rate of diffusion of soluble components from the Sediments to the Water Column.
Ratio of saturation for ebullition in water column	1.5	unitless	Bubble forming of oxygen generated from photosynthesis is modeled at a multiple of the saturation concentration calculated from liquid temperature and atmospheric partial pressure.
Ratio of saturation for ebullition in sediments	10	unitless	Bubble forming of methane generated from anaerobic digestion is modeled at a multiple of the saturation concentration calculated from liquid temperature and atmospheric partial pressure.

Environmental parameters

The environmental model parameters which govern photosynthesis and heat exchanges in the Gen3 model are presented in the Table below.

Name	Default	Units	Comments
Solar radiation for algal photosynthesis - depth averaged	100	$W.m^{-2}$	Depth averaged solar radiation in wavelength spectrum useful for photosynthetic activity. Specify as a dynamic input to account for diurnal and seasonal variations.
Optimal irradiation for photosynthesis - depth averaged	100	$W.m^{-2}$	Solar radiation for optimal photosynthetic activity.
TSS concentration for calculating light extinction switching factor	100	$g.m^{-3}$	Accounts for shading effect. For highly loaded ponds with Water Column TSS concentrations above this value, no photosynthetic growth will be simulated. For low loaded pond, algal growth will occur until Water Column TSS (including algal component) reaches this value. This value varies based on depth and can be used as a calibration parameter.
Solar radiation for pond heating	200	$W.m^{-2}$	Solar radiation used in heat model.
Wind speed	10	$km.h^{-1}$	Used for calculating convection in heat model.
Air temperature	15	°C	Used in heat model and aeration model.
Ground temperature	15	°C	Used in heat model.
Relative humidity	70	%	Used in heat model.

Mechanical aeration settings

The model parameters which govern mechanical aeration in the Gen3 model are presented in the Table below.

Name	Default	Units	Comments
Wire power of aeration system	50	kW	
Standard aeration efficiency	1.5	kg O_2/kWh	

Name	Default	Units	Comments
Motor efficiency	70	%	
Alpha (wastewater/clean water) factor	0.9	unitless	
Elevation above sea level	200	m	

Heat transfer parameters

The model parameters which govern heat exchange in the Gen3 model are presented in the Table below. Note that this table only appears if the option “Calculate heat loss and gain” is selected in the SUMO “CONFIGURE” tab.

Name	Default	Units	Comments
Heat transfer velocity of the wind of walls	8.37E+04	$J.m^{-2}.K$	
Stefan Boltzman constant for long wave atmospheric radiation heat term	5.67E-08	$J.m^{-2}.s^{-1}.K^{-4}$	
Emissivity of water surface for long wave atmospheric radiation heat term	9.70E-01	unitless	
Atmospheric radiation factor for long wave atmospheric radiation heat term	8.50E-01	unitless	
Reflectivity of water for long wave atmospheric radiation heat term	3.00E-02	unitless	
Heat capacity of air	1.00E+00	$J.g^{-1}.K^{-1}$	
Heat of biological reaction	8.00E-03	$MJ.g\ COD^{-1}$	

Biological model

The Gen3 pond model is compatible with all the standard SUMO biokinetic models including Sumo1, Sumo2, Mini_Sumo, Sumo2C, Sumo2S and Sumo4N with the added feature that it also includes algal photosynthesis.

Growth is dependent on the user input "Solar radiation for algal photosynthesis - depth averaged" which may vary depending on time of day (there is no sunlight at night), latitude and season, cloud cover as well as the depth of the pond. It is the user's responsibility to account for these factors when specifying the depth averaged solar radiation. Specifying diurnal and seasonal variations of solar radiation is possible using Input Dynamics.

The effect of shading in the water column due to influent particulate material, as well as algae itself, is accounted for using the parameter "TSS concentration for calculating light extinction switching factor". When the simulated TSS concentration in the water column approaches this value, the growth rate of algae switches to zero regardless of what the specified value is for "Solar radiation for algal photosynthesis - depth averaged".

Growth of algae is accompanied by assimilation of ammonia as a nutrient source unless ammonia becomes limiting in which case nitrate is assimilated. Phosphorus and carbon dioxide are also assimilated for growth.

Respiration of algae is simulated when oxygen is available. Respiration means the conversion of algae into water, CO2, ammonia and phosphate by oxydation using oxygen. In the absence of oxygen, the respiration rate switches to zero and decay of algae is switched on. Decay means the lysis of algae into particulate organic material, ammonia and phosphate and occurs in the pond sediments where oxygen is absent.

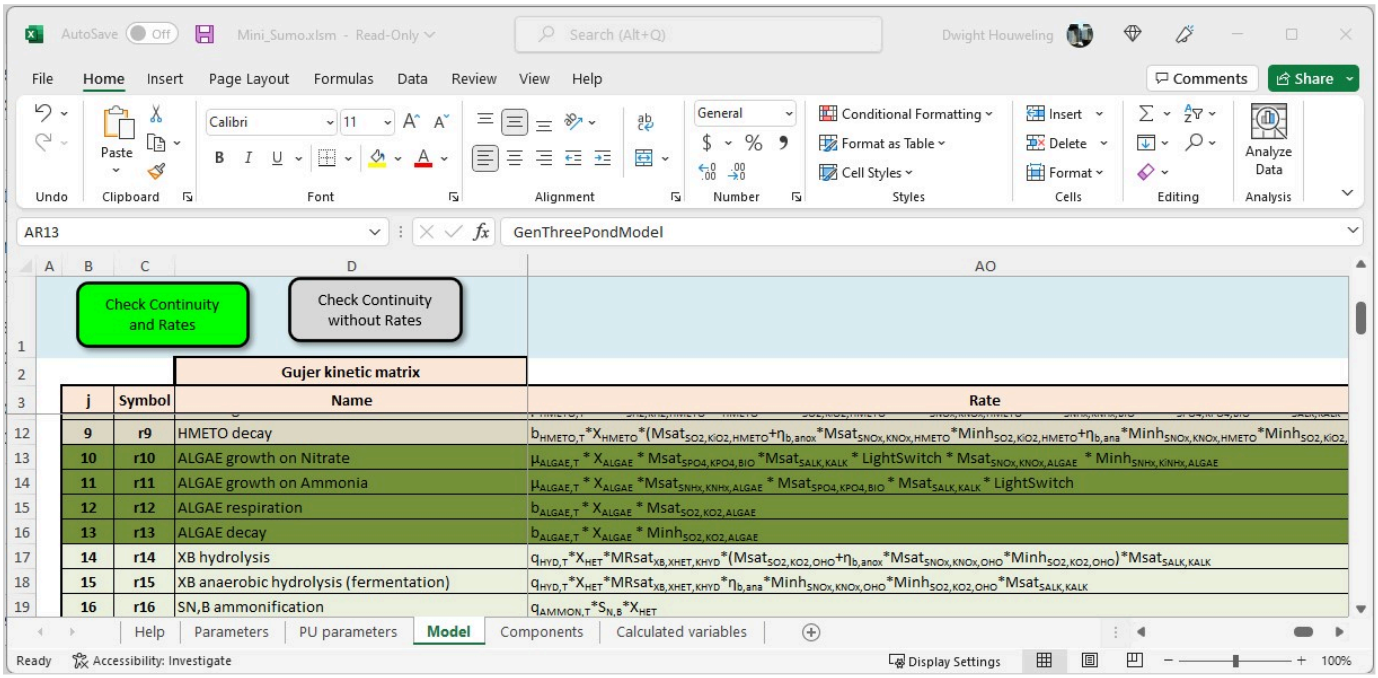
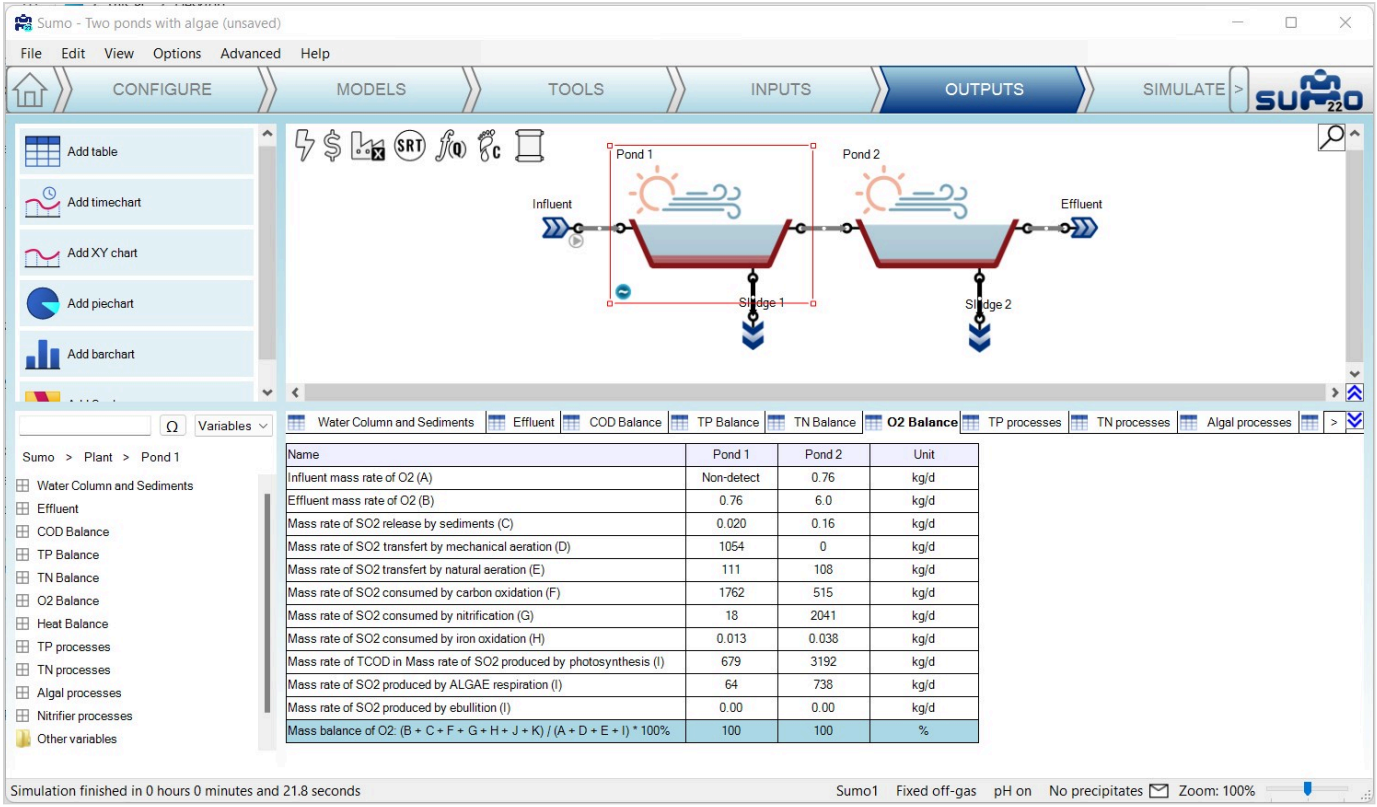


Figure: Algal growth model including “LightSwitch” parameter which accounts for solar radiation input by the user and shading factor as calculated based on simulated Water Column TSS

Mass balances

Mass balances for COD, TP, TN, O2 and Heat are provided for convenient output to tables, bar charts or pie charts. These data represent the mass balance for the Water Column and not the entire Pond. As illustrated in the Figure below, the bottom line item should be at or near 100% when the pond is at steady state.

In addition to indicating whether the Pond is in steady state, this table can indicate the most significant processes governing Pond behavior. In this case we see that mechanical aeration (line item D) is more significant than photosynthesis (line item I) in Pond 1 but not in Pond 2.



Name	Pond 1	Pond 2	Unit
Influent mass rate of O2 (A)	Non-detect	0.76	kg/d
Effluent mass rate of O2 (B)	0.76	6.0	kg/d
Mass rate of SO2 release by sediments (C)	0.020	0.16	kg/d
Mass rate of SO2 transfert by mechanical aeration (D)	1054	0	kg/d
Mass rate of SO2 transfert by natural aeration (E)	111	108	kg/d
Mass rate of SO2 consumed by carbon oxidation (F)	1762	515	kg/d
Mass rate of SO2 consumed by nitrification (G)	18	2041	kg/d
Mass rate of SO2 consumed by iron oxidation (H)	0.013	0.038	kg/d
Mass rate of TCOD in Mass rate of SO2 produced by photosynthesis (I)	679	3192	kg/d
Mass rate of SO2 produced by ALGAE respiration (I)	64	738	kg/d
Mass rate of SO2 produced by ebullition (I)	0.00	0.00	kg/d
Mass balance of O2: (B + C + F + G + H + J + K) / (A + D + E + I) * 100%	100	100	%

Conversion processes

Conversion rates of interest to TP, TN, Algal and Nitrifier processes provide additional insight into Pond behavior. As illustrated in the Figure below, the purple bar "Settling of TN to sediments" is larger than the turquoise bar "Release of ammonia from sediments" indicating net accumulation of nitrogen in the Sediment layer. In addition the pink bar "Assimilation rate for TN by all OHOs" is of a similar magnitude to the settling rate of TN indicating the role of heterotrophic assimilation in the overall TN balance.

Investigating "Algal processes" and "Nitrifier processes" can provide insights into relative magnitude or growth rates, settling and washout rates into the effluent.

Tools in Sumo

Description of available tools in Sumo.

Introduction

Sumo comes with a set of Excel-based tools to assist your work. This page contains more in-depth information about the available tools in Sumo. We are continuously working on this content to have all the details you are looking for.

How to work with Sumo Excel Tools

In general, Sumo tools are accessible via buttons on the Inputs tab of the relevant process units (e.g. the Influent tool can be opened from the Influent process unit). When you start up a tool from a Sumo project, an Excel file will be opened with the default values. This file will have a unique filename, so that Sumo can assign it to the actual unit and store it within the sumo project file (.sumo, .msumo, etc.) for later use, when it is saved. Thus, multiple Excel tool files can be stored with the project (imagine having multiple influents, each with their own setup, based on data in individual Influent Tool files). This way you can keep all project-related changes to the Excel Tool file(s) within the Sumo project, which comes handy for archiving purposes, as well as when you are working in a group.

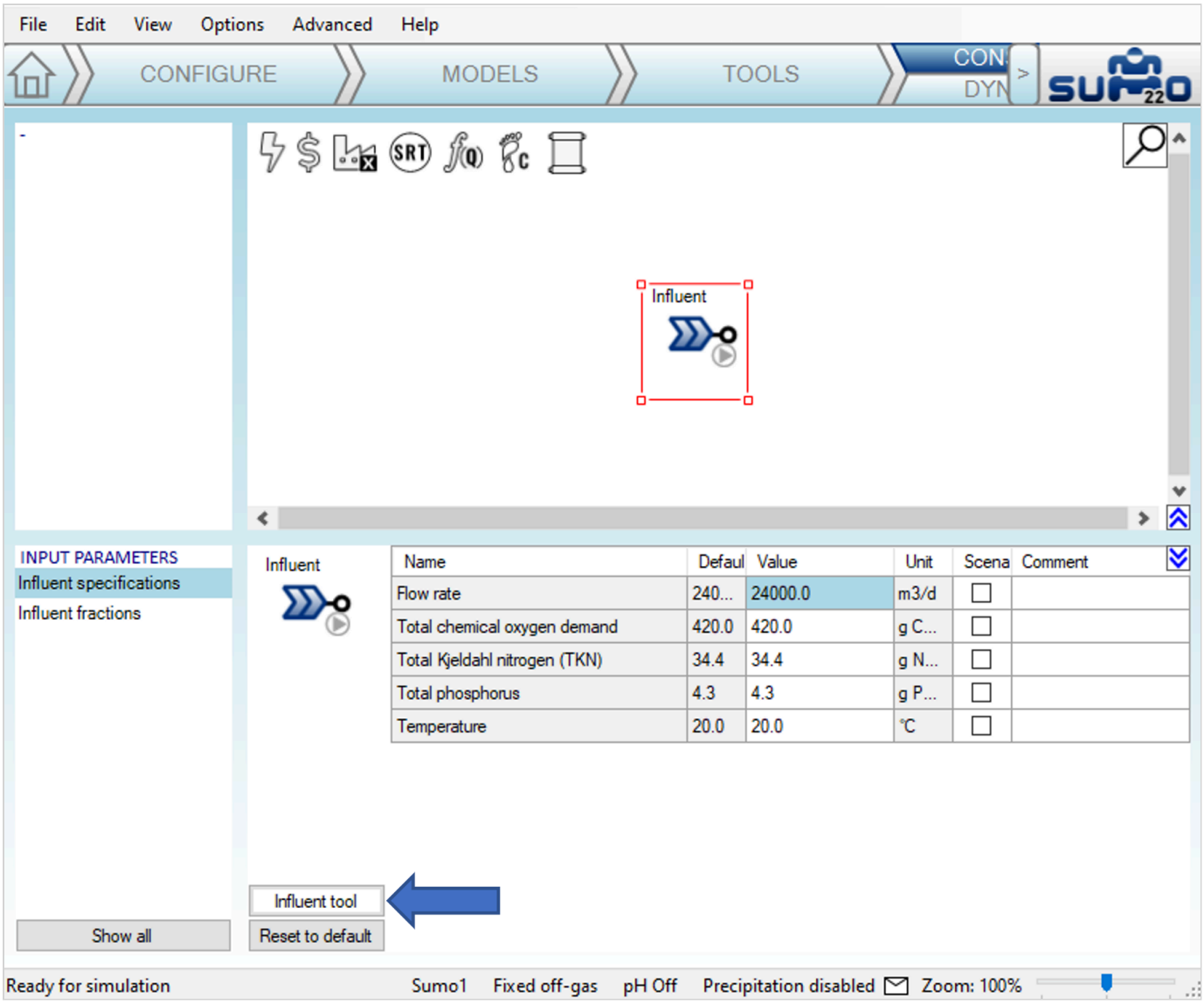
If you modify the contents of an Excel Tool file (which is very likely to happen), please make sure that you save it in Excel before saving your project in Sumo, as a project save command in Sumo will pack the saved version of any Excel Tool file that has been associated with the project. So the correct way to handle the management of project-assigned Excel Tool files, is to 1) always save all changes while the tool files are open in Excel and then 2) save your Sumo project.

When a process unit has a saved version of an Excel Tool file in a project, it is indicated by the blue color of the tool button (otherwise being white). If the project is opened again, by clicking the blue tool button on the Input tab, it will open up the relevant file with the last saved data in it.

Influent tool

The purpose of this tool is to help users fractionate their measured influent data into different COD, TKN, and TP fractions that is needed to properly set up the influent model input. Each of the Sumo full plant and focus models have a raw influent and a primary effluent tool which can be accessed by clicking on the influent unit in the Input tab (it is available at the bottom of the screen). The tool is Excel based and is specific to the project and the influent unit. Once the fractionation has been performed, the values should be saved in Excel and become part of the project. This tool will allow users to identify fractions for a constant dataset, meaning, it should be used for average values of a dataset. If multiple datasets are to be fractionated such as winter

versus summer, then two tools must be used and saved with different names as part of the project. If the file name is changed, the file can be retrieved from the project directory.

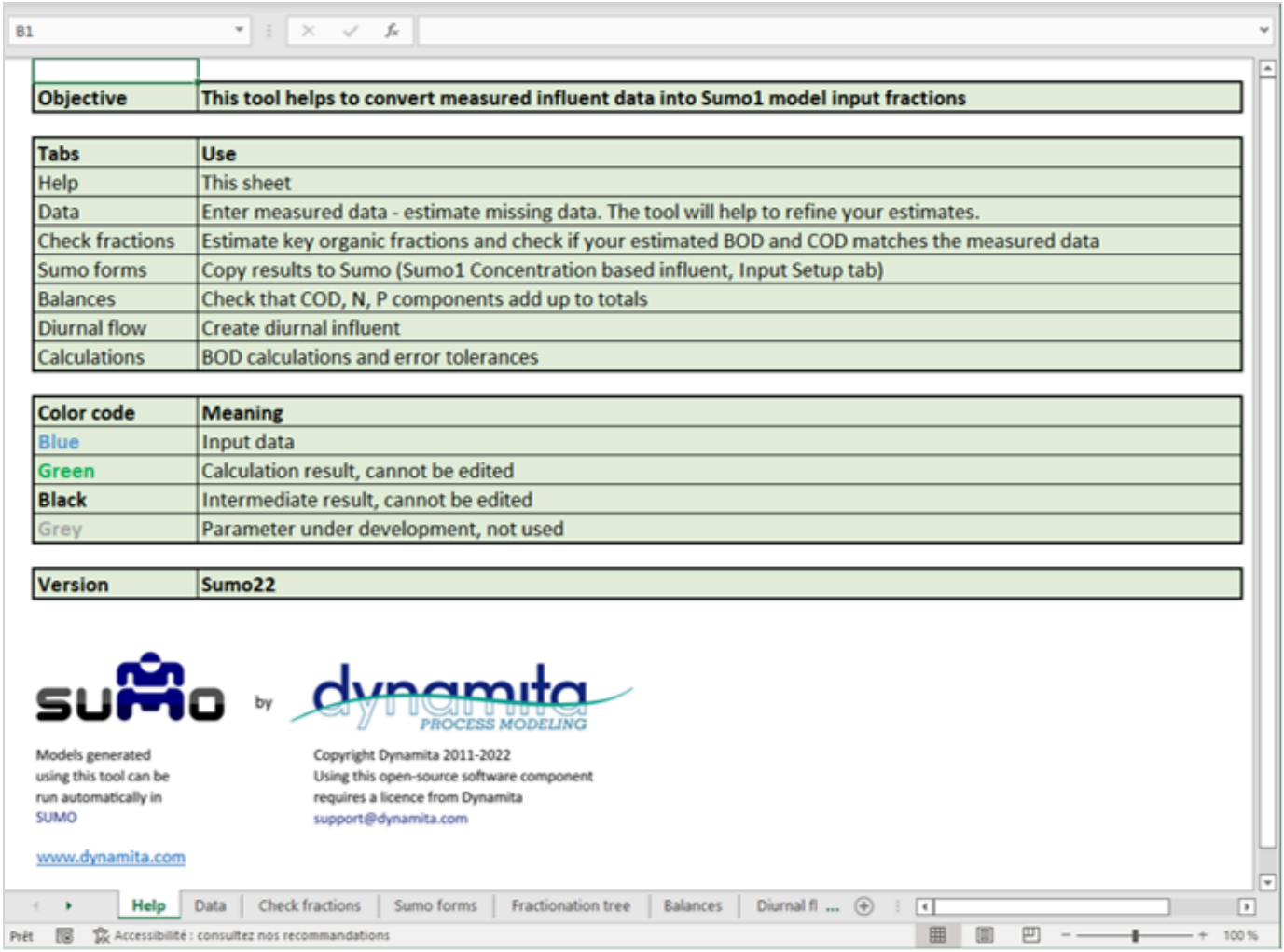


Influent Tool Figure 1 - Open from Sumo

Influent fractionation is one of the key tasks in process modeling and it is very important for users to familiarize themselves with the fractions and the fractionation workflow process. More details can be found in the Influent characterization chapter. Here we present a brief overview of the workflow a user must follow to achieve a successful fractionation and the logic behind the fractionation tool.

Step 1 - Help sheet

Read the **Help** sheet, it provides brief information regarding the use of the tool.



Objective	This tool helps to convert measured influent data into Sumo1 model input fractions

Tabs	Use
Help	This sheet
Data	Enter measured data - estimate missing data. The tool will help to refine your estimates.
Check fractions	Estimate key organic fractions and check if your estimated BOD and COD matches the measured data
Sumo forms	Copy results to Sumo (Sumo1 Concentration based influent, Input Setup tab)
Balances	Check that COD, N, P components add up to totals
Diurnal flow	Create diurnal influent
Calculations	BOD calculations and error tolerances

Color code	Meaning
Blue	Input data
Green	Calculation result, cannot be edited
Black	Intermediate result, cannot be edited
Grey	Parameter under development, not used

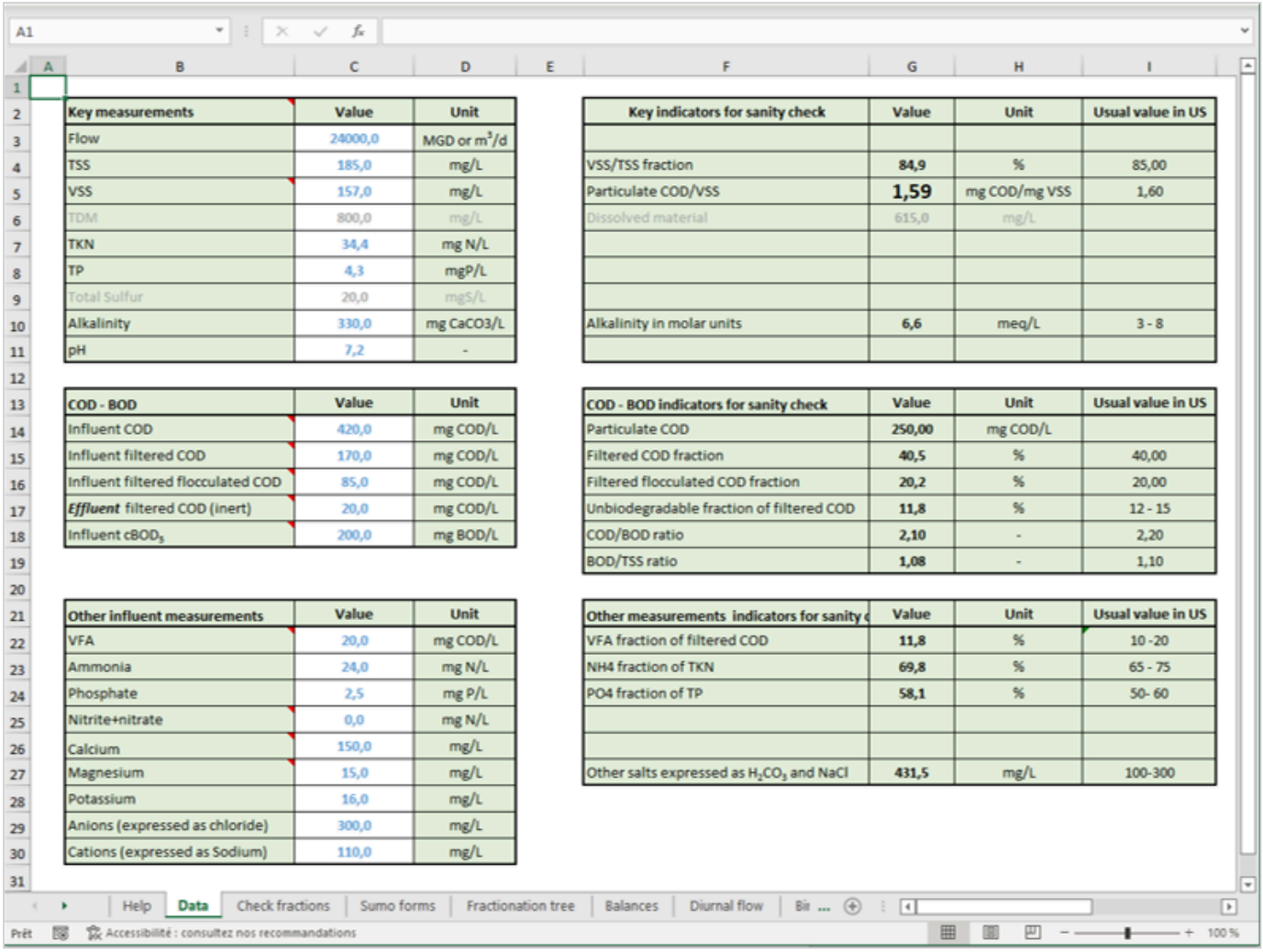
Version	Sumo22

Influent Tool Figure 2 - Help sheet

Step 2 - Data sheet

In the **Data** sheet tool input the available dataset wherever the values are blue (Column C).

- If any of the values are missing, then use the key indicators for sanity check as a guide to estimate the missing values. For instance, if the total COD value is not available then use a typical COD/BOD ratio of your plant or use our recommended value of 2.2-2.5.
- Once all values are provided, the tool calculates key indicators for a sanity check in Column H. One must make sure that they seem reasonable before proceeding.



Key measurements	Value	Unit
Flow	24000,0	MGD or m^3/d
TSS	185,0	mg/L
VSS	157,0	mg/L
TDM	800,0	mg/L
TKN	34,4	mg N/L
TP	4,3	mgP/L
Total Sulfur	20,0	mgS/L
Alkalinity	330,0	mg CaCO3/L
pH	7,2	-

Key indicators for sanity check	Value	Unit	Usual value in US
VSS/TSS fraction	84,9	%	85,00
Particulate COD/VSS	1,59	mg COD/mg VSS	1,60
Dissolved material	615,0	mg/L	
Alkalinity in molar units	6,6	meq/L	3 - 8

COD - BOD	Value	Unit
Influent COD	420,0	mg COD/L
Influent filtered COD	170,0	mg COD/L
Influent filtered flocculated COD	85,0	mg COD/L
Effluent filtered COD (inert)	20,0	mg COD/L
Influent $cBOD_5$	200,0	mg BOD/L

COD - BOD indicators for sanity check	Value	Unit	Usual value in US
Particulate COD	250,00	mg COD/L	
Filtered COD fraction	40,5	%	40,00
Filtered flocculated COD fraction	20,2	%	20,00
Unbiodegradable fraction of filtered COD	11,8	%	12 - 15
COD/BOD ratio	2,10	-	2,20
BOD/TSS ratio	1,08	-	1,10

Other influent measurements	Value	Unit
VFA	20,0	mg COD/L
Ammonia	24,0	mg N/L
Phosphate	2,5	mg P/L
Nitrite+nitrate	0,0	mg N/L
Calcium	150,0	mg/L
Magnesium	15,0	mg/L
Potassium	16,0	mg/L
Anions (expressed as chloride)	300,0	mg/L
Cations (expressed as Sodium)	110,0	mg/L

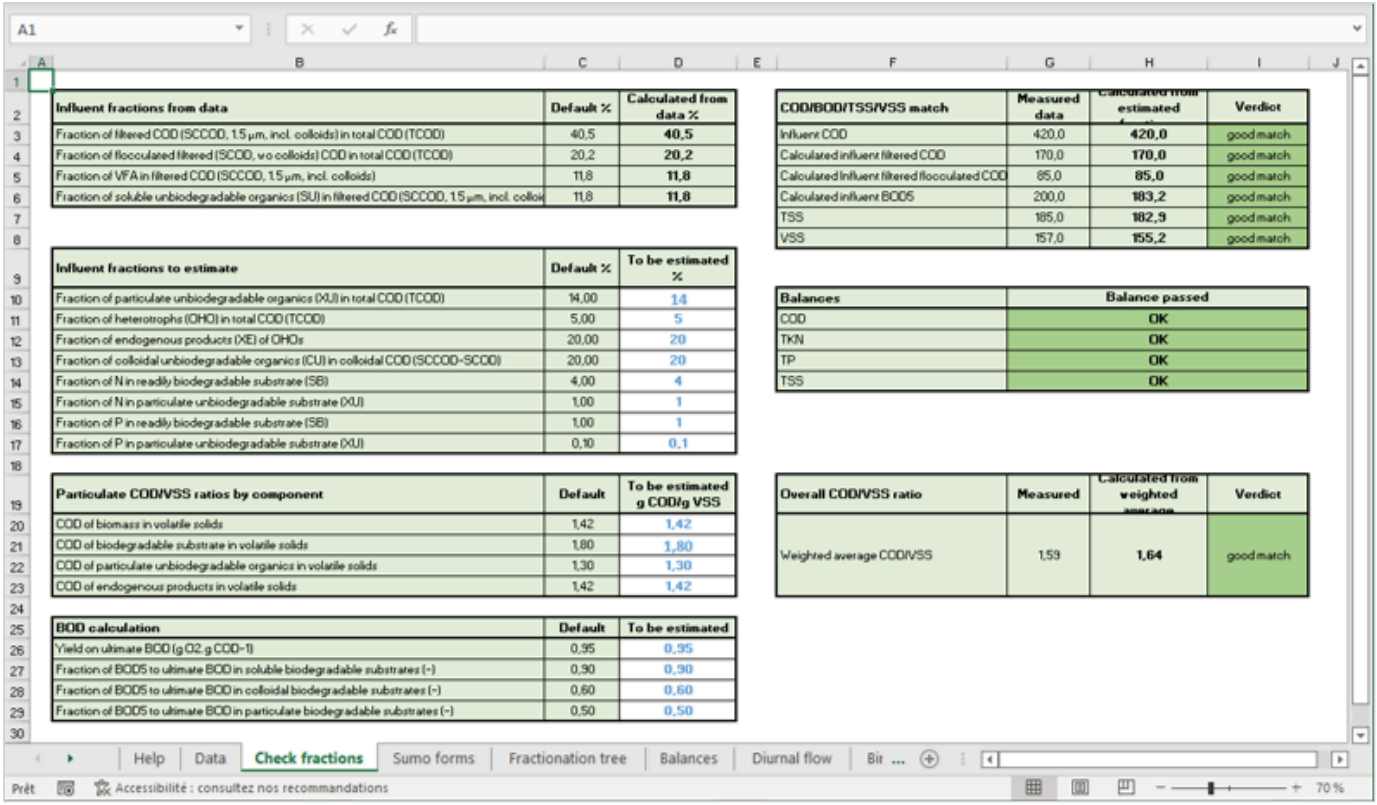
Other measurements indicators for sanity c	Value	Unit	Usual value in US
VFA fraction of filtered COD	11,8	%	10 -20
NH4 fraction of TKN	69,8	%	65 - 75
PO4 fraction of TP	58,1	%	50- 60
Other salts expressed as H_2CO_3 and NaCl	431,5	mg/L	100-300

Influent Tool Figure 3 - Data sheet

Step 3 - Check fractions sheet

The **Check fractions** sheet is for:

- Comparing three main parameters (Calculated influent BOD_5, TSS, and VSS) that are provided by the user and calculated based on the fractions identified in Column D of table named Influent fractions to estimate. These fractions can be adjusted to improve the match between data and calculated parameters indicated in COD/BOD/TSS/VSS match table on the right. If comparison is off for BOD by 25% and TSS&VSS by 15% then the verdict will be a no match. Details of the decision matrix can be seen in the Error tolerances table on sheet named **Calculations**.
  The values in the Table called Particulate COD/VSS ratios by component and BOD calculation are used for estimating the parameters as well. These should be adjusted based understanding the type of wastewater user is dealing with.



Influent fractions from data	Default %	Calculated from data %
Fraction of filtered COD (SCCOD, 1.5 µm, incl. colloids) in total COD (TCOD)	40,5	**40,5**
Fraction of flocculated filtered (SCOD, w o colloids) COD in total COD (TCOD)	20,2	**20,2**
Fraction of VFA in filtered COD (SCCOD, 1.5 µm, incl. colloids)	11,8	**11,8**
Fraction of soluble unbiodegradable organics (SU) in filtered COD (SCCOD, 1.5 µm, incl. colloi	11,8	**11,8**

COD/BOD/TSS/VSS match	Measured data	Calculated from estimated	Verdict
Influent COD	420,0	**420,0**	good match
Calculated influent filtered COD	170,0	**170,0**	good match
Calculated influent filtered flocculated COD	85,0	**85,0**	good match
Calculated influent BOD5	200,0	**183,2**	good match
TSS	185,0	**182,9**	good match
VSS	157,0	**155,2**	good match

Influent fractions to estimate	Default %	To be estimated %
Fraction of particulate unbiodegradable organics (XU) in total COD (TCOD)	14,00	14
Fraction of heterotrophs (OHO) in total COD (TCOD)	5,00	5
Fraction of endogenous products (XE) of OHOs	20,00	20
Fraction of colloidal unbiodegradable organics (CU) in colloidal COD (SCCOD-SCOD)	20,00	20
Fraction of N in readily biodegradable substrate (SB)	4,00	4
Fraction of N in particulate unbiodegradable substrate (XU)	1,00	1
Fraction of P in readily biodegradable substrate (SB)	1,00	1
Fraction of P in particulate unbiodegradable substrate (XU)	0,10	0,1

Balances	Balance passed
COD	OK
TKN	OK
TP	OK
TSS	OK

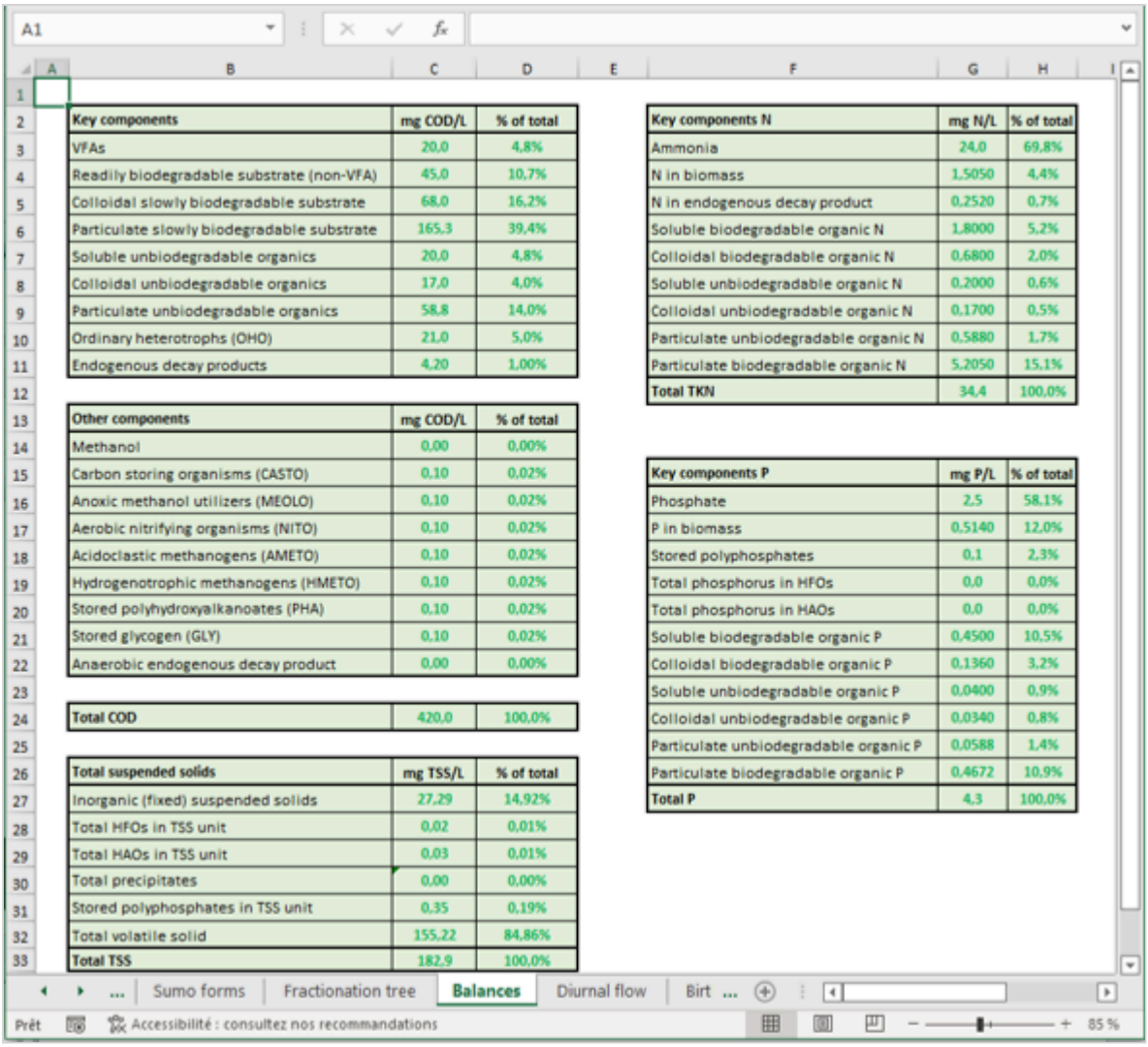
Particulate COD/VSS ratios by component	Default	To be estimated g COD/g VSS
COD of biomass in volatile solids	1,42	1,42
COD of biodegradable substrate in volatile solids	1,80	1,80
COD of particulate unbiodegradable organics in volatile solids	1,30	1,30
COD of endogenous products in volatile solids	1,42	1,42

Overall COD/VSS ratio	Measured	Calculated from weighted	Verdict
Weighted average COD/VSS	1,59	**1,64**	good match

BOD calculation	Default	To be estimated
Yield on ultimate BOD (g O2 g COD-1)	0,95	0,95
Fraction of BOD5 to ultimate BOD in soluble biodegradable substrates (-)	0,90	0,90
Fraction of BOD5 to ultimate BOD in colloidal biodegradable substrates (-)	0,60	0,60
Fraction of BOD5 to ultimate BOD in particulate biodegradable substrates (-)	0,50	0,50

Influent Tool Figure 4 - Check fractions

- Checking for the Balances of COD, TKN, TP, and TSS. All the balances must be OK before proceeding. The balance can be off if data or the fractions do not make sense, for instance in the following example: if TCOD is 420 g COD/m^3, TKN is 20 g N/m^3, and S_{NHx} is 15 g N/m^3, there is too little N left for organic nitrogen, and the Tool will tell us that **No, please check the data (TKN, Ammonia) and the fractions** in the **Balances** sheet. The details regarding by how much the balance is off can be reviewed in the sheet named Balances. In this case, Particulate biodegradable organic N is -0.1950, which would be incorrect. This can be remedied by either decreasing the fraction of N in readily biodegradable substrate (SB) and fraction of N in particulate unbiodegradable substrate (XU), decreasing the N content of other organics (see table Model parameters in sheet Balances) or the data should be checked for measurement errors.



Key components	mg COD/L	% of total
VFAs	20,0	4,8%
Readily biodegradable substrate (non-VFA)	45,0	10,7%
Colloidal slowly biodegradable substrate	68,0	16,2%
Particulate slowly biodegradable substrate	165,3	39,4%
Soluble unbiodegradable organics	20,0	4,8%
Colloidal unbiodegradable organics	17,0	4,0%
Particulate unbiodegradable organics	58,8	14,0%
Ordinary heterotrophs (OHO)	21,0	5,0%
Endogenous decay products	4,20	1,00%

Other components	mg COD/L	% of total
Methanol	0,00	0,00%
Carbon storing organisms (CASTO)	0,10	0,02%
Anoxic methanol utilizers (MEOLO)	0,10	0,02%
Aerobic nitrifying organisms (NITO)	0,10	0,02%
Acidoclastic methanogens (AMETO)	0,10	0,02%
Hydrogenotrophic methanogens (HMETO)	0,10	0,02%
Stored polyhydroxyalkanoates (PHA)	0,10	0,02%
Stored glycogen (GLY)	0,10	0,02%
Anaerobic endogenous decay product	0,00	0,00%

Total COD	420,0	100,0%

Total suspended solids	mg TSS/L	% of total
Inorganic (fixed) suspended solids	27,29	14,92%
Total HFOs in TSS unit	0,02	0,01%
Total HAOs in TSS unit	0,03	0,01%
Total precipitates	0,00	0,00%
Stored polyphosphates in TSS unit	0,35	0,19%
Total volatile solid	155,22	84,86%
Total TSS	182,9	100,0%

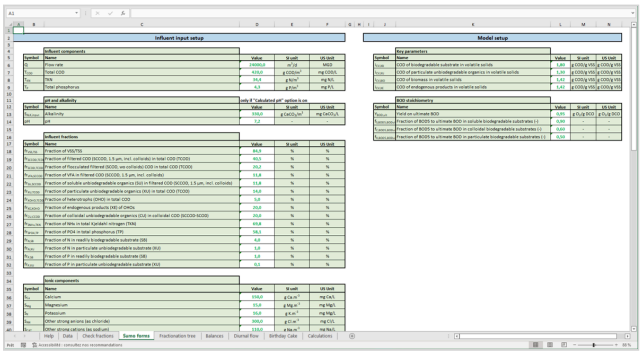
Key components N	mg N/L	% of total
Ammonia	24,0	69,8%
N in biomass	1,5050	4,4%
N in endogenous decay product	0,2520	0,7%
Soluble biodegradable organic N	1,8000	5,2%
Colloidal biodegradable organic N	0,6800	2,0%
Soluble unbiodegradable organic N	0,2000	0,6%
Colloidal unbiodegradable organic N	0,1700	0,5%
Particulate unbiodegradable organic N	0,5880	1,7%
Particulate biodegradable organic N	5,2050	15,1%
Total TKN	34,4	100,0%

Key components P	mg P/L	% of total
Phosphate	2,5	58,1%
P in biomass	0,5140	12,0%
Stored polyphosphates	0,1	2,3%
Total phosphorus in HFOs	0,0	0,0%
Total phosphorus in HAOs	0,0	0,0%
Soluble biodegradable organic P	0,4500	10,5%
Colloidal biodegradable organic P	0,1360	3,2%
Soluble unbiodegradable organic P	0,0400	0,9%
Colloidal unbiodegradable organic P	0,0340	0,8%
Particulate unbiodegradable organic P	0,0588	1,4%
Particulate biodegradable organic P	0,4672	10,9%
Total P	4,3	100,0%

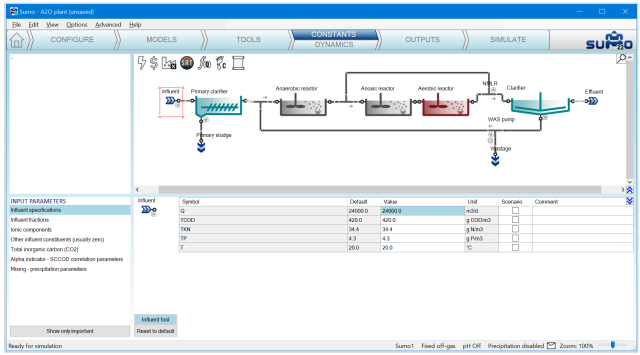
Influent Tool Figure 5 - Balances

Step 4 - Feed the parameters to Sumo

Copying the values from the tool's Sumo form to the Sumo influent unit can be done by selecting, copying (Ctrl-C), and pasting (Ctrl-V) in Sumo.

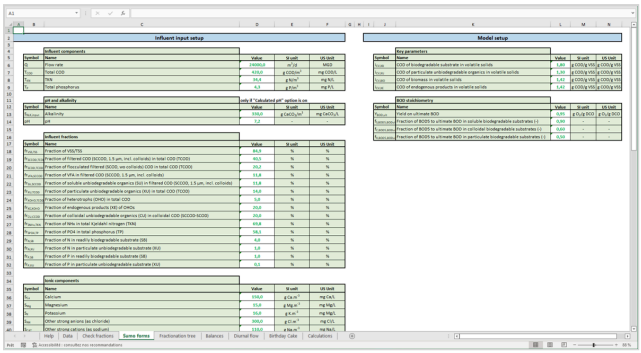


Influent Tool Figure 6 - Copy parameters from Sumo forms sheet (Ctrl - C)

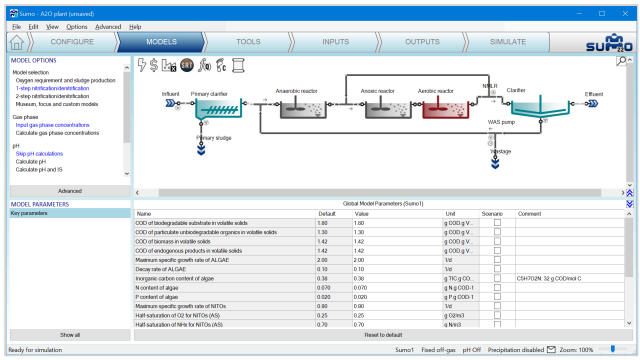


Influent Tool Figure 7 - Paste into Sumo for the relevant table (Ctrl - V)

If any of the model parameters including COD/VSS ratios were adjusted, then they should be copied to the Model Setup tab in Sumo.



Influent Tool Figure 8 - Copy parameters from Sumo forms sheet (Ctrl - C)

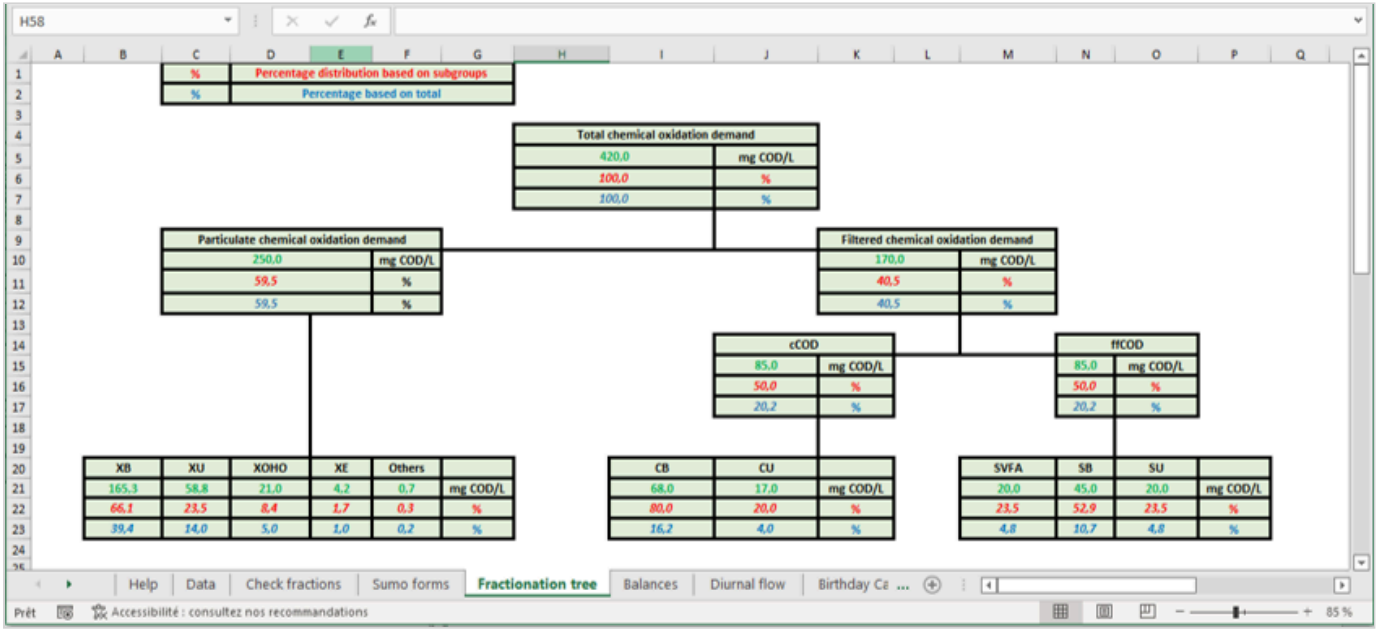


Influent Tool Figure 9 - Paste into Sumo Model setup (Ctrl - V)

Other features of the tool

Fractionation tree

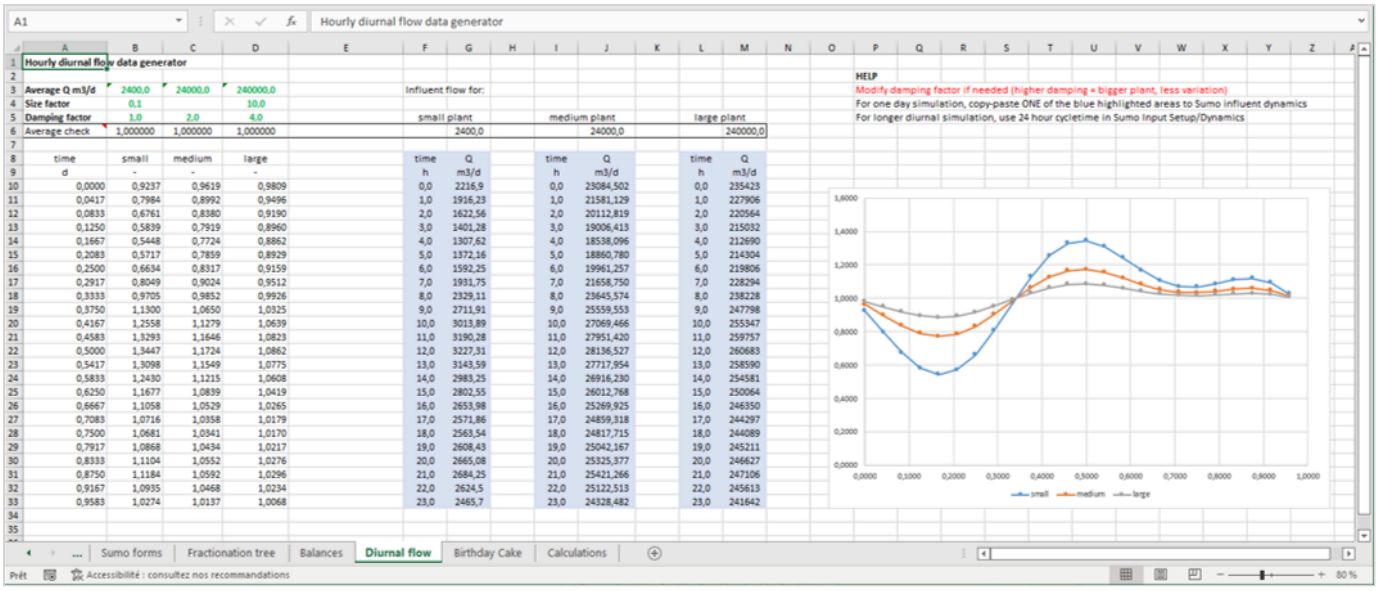
The fractionation tree sheet helps you visualize fractions and are useful for documentation.



Influent Tool Figure 10 - Fractionation tree

Diurnal flow

The **Diurnal flow** sheet creates three types of hourly dynamic influent data (small, medium and large plants) for 24 hours using the Flow value provided in the C3 of **Data** sheet. This dynamic table is useful for setting up dynamic simulation in case no diurnal data is available.



Influent Tool Figure 11 - Diurnal flow

Birthday cake

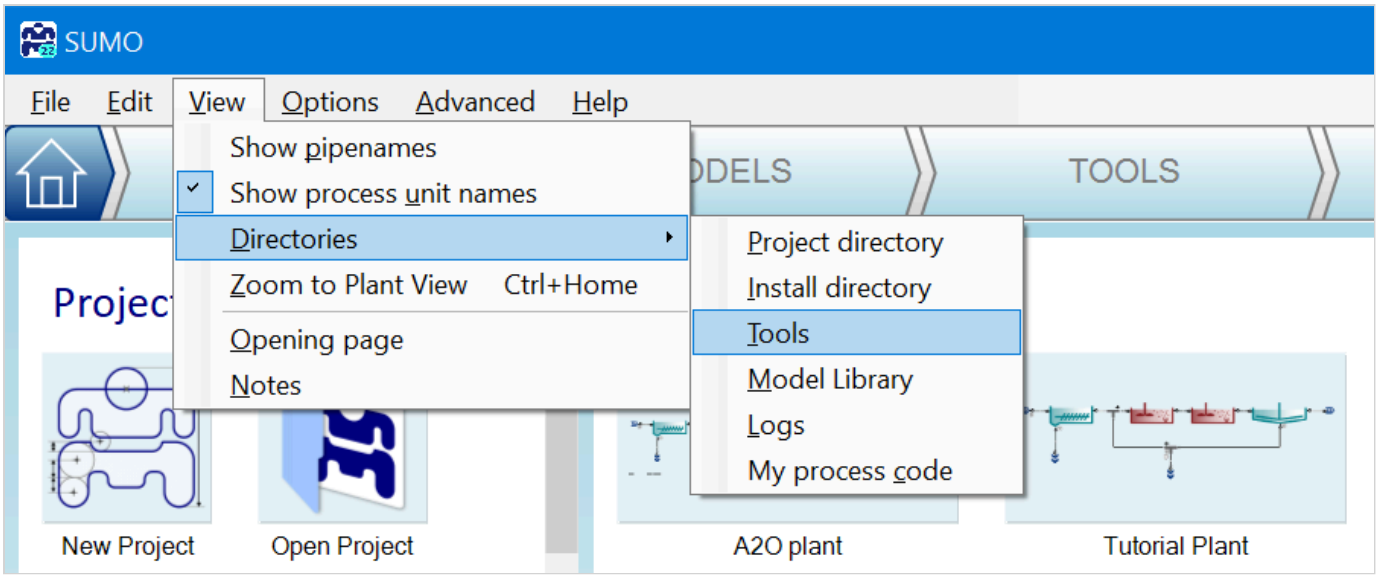
The **Birthday cake** sheet provides hourly data for a simplified birthday cake analysis of 16 days. This is useful for sizing and evaluating plant performance under diurnal variation, monthly maximum load and peak daily load conditions. For further details we suggest to look into the Guidelines for Using Activated Sludge Models published by IWA .

Note

There are multiple situations all of which can not be described comprehensively in this document, so refer to the Influent characterization chapter and feel free to write to support@dynamita.com.

Aeration (SOTE) tool

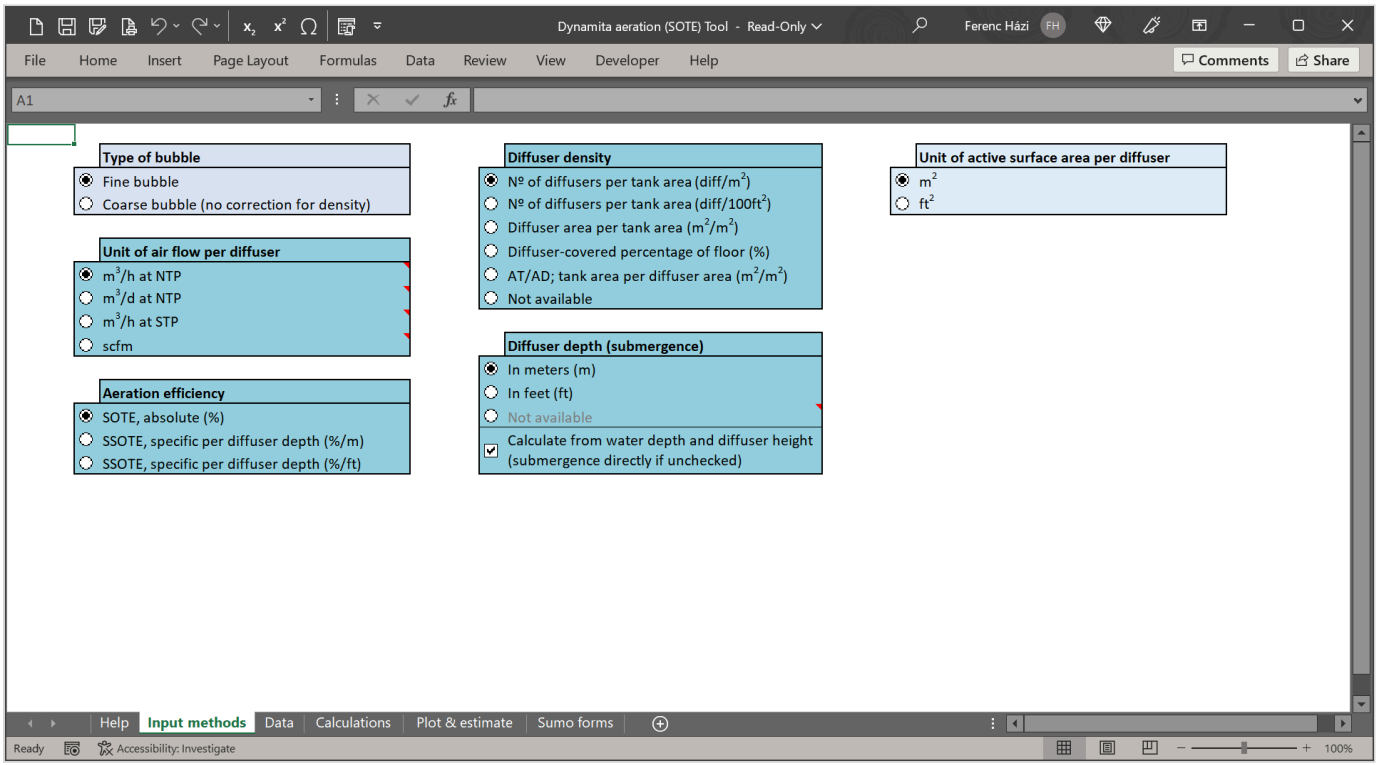
The purpose of this tool is to identify parameters for the clean water oxygen transfer modeling function through curve fitting using diffuser equipment testing data. The tool can be reached from View|Directories|Tools folder by opening ***Dynamita aeration (SOTE) tool.xlsm***. Be aware that the tool is using VBA macros. You can save the tool anywhere, even drag and drop the file to the Notes (bottom right panel) on the **Configure** tab in Sumo so it will be stored with your project.



SOTE Tool Figure 1 - Open aeration tool

Step 1 - input parameter set definition

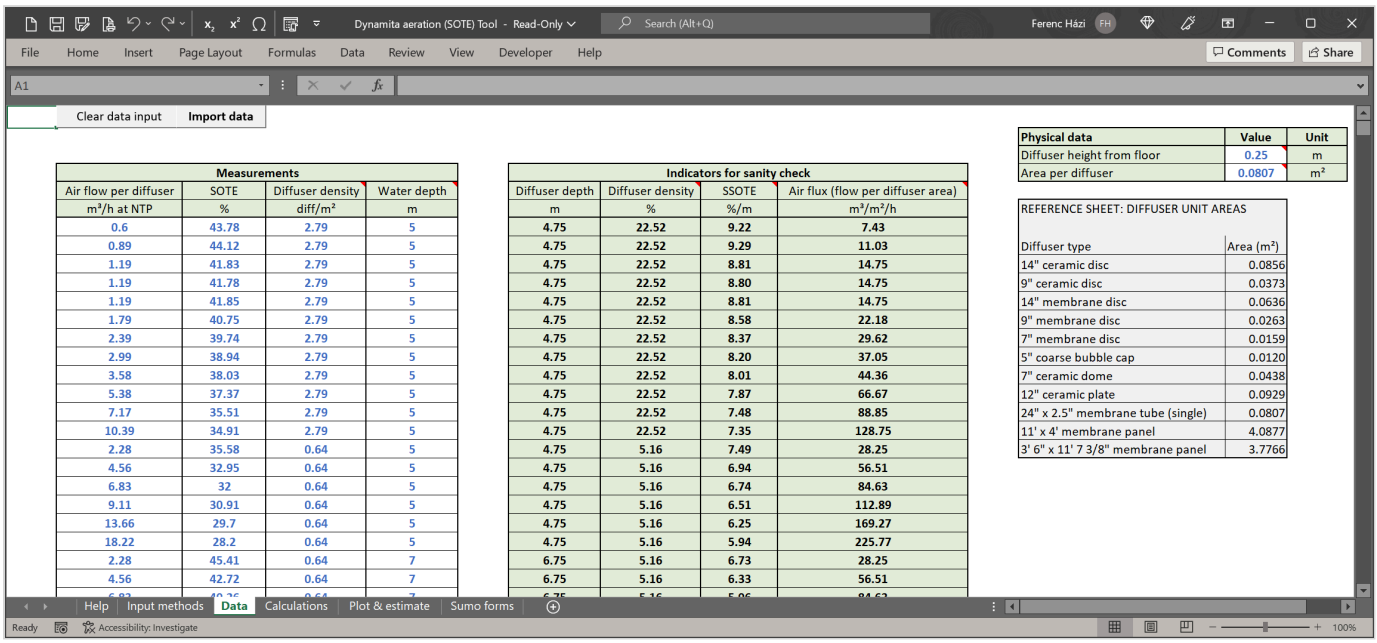
The parameters identified are plugged into the *Oxygen transfer efficiency correlation parameters* table in the reactor model for calibration of the plant's diffuser system. In the **Input methods** sheet, users start by selecting the type of diffuser and the units for key information to be processed by the tool. The selection criteria are presented below.



SOTE Tool Figure 2 - Select input parameter set

Step 2 - Provide data

Next step is to switch to the **Data** sheet and provide data from manufacturer specifications or plant measurement campaigns within the Measurements table and provide the Physical data such as *Diffuser height from floor* and *Area per diffuser*. The tool comes with a default set of demonstratory data which must be removed by clicking the ***Clear data input*** button at the upper left corner of the sheet. Also available is a reference sheet containing common diffuser type unit areas, for estimating the active surface area. Once the new data is entered, users must press the ***Import data*** button to start the automated data manipulation. The details of these calculations can be seen in the **Calculations** sheet where the dataset is processed for curve fitting.



Clear data input | Import data

Measurements

Air flow per diffuser	SOTE	Diffuser density	Water depth
m³/h at NTP	%	diff/m²	m
0.6	43.78	2.79	5
0.89	44.12	2.79	5
1.19	41.83	2.79	5
1.19	41.78	2.79	5
1.19	41.85	2.79	5
1.79	40.75	2.79	5
2.39	39.74	2.79	5
2.99	38.94	2.79	5
3.58	38.03	2.79	5
5.38	37.37	2.79	5
7.17	35.51	2.79	5
10.39	34.91	2.79	5
2.28	35.58	0.64	5
4.56	32.95	0.64	5
6.83	32	0.64	5
9.11	30.91	0.64	5
13.66	29.7	0.64	5
18.22	28.2	0.64	5
2.28	45.41	0.64	7
4.56	42.72	0.64	7

Indicators for sanity check

Diffuser depth	Diffuser density	SSOTE	Air flux (flow per diffuser area)
m	%	%/m	m³/m²/h
4.75	22.52	9.22	7.43
4.75	22.52	9.29	11.03
4.75	22.52	8.81	14.75
4.75	22.52	8.80	14.75
4.75	22.52	8.81	14.75
4.75	22.52	8.58	22.18
4.75	22.52	8.37	29.62
4.75	22.52	8.20	37.05
4.75	22.52	8.01	44.36
4.75	22.52	7.87	66.67
4.75	22.52	7.48	88.85
4.75	22.52	7.35	128.75
4.75	5.16	7.49	28.25
4.75	5.16	6.94	56.51
4.75	5.16	6.74	84.63
4.75	5.16	6.51	112.89
4.75	5.16	6.25	169.27
4.75	5.16	5.94	225.77
6.75	5.16	6.73	28.25
6.75	5.16	6.33	56.51

Physical data	Value	Unit
Diffuser height from floor	0.25	m
Area per diffuser	0.0807	m²

REFERENCE SHEET: DIFFUSER UNIT AREAS

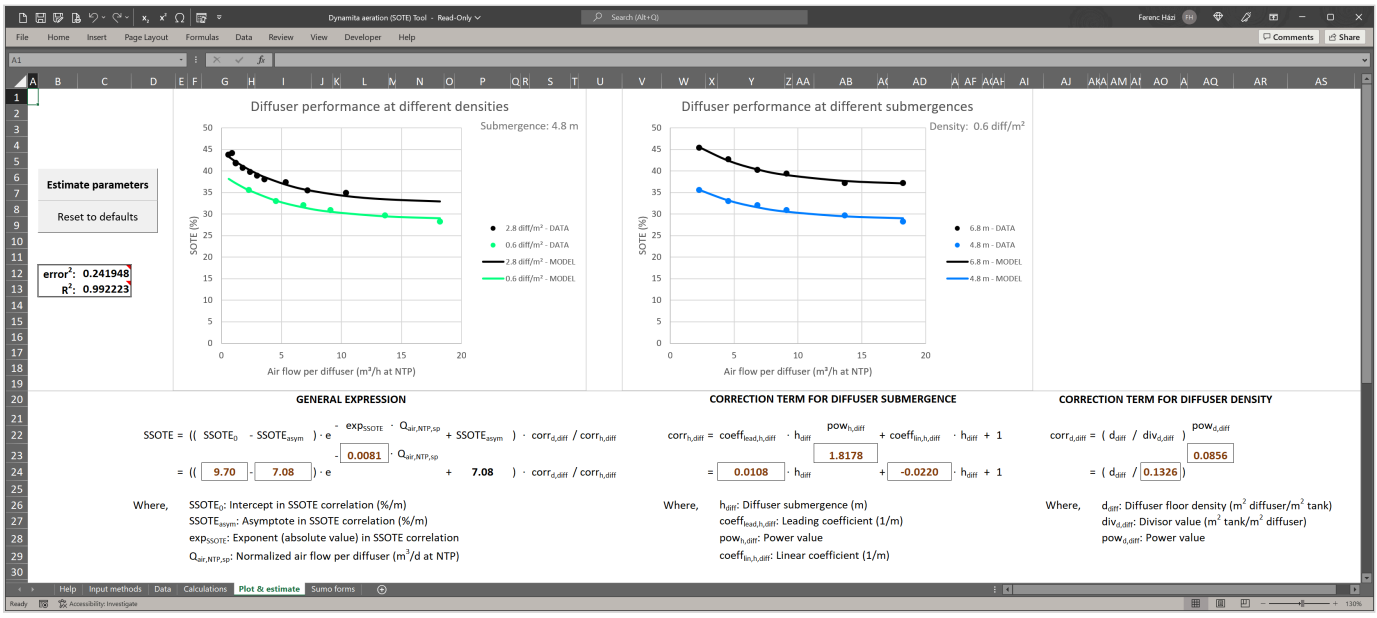
Diffuser type	Area (m²)
14" ceramic disc	0.0856
9" ceramic disc	0.0373
14" membrane disc	0.0636
9" membrane disc	0.0263
7" membrane disc	0.0159
5" coarse bubble cap	0.0120
7" ceramic dome	0.0438
12" ceramic plate	0.0929
24" x 2.5" membrane tube (single)	0.0807
11' x 4' membrane panel	4.0877
3' 6" x 11' 7 3/8" membrane panel	3.7766

Help | Input methods | Data | Calculations | Plot & estimate | Sumo forms

SOTE Tool Figure 3 - Data input sheet

Step 3 - Check parameter fitting

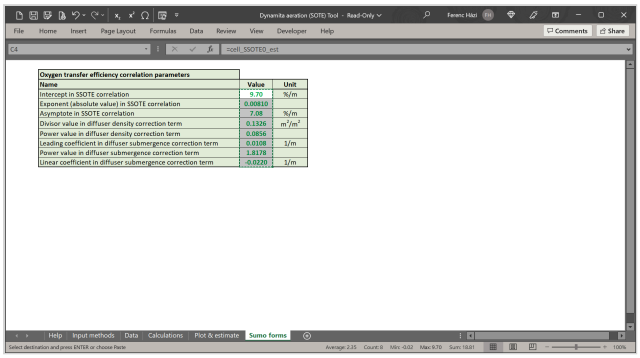
In the **Plot & estimate** sheet the parameters are estimated for the expression predicting SSOTE, including the correction term for diffuser submergence and the diffuser density by adjusting the function parameters to match the measured data (***Estimate parameters*** button on the left side of the sheet). See the figure below showing the fitted curve.



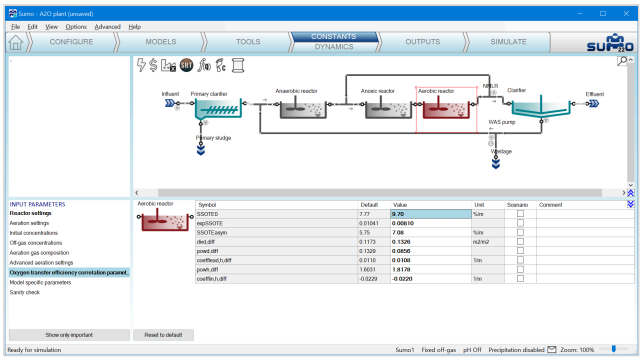
SOTE Tool Figure 4 - Estimated parameters for SOTE curve

Step 4 - Feed the parameters to Sumo

The last step is to copy the values from the **Sumo forms** sheet in the tool into the reactor's *Oxygen transfer efficiency correlation parameters* in Sumo within the **Inputs** tab.



SOTE Tool Figure 5 - Copy from the Sumo forms (Ctrl - C)



SOTE Tool Figure 6 - Paste into Sumo (Ctrl - V)

Add-ons for Sumo

Description of available add-on packages for Sumo

Introduction

Add-on packages are dedicated process units to cover different technologies or areas such as mobile carrier technologies or detailed sewer network modeling. The chapter provides description about these models.

The addons are available for download on our website .

Mobile carrier model

Mobile carrier can be described as free moving, submerged biofilm carrier which can leave the reactor boundaries with the biofilm attached to it.

Mobile carrier (MC) model is the extension of the SumoBioFilm© model by allowing the carrier and the attached biofilm to move between process units. The model uses Xcarrier variable to calculate the amount of carrier and attached biofilm transported via connections. The sub-model allows the simulation of recirculation, back mixing, media removal and addition.

Biofilm carrier migration model describes reactor performance, Water Science & Technology, 75.12, 2017, Joshua P. Boltz, Bruce R. Johnson, Imre Takács, Glen T. Daigger, Eberhard Morgenroth, Doris Brockmann, Róbert Kovács, Jason M. Calhoun, Jean-Marc Choubert and Nicolas Derlon

Sewer model

The sewer network add-on contains a pipe segment process unit, a service cover and compatible gas flow element. The pipe segment is consider as a plug flow reactor and can model force main and gravity sewers with fixed biofilm or sediments.

In gravity sewers, the gas phase is allowed to flow both directions – same as sewage and counter direction as well. The service cover predicts fresh air intrusion and gas transfer.

Densified Sludge Model

This add-on includes a Densified sludge separator process unit to simulate the granules selection obtained with a hydrocyclone. A specific model extension is required to simulate separate biological reactions in the flocs and granules: the user can choose from either the Sumo2 or Sumo4N with granule extension models.

Model description

The concept is based on the aerobic granular sludge modeling approach described by Baeten *et al.* (2018) wherein separate modelling state variable components are assigned for floccular and granular organism groups. The diffusion resistance of substrate into the granules is accounted for using higher “apparent” half-saturation coefficients for granular components. The selective retention and accumulation of granules is predicted by the model as a result of the differential effect on the floccular and granular organism groups of biological selector zones and external selectors, for example wasting from the overflow of hydrocyclones.

The granule fraction is calculated as a function of the relative ratio of granular to total organism groups (granules + flocs) and by assigning portions of influent particulate material to either the floccular or granular groups.

Under normal circumstances, the floccular components of ordinary heterotrophs (X_{OHO}), and PAO and GAO carbon storing organisms (X_{CASTO}) will dominate the growth processes because the model applies a “Diffusion Resistance” parameter to the growth of granular organisms. This diffusion resistance accounts for the reduced access to substrate and oxygen in the inner layers of the granules. It is applied using the “apparent Ks” concept described by Baeten et al. (2018). For example, in the equation below the Monod saturation term for some substrate “S” is defined with the half-saturation coefficient “$Msat_S$” increased proportionally to the diffusion resistance “DR”. The default value of DR is 1.2 which implies a 20% increase in the half-saturation coefficient.

$$Msat_S = \frac{S}{(S + K_S * DR)}$$

In fact the term (Ks*DR) acts as the “apparent Ks” investigated by Baeten et al. Table 1 shows how this might be applied in a simplified model matrix. Figure 1 provides a conceptual framework for how modeling direction of influent substrate to growth of floccular and granular organisms in the mixed liquor can then be used to calculate the densified fraction of the mixed liquor.

Table 1 - Gujer matrix presenting separate state components for floccular and granular PAOs, storage products (PHA) as well as “apparent Ks” applied to VFA sequestration and O_2 utilization in granules

Process name	$X_{PAO,floc}$	$X_{PAO,granule}$	$X_{PHA,floc}$	$X_{PHA,granule}$	S_{VFA}	S_{O2}	Kinetic rate
Sequestration of PHA in flocular PAOs			+1		-1		$q_{max} * X_{PAO,floc} * S_{VFA}/(S_{VFA} + K_{VFA})$
Sequestration of PHA in granular PAOs				+1	-1		$q_{max} * X_{PAO,granule} * S_{VFA}/(S_{VFA} + K_{VFA,apparent})$
Growth of flocular PAOs	+Y		-1			-(1-Y)	$\mu_{max} * X_{PAO,floc} * S_{O2}/(S_{O2} + K_{O2})$
Growth of granular PAOs		+Y		-1		-(1-Y)	$\mu_{max} * X_{PAO,granule} * S_{O2}/(S_{O2} + K_{O2,apparent})$

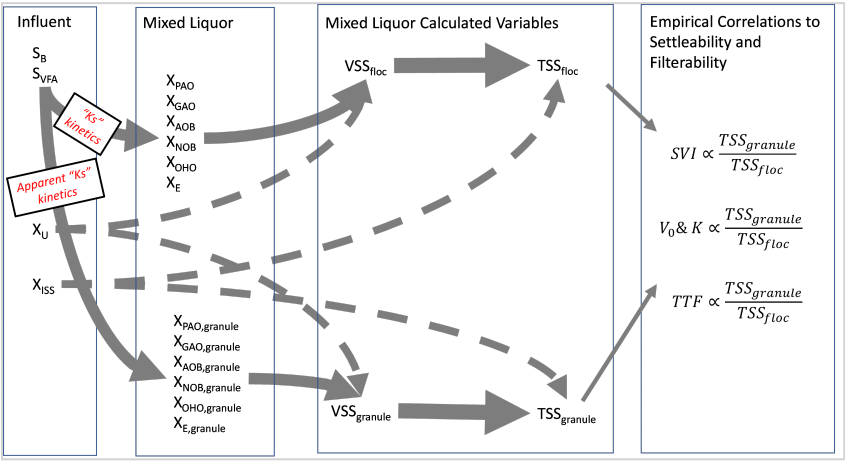


Figure 3 - Conceptual overview of the apparent Ks model application to sludge densification

Because the higher “apparent Ks” has less impact when substrate concentrations are high, the model will simulate the beneficial effects of an internal selector for sludge densification. It is then easy to model the benefits of an external selector to enhancing densification, such as a hydrocyclone, in which granular state variables are selectively retained.

J. Baeten, M.C.M. van Loosdrecht, E. Volcke (2018) “Modelling aerobic granular sludge reactors through apparent half-saturation coefficients.” 146. 134-145. Water Research.

Quick tutorial: How to use Sumo Densified Sludge Model

Opening an existing example in Sumo

You can modify an existing Sumo model to work with the densification model. In this example, we will select the A2O plant from the list of Examples in the home screen.

Figure 1 - Opening the A2O example in Sumo

Selecting the Sumo2_Granules biokinetic model

To select the densification biokinetic model, go to the MODELS tab in the Sumo ribbon, select the “Advanced” option, and then the Sumo2_Granules option from the Focus models. This model is based on Sumo2, a 2-step nitrification model, with the modification that certain particulate state variables are divided between floccular and granular components.

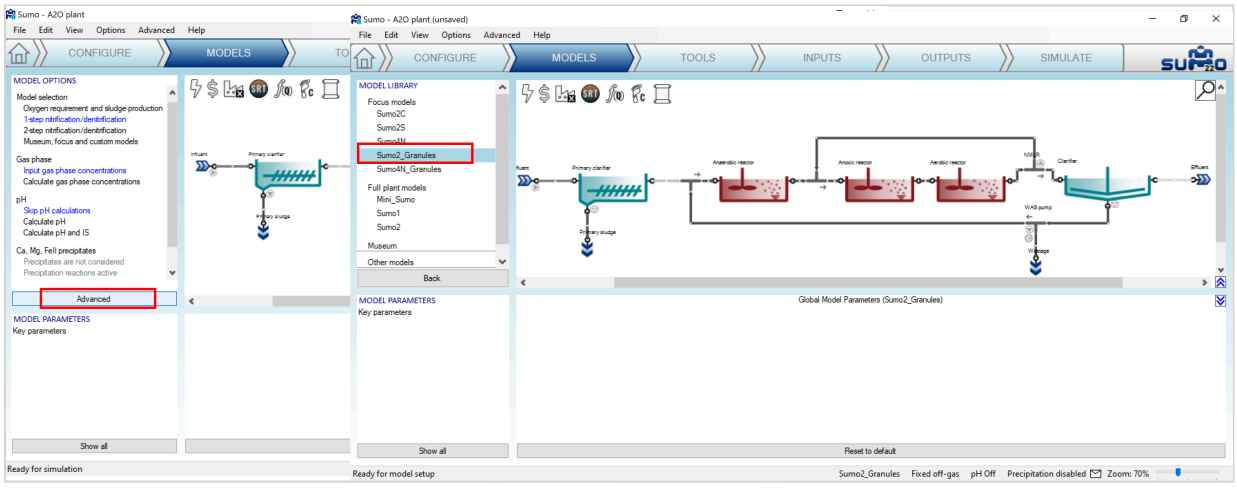


Figure 3 - Selecting Densified Sludge Model

Adding a Cyclone from the Separators elements

To add a hydrocyclone to the flowsheet, select it from the “Separators” in the CONFIGURE tab of the Sumo ribbon. Make sure to select “Densified sludge separator” from the Options in the bottom left pane.

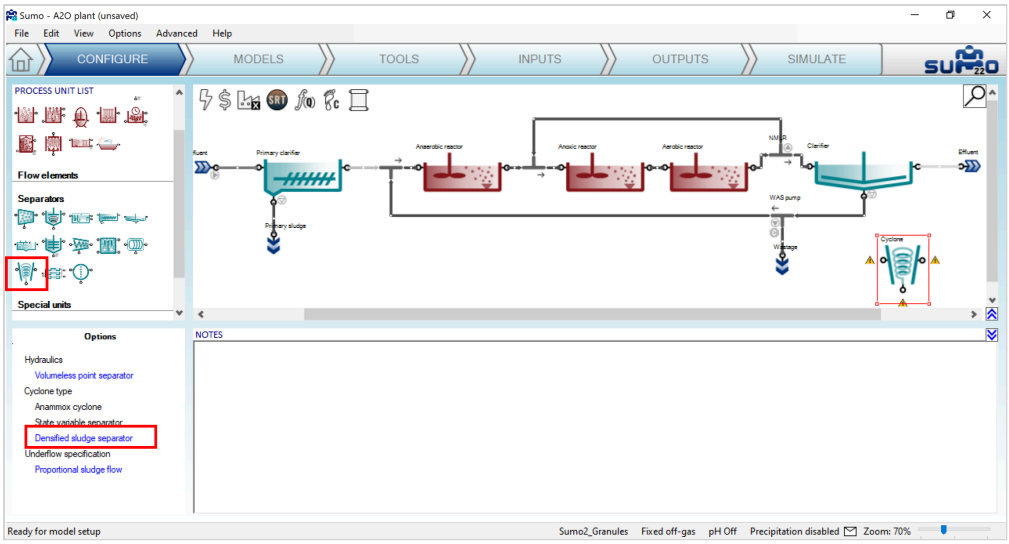


Figure 5 - adding a cyclone

The hydrocyclone is added to the WAS stream together with a “Proportional side flow divider” to enable easy switching “On” and “Off” of the cyclone operations.

Displaying the Densified Fraction of TSS

In the OUTPUTS tab, select the Cyclone element. Create a table and drag and drop the “Contributors to granular TSS” into the table for each of the Feed, Overflow and Underflow. You can drag and drop the input and output ports of the cyclone to create the different columns.

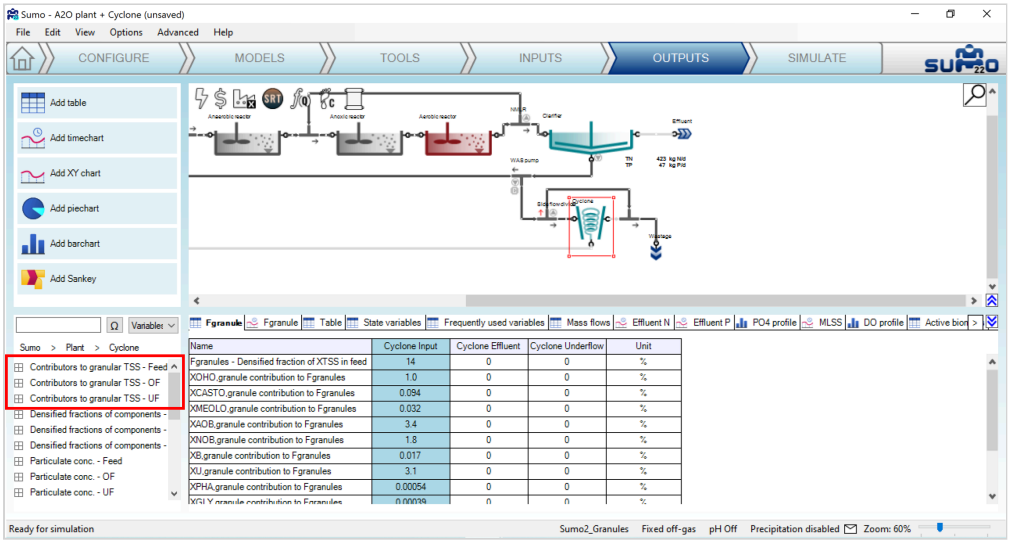


Figure 6 - Displaying the Densified Fraction of TSS

Create scenarios for Cyclone “On” and “Off” scenarios

In the INPUTS tab of the Sumo ribbon, select the proportional side flow divider immediately upstream of the cyclone and check the “Scenario” box.

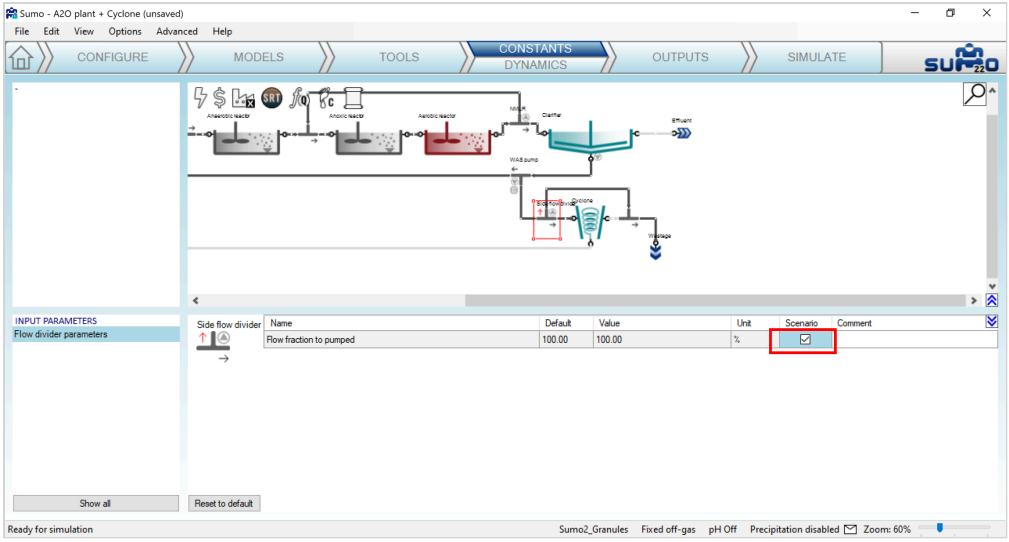


Figure 7 - Adding pump flow fraction to scenarios to represent Cyclone “on” and “off” operations

In the SIMULATE tab, this parameter will now appear as an option in the bottom left pane. Create and name two scenarios to represent Cyclone “On” and “Off” operations.

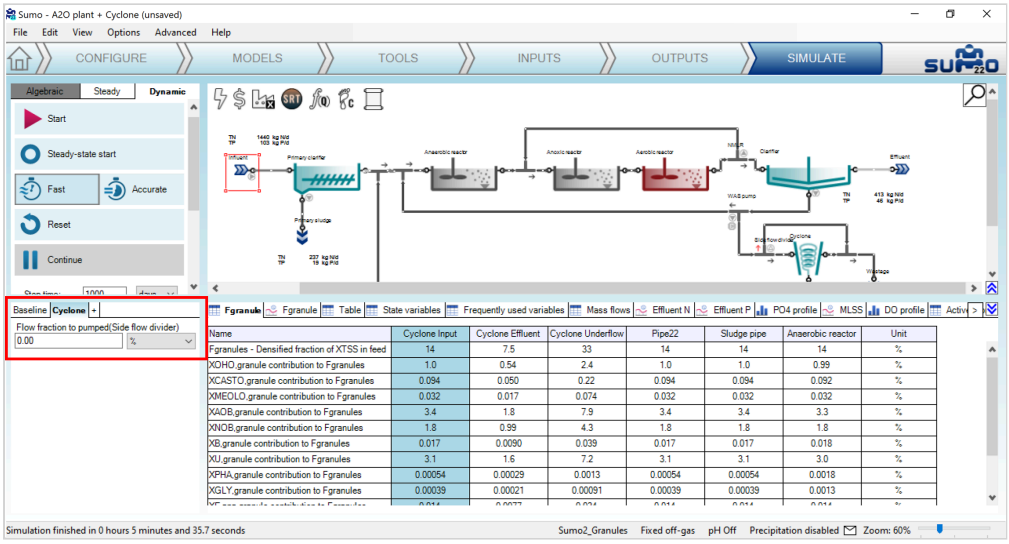


Figure 8 - Scenario to represent Cyclone “on” and “off” operations

Calibrating influent characteristics

The model includes fractions to represent the amount of particulate inorganic (X_{INORG}), particulate unbiodegradable (X_U), particulate biodegradable (X_B) and heterotrophs (X_{OHO}) that are granular. The default values are 20%, 10%, 0% and 1%, respectively. The fractions are applied in the following manner: if the amount of influent X_{INORG} is 75 mg/L then 15 mg/L (20%) will be assigned to $X_{INORG,granule}$ and the remaining 60 mg/L (80%) to regular “floccular” X_{INORG}.

By including these in the scenarios we can use them to calibrate the amount unbiodegradable material that contributes to the densified fraction. For example, changing the fraction of influent unbiodegradable organics (X_U) that meets the granule definition from 10% to 5% reduces the Densified fraction from 7.5% to 6% in the Baseline scenario (Cyclone Off).

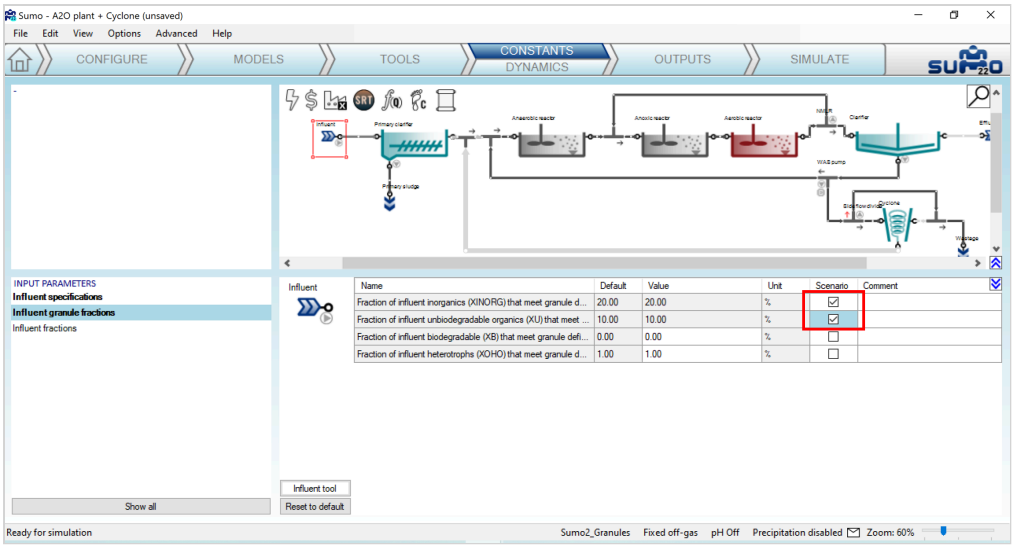


Figure 9 - Selecting influent characteristics for scenarios to calibrate them

Calibrating Diffusion Resistance (DR)

The diffusion resistance (DR) parameters are defined in the MODELS tab of the Sumo ribbon in the bottom left pane after selecting “Show all” under the heading “Granule diffusion resistance”. We can calibrate the impact of these parameters by selecting the “Scenario” boxes as shown below.

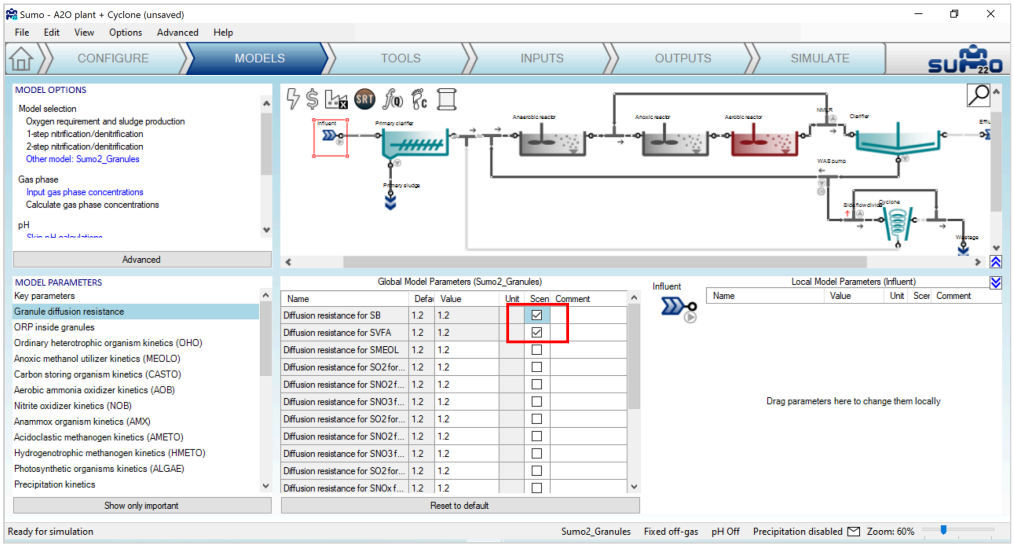


Figure 9 - Selecting diffusion resistance for scenarios to calibrate them

After changing the DR for susbtrates S_B and S_{VFA} from 1.2 to 2, simulating dynamically for 100 days shows the Baseline densified fraction ($F_{granule}$) decreasing from 7.5% to 6.5%.

Note that the steady state solver does not always accurately find the “true” long term stable state condition, particularly when the previous solution state was “far” from the current one. It may be advisable to use the “Reset” button in some cases to reinitialize the model to a state closer to a “normal” condition or run long term dynamic simulations until time series charts show stabilizing variables of interest.

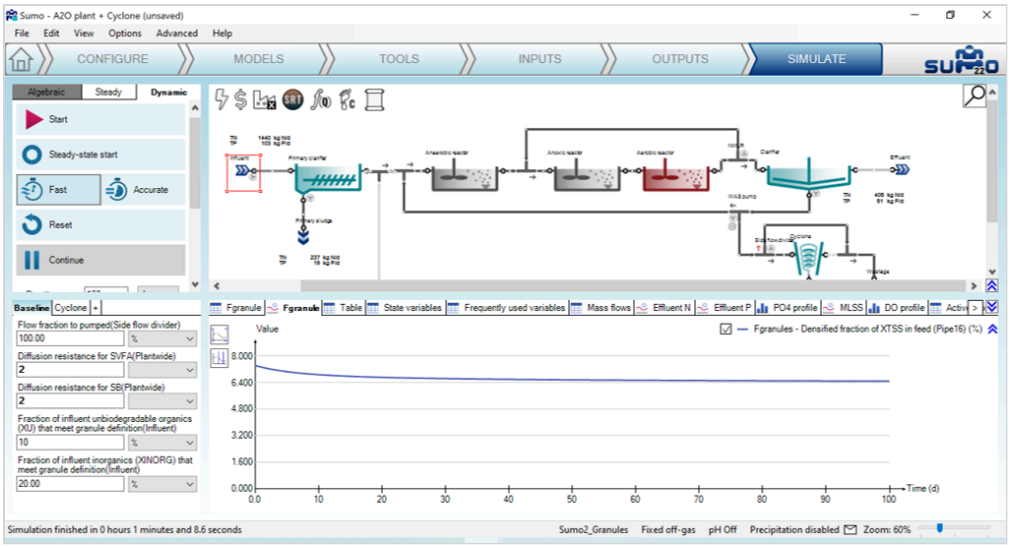


Figure 10 - Baseline simulation after changing the diffusion resistance in scenario

On switching to the “Cyclone” scenario, and including the changes to the diffusion resistance parameters from 1.2 to 2, we see the dynamic changes in Densified fraction “$F_{granules}$” decreasing from 28.8% to 21.2% over 100 days of simulation.

Oxidation-reduction potential (ORP)

The model calculates a difference in ORP for fermentative organisms in the floc and the granules. The ORP for the flocs and granules can be viewed in a table by typing “Oxidation-reduction” into the dialog box in the bottom left pane of the OUTPUTS tab of the Sumo ribbon. As long as the “Variables” option is selected from the drop-down menu then the “Oxidation-reduction potential” for the flocs and granules should be displayed. As can be seen below, the ORP in the granules is lower than in the flocs.

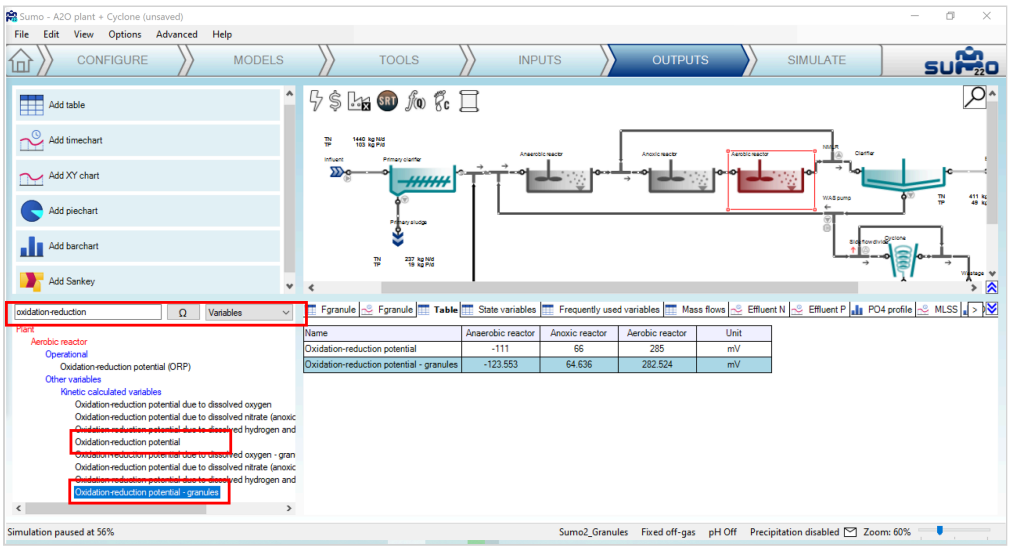


Figure 11 - Displaying ORP potential in bulk and granules

Cyclone operations calibration

The Cyclone operating parameters can be accessed in the INPUTS tab of the Sumo ribbon. The cyclone model is defined with only four parameters. The first specifies the hydraulic or volumetric split between the overflow and the underflow and has a default value of 10%. The second parameter represents the mass fraction of floccular particulate material captured in the underflow and has a default value of 20%. The last two parameters represent a multiplier applied to this mass capture for granular material and inorganic granular material. So for a default capture of 20% of flocs in the underflow, a “Ratio of granule to flow captured in underflow” of 3 will result in a mass capture of 66% of granules in the underflow.

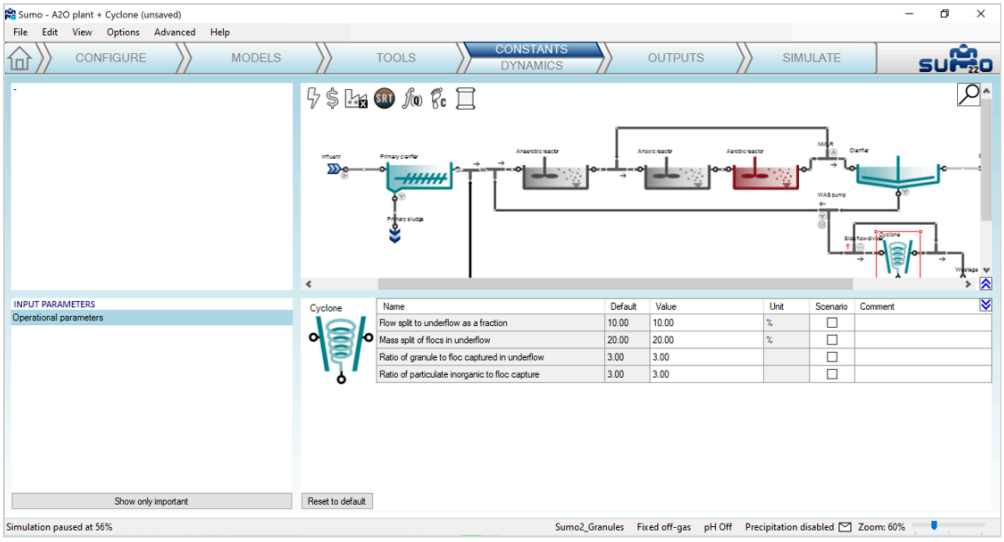


Figure 12 - Cyclone operating parameters

Plant and granules SRT calculation

The plant SRT calculation can be calculated as usual in the TOOLS ribbon, selecting the “Sludge Retention Time” feature and selecting the proper units with drag and drop method.

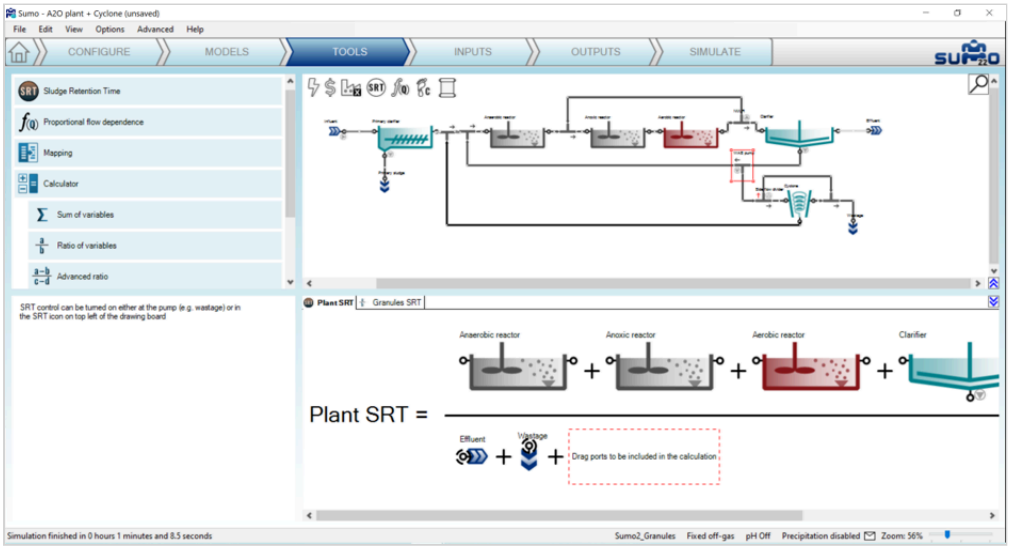


Figure 13 - Setting the plant SRT calculation

The calculation of granule SRT can be done on the basis of one of the granular biomass, as $X_{AOB,\ granule}$ for example. The “Ratio of variables” calculation has to be selected in the top left panel, and “custom” numerator

and denominator variables should be set in the bottom left panel as “M_X_AOB_granule” and “F_X_AOB_granule” respectively. In the bottom right panel, the appropriate process units should be drag ant drop at numerator and denominator.

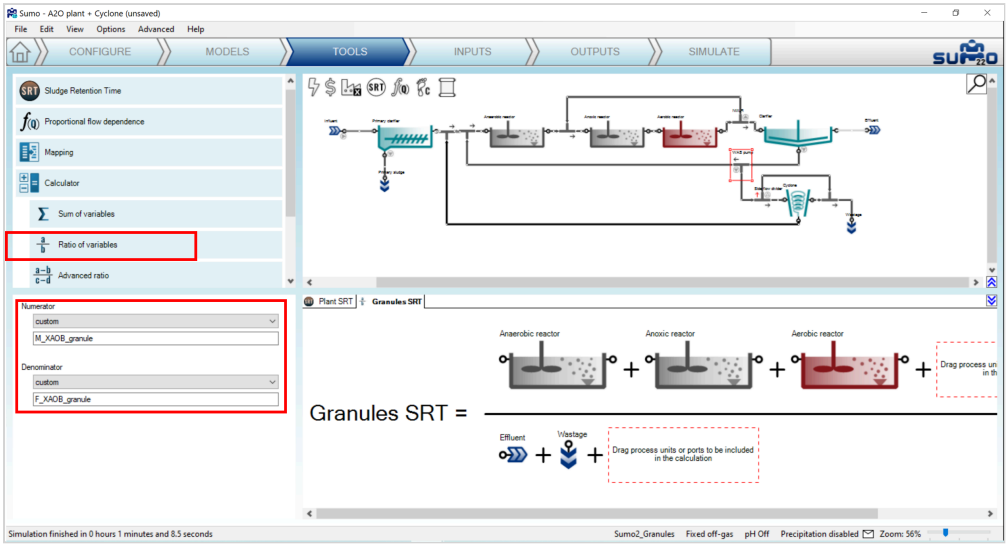


Figure 14 - Setting the granules SRT calculation

In the following simulation with the cyclone activated, the process is intensified by increasing the WAS pumped flow from 300 m^3/d to 900 m^3/d. The SRT calculations results in 6.3d SRT for the plant and 8.6d SRT for granules.

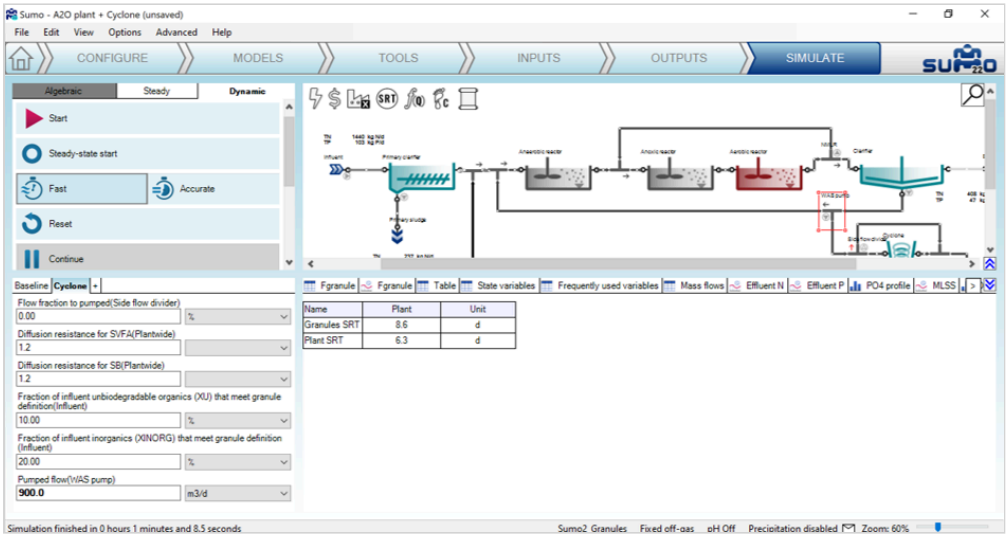


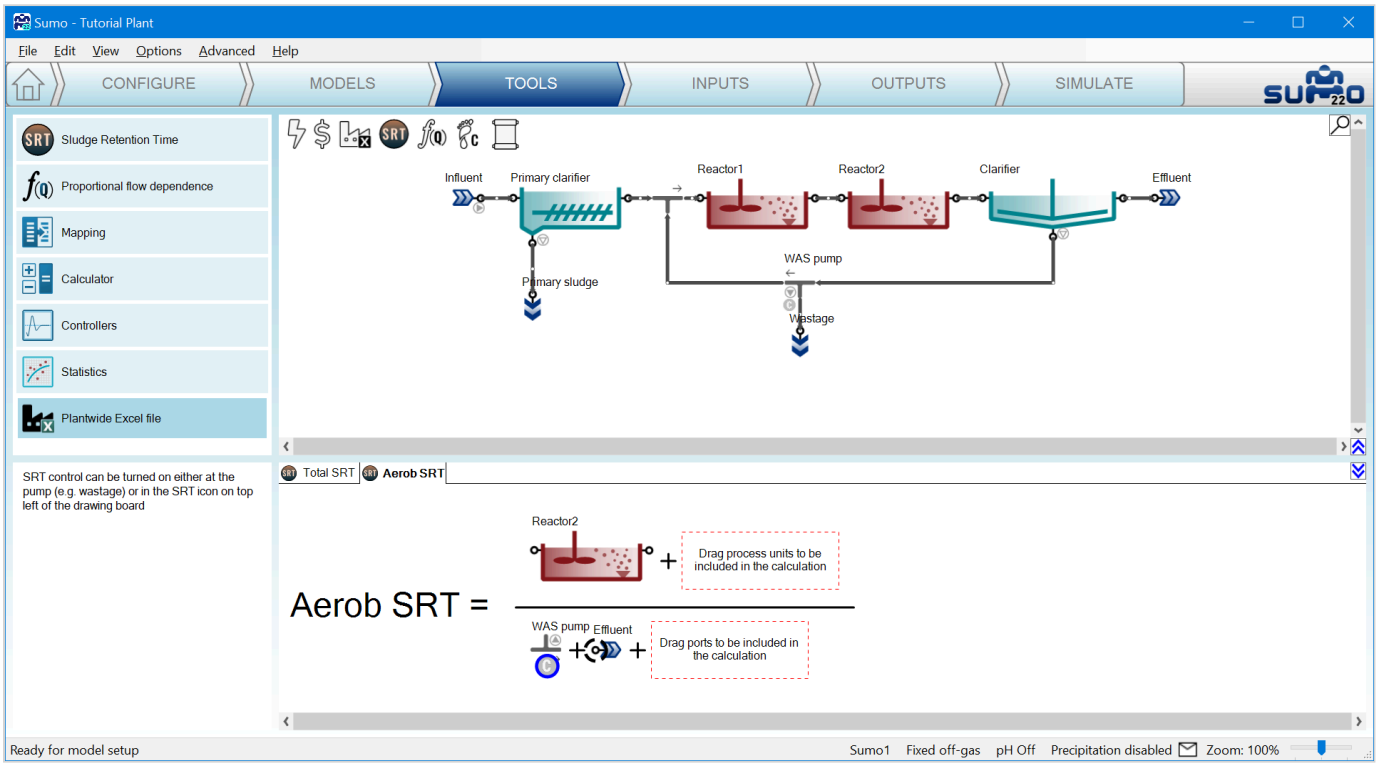
Figure 14 - Plant and granules SRT calculation results

Plantwide Excel calculations

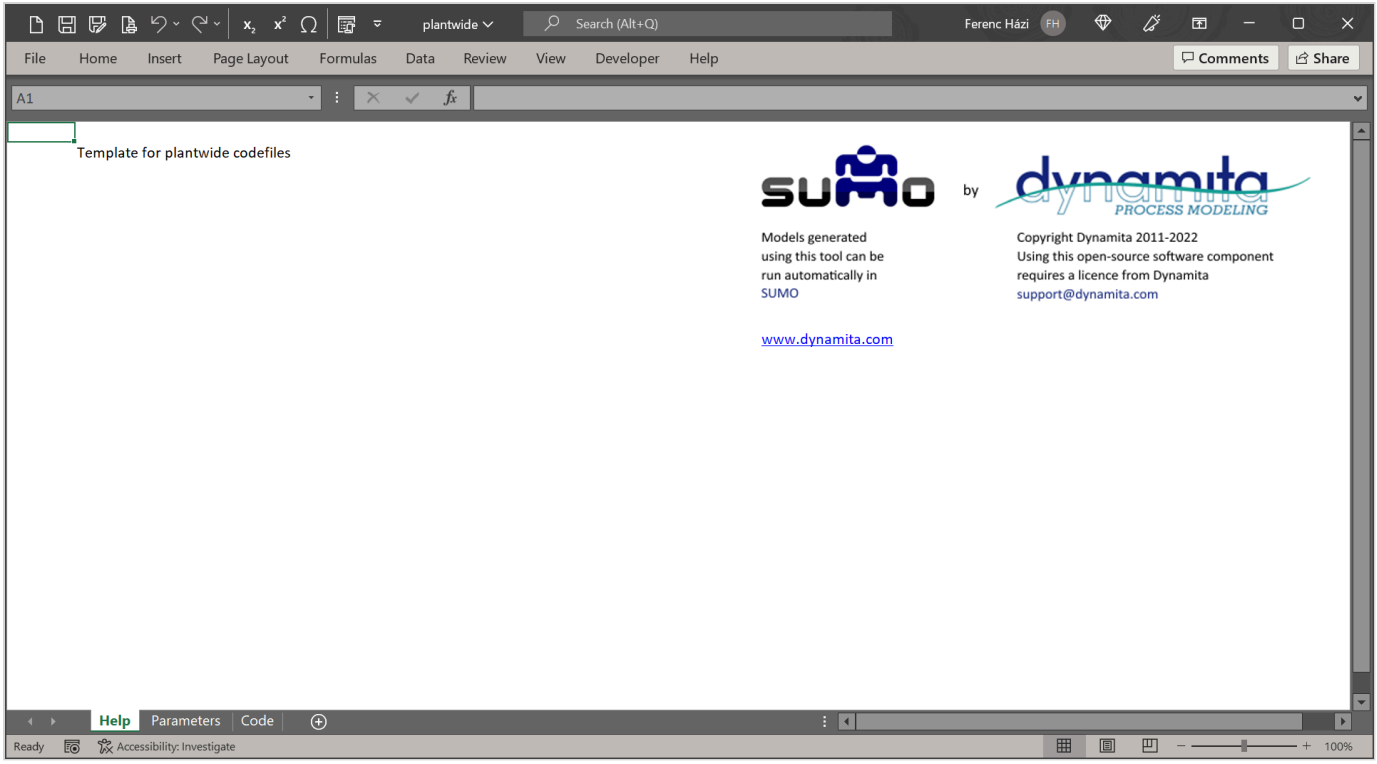
How to write calculations in the plantwide excel? Find the answer in the chapter.

Introduction

Plantwide code is not confined to one process unit (PU) but uses variables from all over the plant model. A template plantwide Excel file for the plantwide code can be opened from the GUI directly or from the Project directory (View|Directories|Project directory|plantwide.xlsx). In this tutorial the observed sludge yield is calculated using SumoSlang on the example of Tutorial plant.



PWE Figure 1 - Open the Plantwide excel file



PWE Figure 2 - Plantwide excel template

IMPORTANT NOTE

Before proceeding further, remove the control flags from both SRT calculations in the example file using the method from the User manual , Figure 3.13 – Toggling between pump selection for target SRT control.

Goal of calculation

The observed sludge production will depend on the SRT (higher SRT leads to lower sludge production) and the SRT directly depends on wastage flow. Total SRT is already defined in Sumo for Tutorial plant. Using the Plantwide Setup tab SRT tool new calculation can be added (see in the User Manual).

The observed yield is defined as solids generated per total COD (or BOD) removed in the plant:

$$Y_{obs} = \frac{F.X_{TSS,wastage} + F.X_{TSS,effluent}}{F.T_{COD,influent} - (F.S_{COD,effluent} + F.S_{COD,wastage})}$$

PWE Equation 1 - Observed yield calculation

Where:

Symbol	Unit	Name
Y_{obs}	gTSS/gCOD removed	Observed yield of sludge production
$F.X_{TSS}$	gTSS/d	Mass flow of total suspended solids
$F.T_{COD}$	gCOD/d	Mass flow of total COD
$F.S_{COD}$	gCOD/d	Mass flow of soluble COD

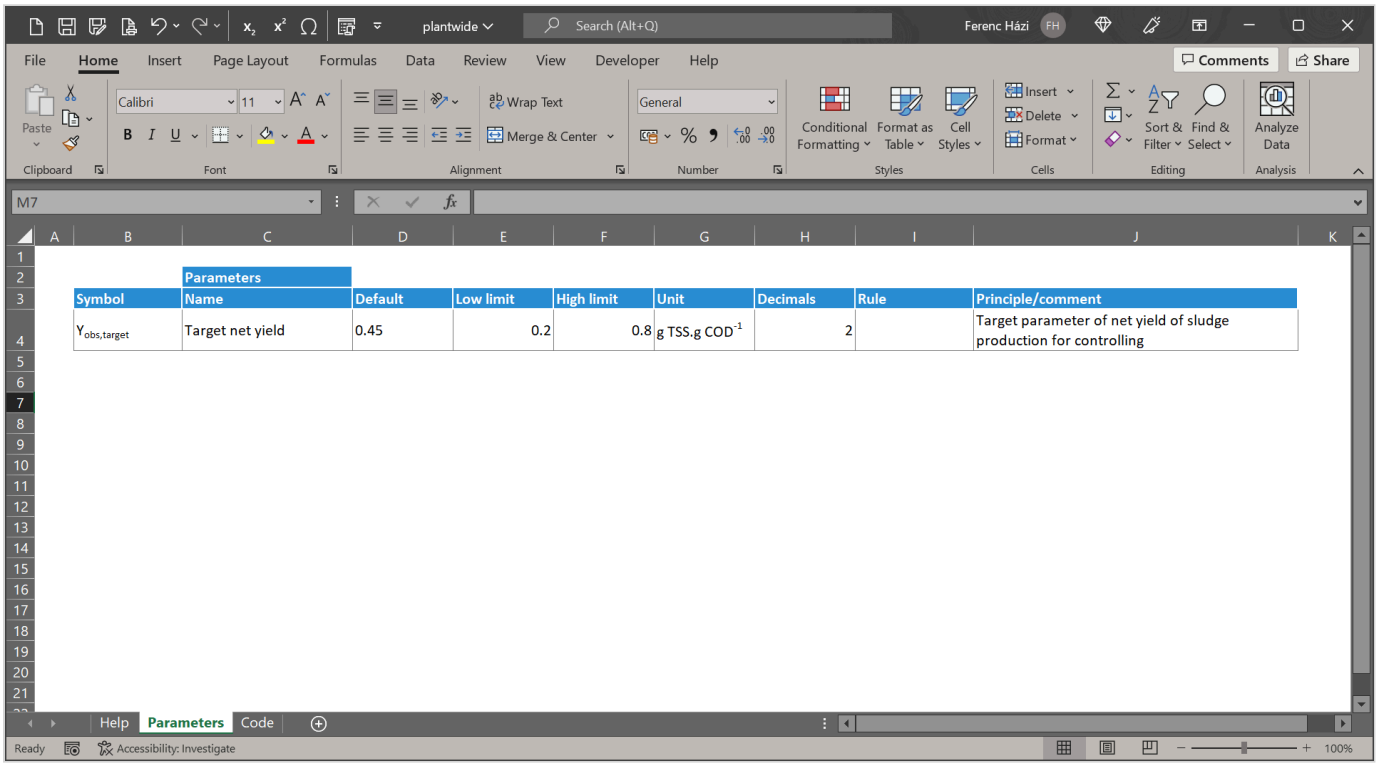
In this example we will be both calculating the net yield and also observe the relationship between wastage flow and sludge retention time.

Using a direct algebraic expression for control

PWE Equation 1. can be solved for the required wastage mass flow rate to maintain a certain $Y_{obs,target}$. Since the model calculates waste solids concentration, the required flow can be expressed.

Definition of the Y_{obs} and wastage control to maintain a desired $Y_{obs,target}$ is carried out by establishing the plantwide code available in Sumo using the necessary variables in the relevant process units.

Define the values for any parameters used in the code on Parameter sheet (PWE Figure 3.). These values can be modified on the Input setup tab in the GUI, without rebuilding the model.



PWE Figure 3 - Parameter table in plantwide file

Variable names used in the code

When writing code, the Incode names of the process units and Symbols of variables have to be used. The general way to write variable names in the plantwide code:

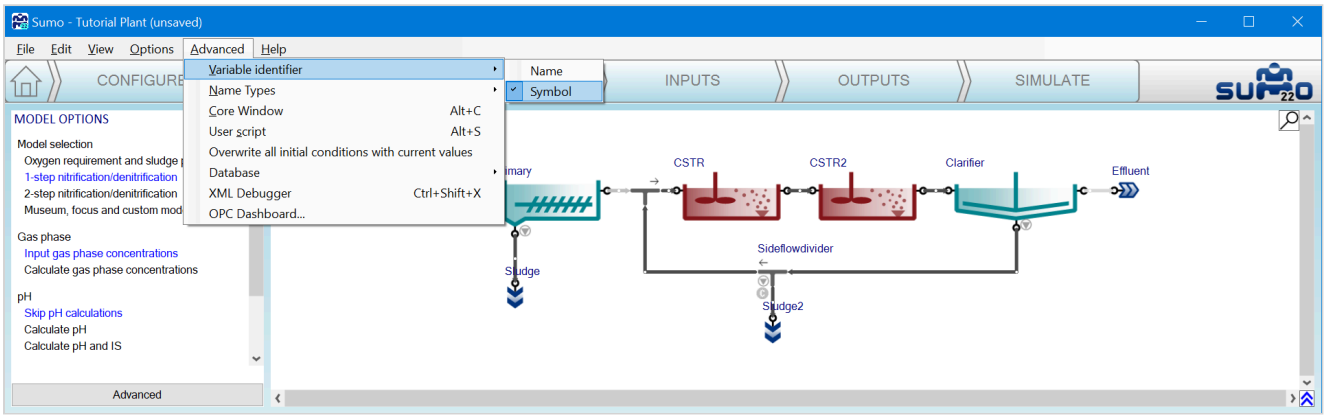
Variables in process units or pipes		Parameters in process units	
Process units	Process unit name..variable	**In expression**	Process unit name..parameter
Pipe	Pipename..variable	**To Control/Set**	

Model parameters	
Global	Model name..parameter
Local	Sumo__Plant__Process unit name__Model name__parameter

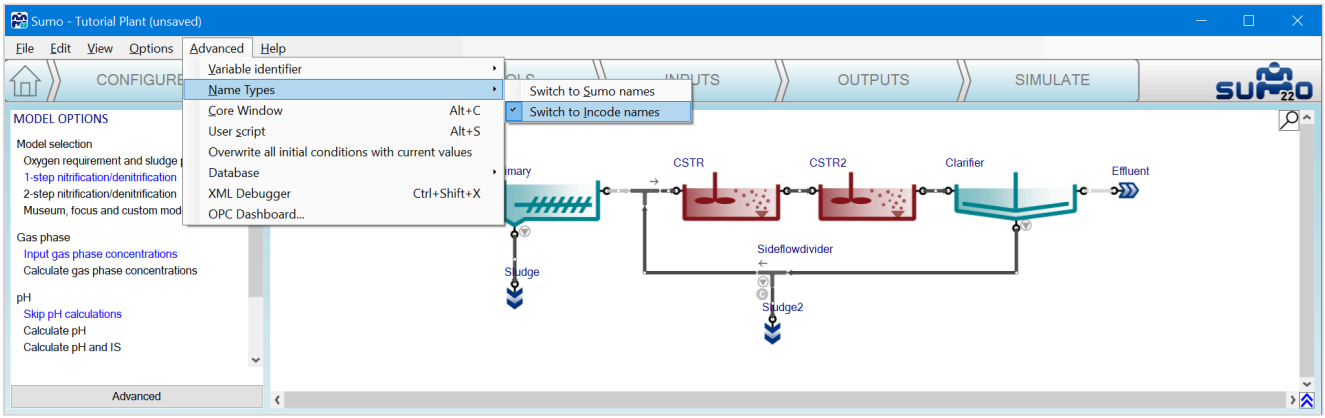
As the engineering names used by the GUI may differ from the names in the code, make sure to use the correct forms, go to:

- View|Advanced|Variable identifier|Switch to Symbol (PWE Figure 4a).
- View|Advanced|Name types|Switch to Incode names (PWE Figure 4b).

The pipe names can be used for calculation therefore pipe names are also need to be shown (View|Show pipenames).



PWE Figure 4a - Changing variable names



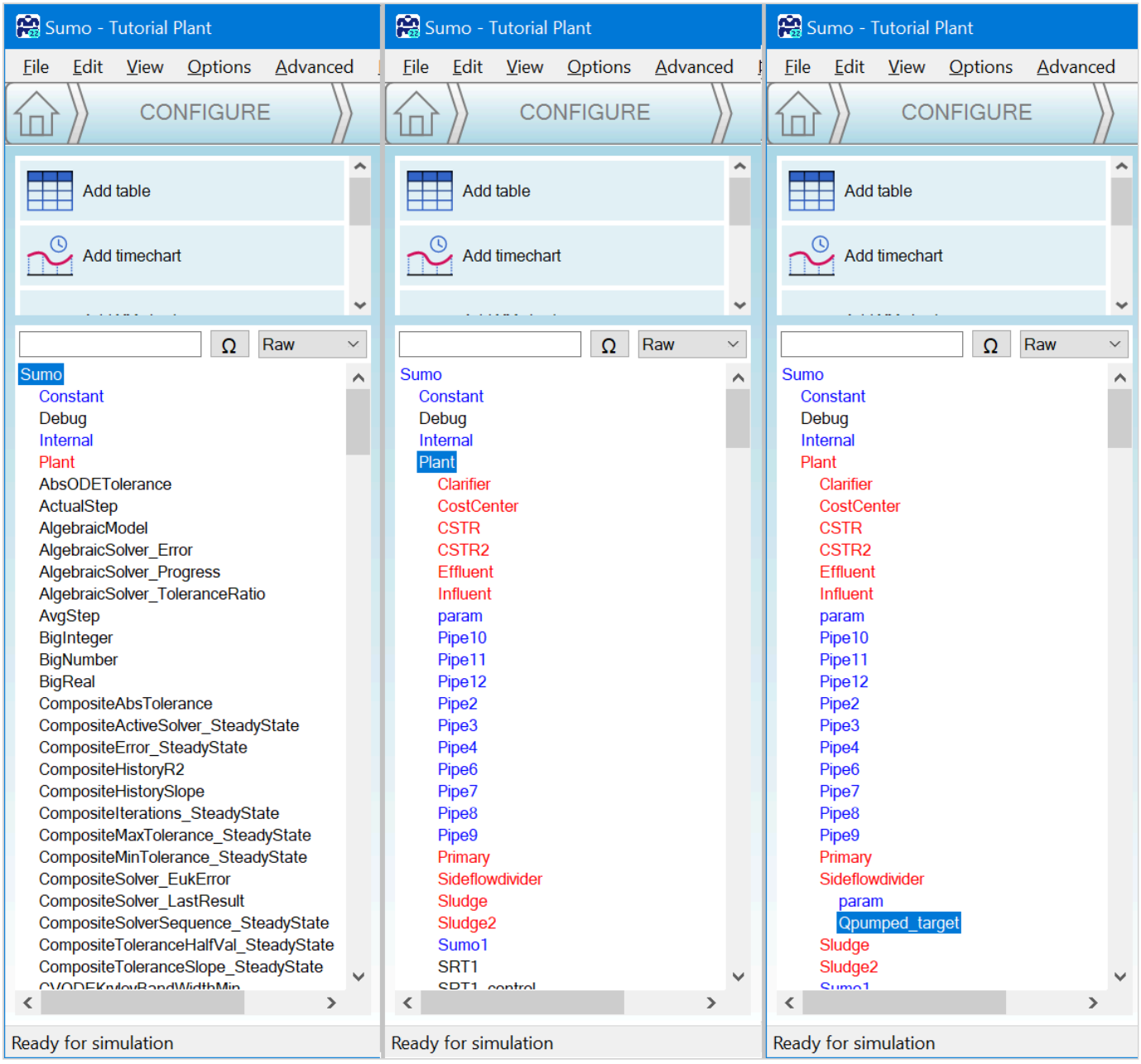
PWE Figure 4b - Changing unit name types

There are different ways to access/verify these valid forms of names.

Output setup

Output Setup tab, left bottom pane, changing the search method to “Raw” and clicking through to the relevant process unit (PWE Figure 5). Here the list shows the Sumo names and proper form of symbols. Concatenate the name with the namespace symbol as shown above:

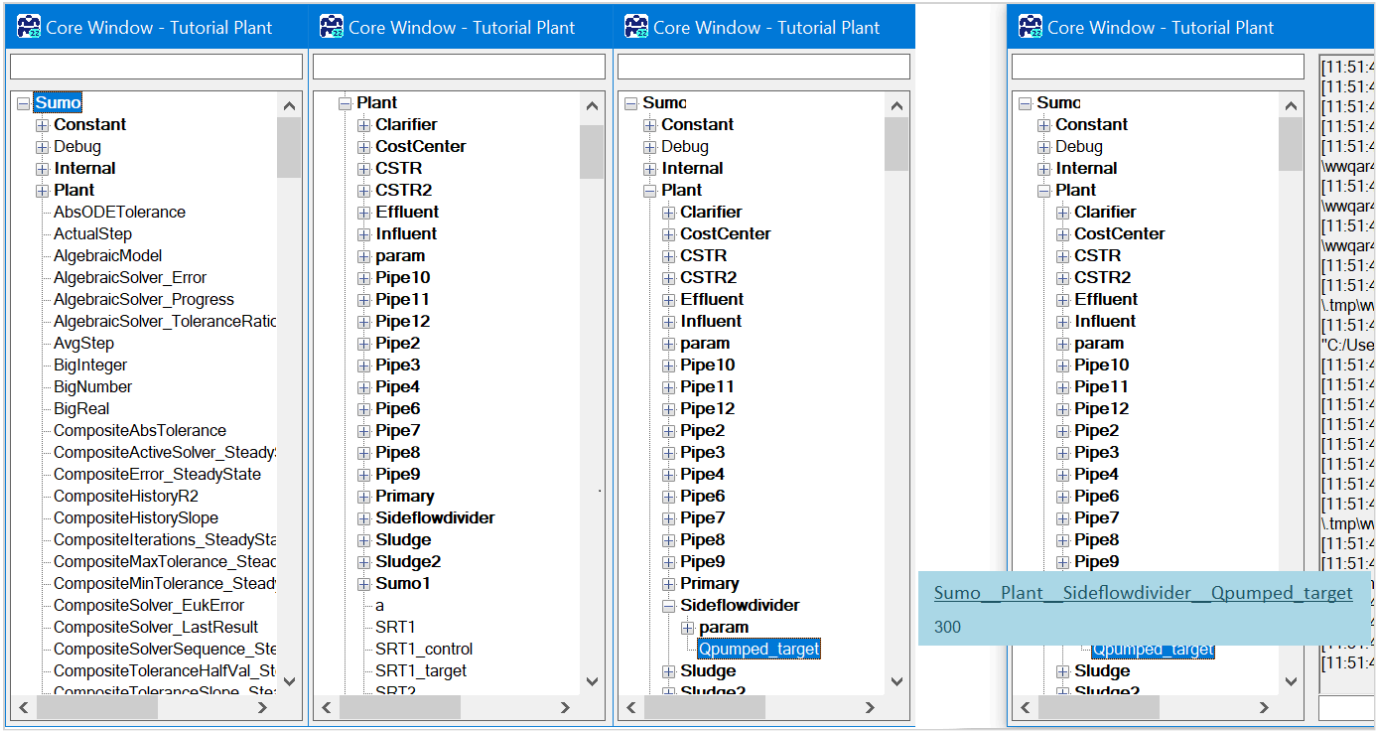
Parameters in process units	
In expression	Sideflowcombiner..Qpumped_target
To Control/Set	



PWE Figure 5 - Find Side flow combiner parameter in Output setup

Advanced core window

Open the advanced core window: View|Advanced|Core window. On the left panel all the variables and constants are listed (PWE Figure 6). Opening the relevant process unit and hovering over the symbol of the variable, the namespaced symbol appears. Use this form excluding the Sumo__Plant namespace. Double underscores are namespace separators.

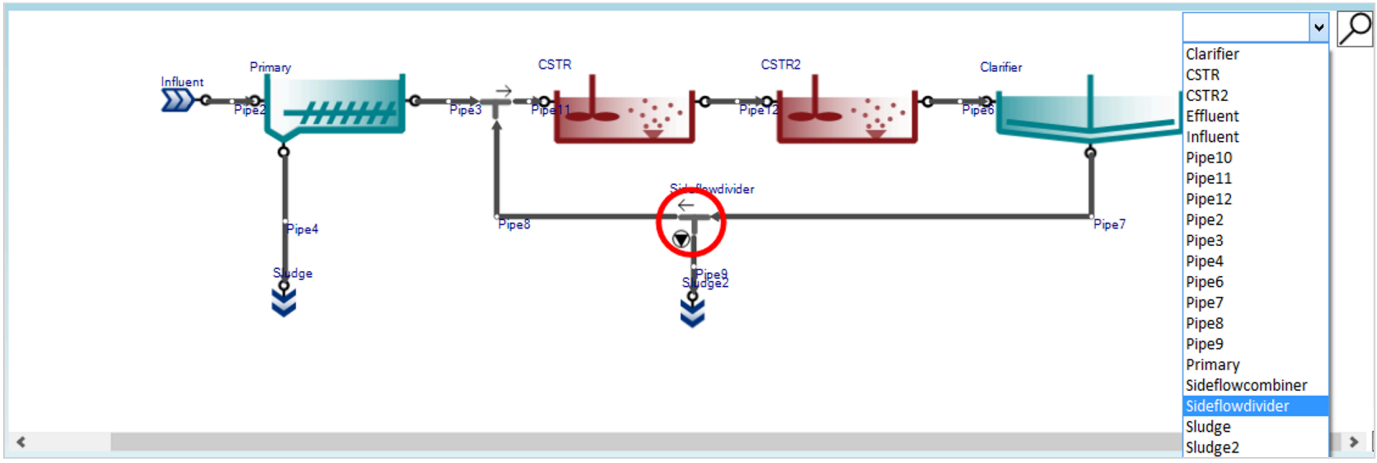


PWE Figure 6 - Find target pumped flow in side flow divider in the Advanced Core window

Process Code

Specific variable names can be found also directly in the code View|Directories|Install directory|Process Code|Process Units the process unit parameters and View|Directories|Model directory for the model parameters and variables. This way the MS Excel sheet is opened where you will find not only the symbols but the descriptive names of the variables to avoid confusion.

During the calculations, the port names are not used in this version, so when a variable is needed from a specific input/output port please look for the connected pipe. In case of large configurations to find the connected pipe, a PU search tool can be found on the drawing board (PWE Figure 7).



PWE Figure 7 - Finding Process Units

Project directory

The complete simulation code is also available after the model was prepared for simulation at any point. It can be found in the Install folder .tmp directory as the varaibles.var file: View|Directories|Project

directory|variables.var. The .var (can be opened with Notepad) is a text file and contains all the variables.

Special cases and namespaces

Array variables

To address array variables in the code (variables for cells of a PFR reactor, phases of flexible SBR cycle, etc) an [i] has to added after the parameter/variable name such as:

PFR3..Qair,NTP[1]	airflow into the 1st cell of the PFR3 reactor
PFR3..Qair,NTP[3]	airflow into the 3rd cell of the PFR3 reactor
PFR3..Qair,NTP[n]	airflow into the last cell of the PFR3 reactor, where n is the Number of cells of the PFR3 unit of the layout

The index starts at 1 for the array variables and goes to the array size defined by the input parameter for the unit specification (input parameter, as Number of PFR segments).

Further details and specification of array variables are in the Book of SumoSlang (Sumo home screen, top left panel).

Sumo__Plant

The Sumo__Plant namespace is only necessary to use in the plantwide code with the above highlighted special cases.

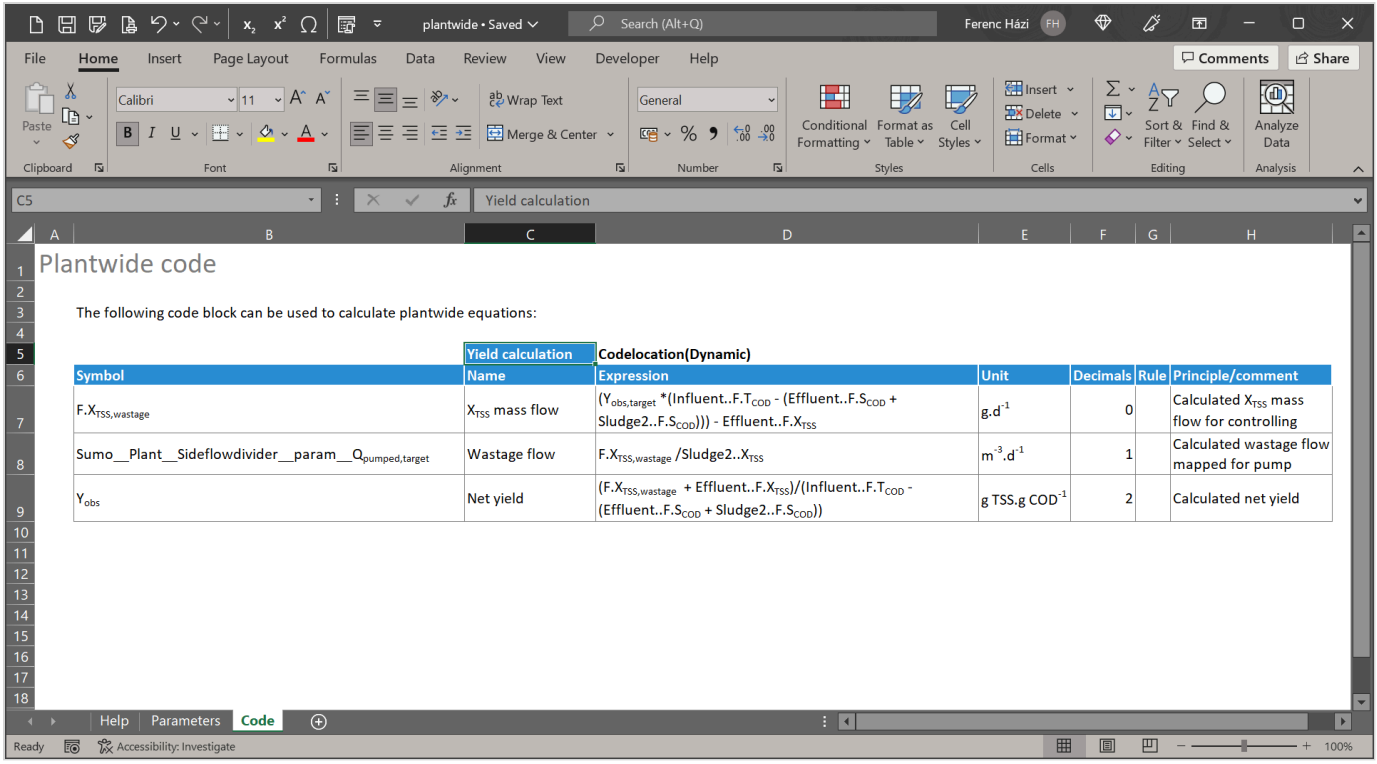
Use of __param__ namespace

The additional **param** namespace was introduced to avoid misconception during control logic building in a project. It has to be used if the parameter is on the left hand side of the equation (under symbol) so the calculation will set/control its value.

Building calculation on the code sheet

Building the plantwide code for this example consists of the following 3 steps (Figure 6):

1. Calculate mass flow of waste TSS ($F.X_{TSS,wastage}$ in equation) from PWE Equation 1.
   The wastage TSS mass flow is expressed from the equation using the target yield. The Influent..$F.T_{COD}$ mass flow rate could be written as Pipe2..$F.T_{COD}$ as Pipe2 is connected to the Influent process unit's output port.
2. Calculate target pumped flow dividing the mass flow by the waste TSS concentration.
   The wastage flow is usually an input parameter in the waste flow divider, but to meet the target yield, it can be calculated as the target flow based on the waste TSS. Remember to use the full namespaced version. As it can be seen the $Q_{pumped,target}$ symbol (as in Process Code excel file) can contain the ‘,’ and it will be converted into ‘_’ automatically.
3. Calculate net yield
   This step calculates the actual net yield which is equal to the target yield in algebraic direct control mode. If rows 7and 8 are deleted, the model will use the wastage flow from the GUI input and simply calculate Y_{obs}.



Plantwide code

The following code block can be used to calculate plantwide equations:

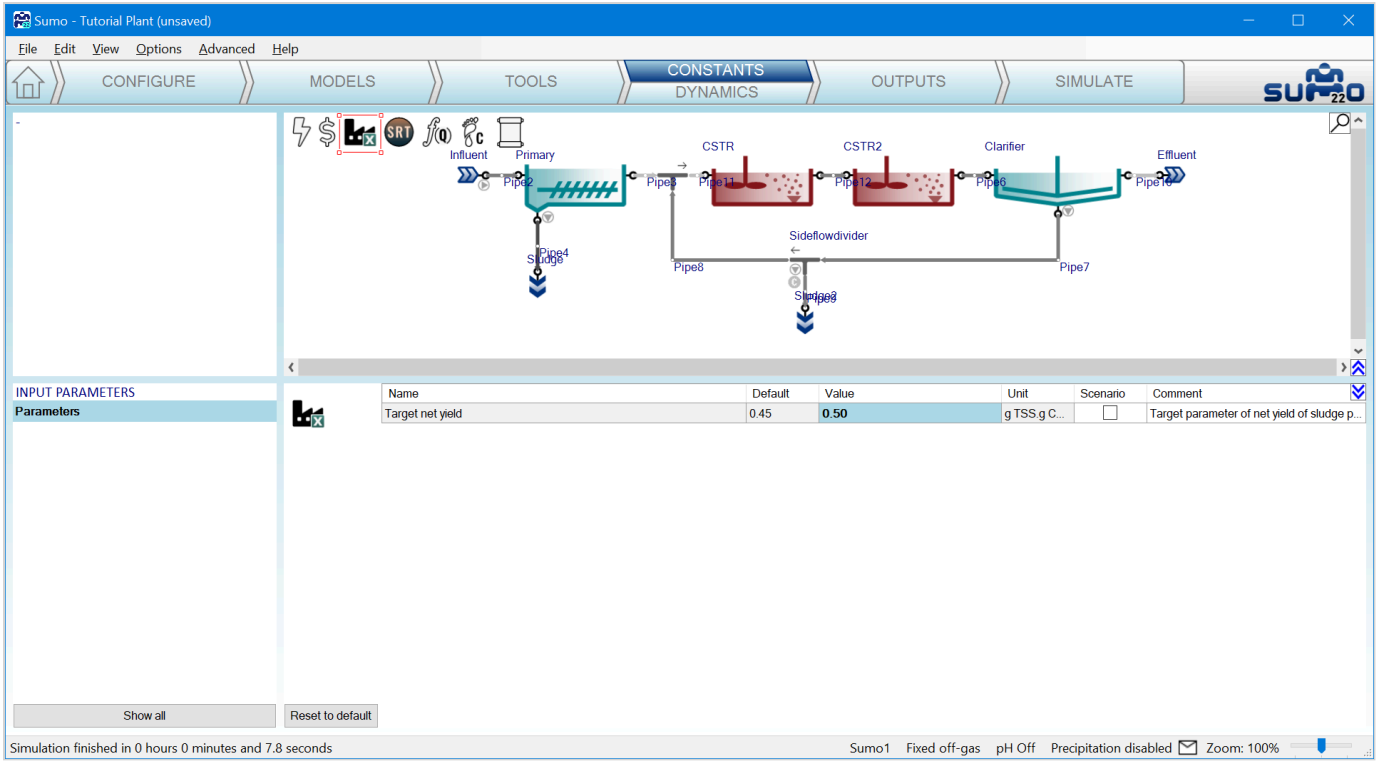
	Yield calculation	Codelocation(Dynamic)				
Symbol	Name	Expression	Unit	Decimals	Rule	Principle/comment
$F.X_{TSS,wastage}$	X_{TSS} mass flow	$(Y_{obs,target}$ *(Influent..F.T_{COD} - (Effluent..F.S_{COD} + Sludge2..F.S_{COD}))) - Effluent..F.X_{TSS}	$g.d^{-1}$	0		Calculated X_{TSS} mass flow for controlling
Sumo__Plant__Sideflowdivider__param__$Q_{pumped,target}$	Wastage flow	F.$X_{TSS,wastage}$ /Sludge2..X_{TSS}	$m^{-3}.d^{-1}$	1		Calculated wastage flow mapped for pump
Y_{obs}	Net yield	(F.$X_{TSS,wastage}$ + Effluent..F.X_{TSS})/(Influent..F.T_{COD} - (Effluent..F.S_{COD} + Sludge2..F.S_{COD}))	g TSS.g COD^{-1}	2		Calculated net yield

PWE Figure 8 - Plantwide code

When saving the file, it must be placed to the autogenerated Project folder - it was opened from there. After saving and closing the Excel file, continue with your workflow. The compilation of the model starts after this point however when changing the plantwide file after the compilation is complete, rebuilding the model is necessary each time.

Set parameters at input setup

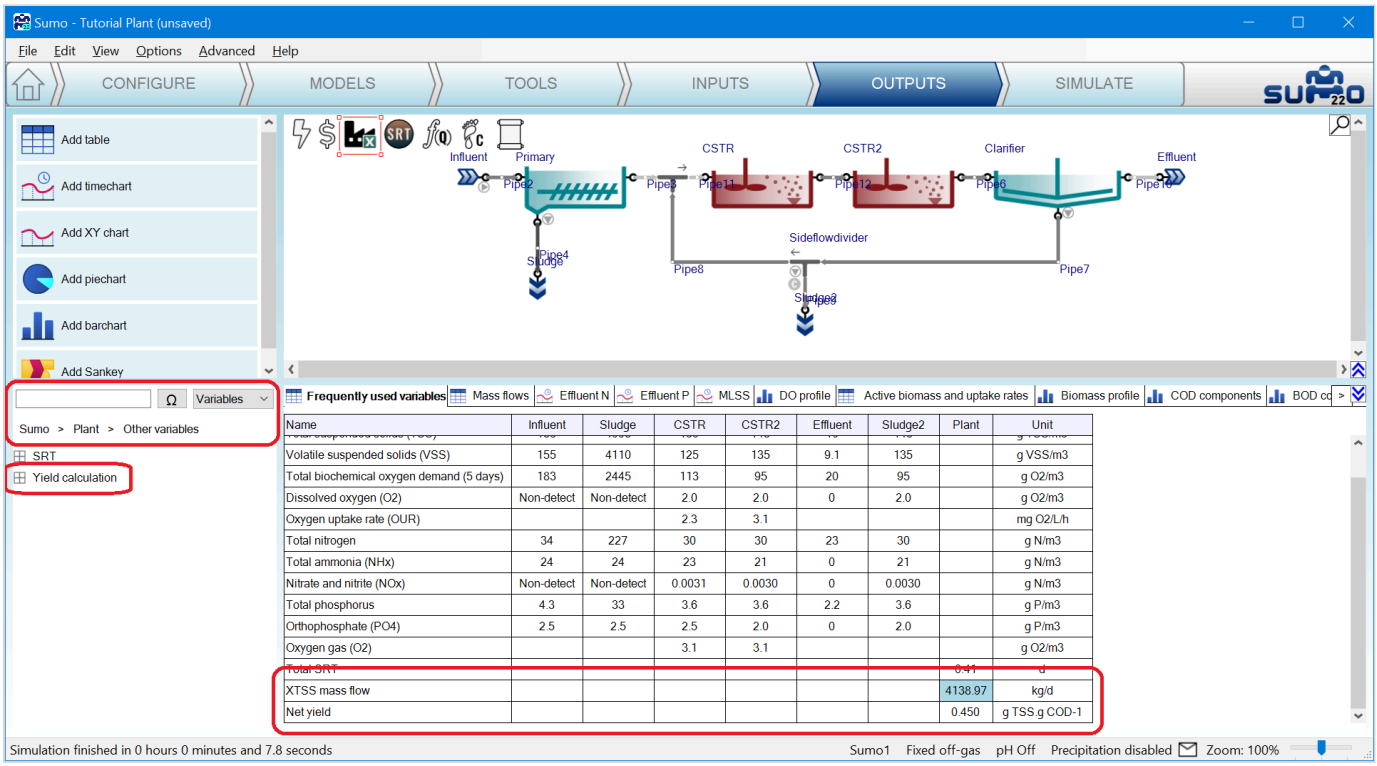
To reach the new parameters of the project, at input setup the Plantwide excel/Factory icon has to be selected. The bottom left panel lists the parameters added to the plantwide excel:



PWE Figure 9 - Plantwide parameters at input setup

Add variables to output setup

To reach the new variables of the project at output setup the Plantwide excel/Factory icon has to be selected. The bottom left panel lists the variables under Sumo|Plant|Other variables|Yield calculations added to the plantwide excel. Note the list name as it is the block header on the code sheet, see cell C9 on PWE Figure 8.



PWE Figure 10 - Plantwide variables at output setup

Advanced User Topics

Keyboard Shortcuts

To speed up workflow, various shortcut commands are available in Sumo, as listed below

The commands marked with general scope are available regardless of which Tab is selected, while the ones with a certain Tab scope are available only when the specified Tab is selected. Some commands are specifically related to the drawing board.

Shortcut	Scope	Effect
Ctrl + N	General	Start new project
Ctrl + O	General	Open existing project
Ctrl + S	General	Save current project
Ctrl + Shift + S	General	Save current project as
Alt + F4	General	Exit Sumo
Ctrl + Z	General	Undo last action
Ctrl + Y	General	Redo last action
Ctrl + Home	General	Zoom to plant
F2	General	Rename selected process unit
Ctrl + A	General	Select all process units
Ctrl + C	General	Copy selection
Ctrl + V	General	Paste
Ctrl + 1...6	General	Select "Configure" ... "Simulate" tabs
Ctrl + M	General	Show/hide message pane
Alt + C	General	Open Core Window
Alt + S	General	Open Userscript
Ctrl + Shift + X	General	Open XML Debugger
ESC	Drawing board	Clear selection
F7	Drawing board	Horizontal mirror
F8	Drawing board	Vertical mirror
F9	Drawing board	Align Ports
Ctrl + W	Drawing board	Show/hide name
Ctrl + F	Drawing board	Find process unit or pipe
Ctrl + scrolling mouse wheel	Drawing board	Zoom in and out the drawing board
Ctrl + middle mouse button	Drawing board	Move configuration around the pane
Del	Configure Tab	Delete selection
Ctrl + click and move	Tools Tab	Move controllers on the drawing board

SumoCore command documentation

A list of Sumo core commands

path

Command	*path <folder>*
Description	Sets the current working directory.
Arguments	**folder** The current working directory will be changed to this folder
Examples	`path c:/;`
Response	530007 Path set to: "\1".

reset

Command	*reset*
Description	Resets all variables to the factory default. Any parameters, dynamic inputs, state variable values are lost.
Response	530011 Reset

set

Command	*set <variable> <value>*
Description	Sets a variable to the given value. Changing a dimension variable will automatically resize all arrays connected to it. If this happens during a simulation, the simulation stops.
Arguments	**variable** Full name of the variable. Only variables with the role of SystemParameter, Parameter, Dimension or Constant can

		be set.
	value	The type of the value must match the type of the variable.

Examples	`set Sumo__Plant__Unit__param__Scalar 1;`
	`set Sumo__Plant__Unit__param__Array 1 2 3;`
	`set Sumo__Plant__Unit__param__Array(0) 1;`

Response	530021 Set: \1 to \2

mode

Command	*mode <mode>*
Description	Sets the simulation mode. Algebraic mode is for very simple calculations in a special Algebraic block. Dynamic mode does dynamic simulation. Steady mode calculates steady-state.

Arguments	**mode**	algebraic, dynamic or steady

Examples	`mode dynamic;`
Response	530053 Mode: \1.

save

Command	*save <filename>*
Description	Saves every variable in an xml format, that you can load back with the load command.

Arguments	**filename**	the name (or full path) of the file you want to create

Examples	`save systemstate.xml;` `save "c:/Users/UserName with Spaces/systemstate.xml";`

Response	530045 Current systemstate saved to "\1".

load

Command	*load <filename> [-partial 1]*
Description	Load every variable from an xml format. Must be used on a systemstate file created with save command from the same model.
Arguments	**filename** the name (or full path) of the file you want to open **-partial 1** optional. If the models doesn't match, loads back any variable that does match. Everything else is ignored.
Examples	`load systemstate.xml;` `load "c:/Users/UserName with Spaces/systemstate.xml" -partial 1;`
Response	530041 Systemstate loaded from "\1".

savestates

Command	*savestates <filename>*
Description	Saves every state variable in an xml format, that you can load back with the loadstates command.
Arguments	**filename** the name (or full path) of the file you want to create
Examples	`savestates state.ss;` `savestates "c:/Users/UserName with Spaces/state.ss";`
Response	530045 Current systemstate saved to "\1".

loadstates

Command	*loadstates <filename> [-partial 1] [-if-better-by <value>] [-maptoic]*
Description	Load every state variable from an xml format. Must be used on a systemstate file created with savestates command from the same model.
Arguments	**filename** the name (or full path) of the file you want to open **-partial 1** optional. If the models doesn't match, loads back any variable that does match. Everything else is ignored. **-if-better-by <value>** optional. If present, the core will not load back the state, if Sumo__MaxAbsDer is larger than the current divided by the given value **-maptoic** optional. If the command is successful, follow it up with a maptoic command
Examples	`loadstates state.ss;` `loadstates "c:/Users/UserName with Spaces/systemstate.xml" -partial 1 -if-better-by 10 -maptoic;`
Response	530041 Systemstate loaded from "\1".

loadtsv

Command	*loadtsv <filename> [-cycletime <value>] [-interpolation <value>]*
Description	Loads a dynamic input table from a tsv file. The file should contain the full name of the target variables, the numbers should be in in-code units and the first column should be Sumo__Time in days. If you modify the file, you need to call unloadtsv on it and then use loadtsv again to refresh the values in the Core.
Arguments	**filename** the name (or full path) of the file you want to open **-cycletime <value>** optional. If set, the dynamic input will restart every <value> msecs. Any value in the dynamic input beyond this time will be ignored with a warning.

	-interpolation <value>	optional. Can be none or linear. If this flag is not set, the default interpolation is none.

Examples

```
loadtsv input.tsv;
```

where *input.tsv* is e.g.

Sumo__Time	Sumo__Plant__Influent__param__Q
0	24000
1	12000
2	24000

Response

530029 TSV file "\1" loaded with \2 interpolation.
530030 TSV file "\1" loaded.
530042 TSV file "\1" loaded with \2 cyclestart and \3 cycletime.
530043 TSV file "\1" loaded with \2 interpolation, \3 cyclestart and \4 cycletime.

unloadtsv

Command	*unloadtsv <filename>*	
Description	Unloads the target dynamic input file that was previously loaded.	
Arguments	**filename**	the name (or full path) of the file that is to be unloaded. It should be the exact same argument that was given to the loadtsv command, even if the file is not there anymore.

Examples

```
unloadtsv input.tsv;
```

Response

530050 TSV file "\1" unloaded.

writetsv

Command	*writetsv <filename> [<variableslist_filename>]*	
Description	Creates a tsv file containing simulation data from every datacomm. A writetsv command is needed without any arguments to release the files that were written.	
Arguments	**filename**	the name (or full path) of the file that is to be written.
	variableslist_filename	optional. The name (or full path) of the file that contain the list of variables (one variable per line). If omitted, all variables are saved to the file.
Examples	`writetsv output.tsv;`	
Response	530037 TSV writer: "\1" all variables. 530038 TSV writer: "\1" variables from file "\2". 530047 TSV writer: writing disabled.	

maptoic

Command	*maptoic*
Description	Maps state variables to initial condition.
Response	530019 Mapping to initial conditions.

execute

Command	*execute <filename>*	
Description	Executes the target sumocore script. The file should contain sumocore commands delimited by semicolon (';').	
Arguments	**filename**	the name (or full path) of the file you want to execute.

Examples	`execute myscript.scs;`
Response	530036 Script file \1 loaded.

start

Command	*start*
Description	Starts the simulation in the mode previously selected by the mode command
Response	530002 Simulation started.

pause

Command	*pause*
Description	Pauses the simulation.
Response	530003 Simulation paused.

continue

Command	*continue*
Description	Resumes the simulation.
Response	530008 Simulation continues...

stop

Command	*stop*
Description	Stops the simulation.
Response	530004 Simulation ended.

Advanced core window

Fuctions and features of the advanced core window

What is the Core window?

The advanced core window is available from the Advanced menu. This gives the capability to execute more advanced functions, such as quickly checking any variable value in the simulation, saving any variables into an Excel file and more. To evaluate the possibilities of the advanced core window open the Tutorial plant from the examples.

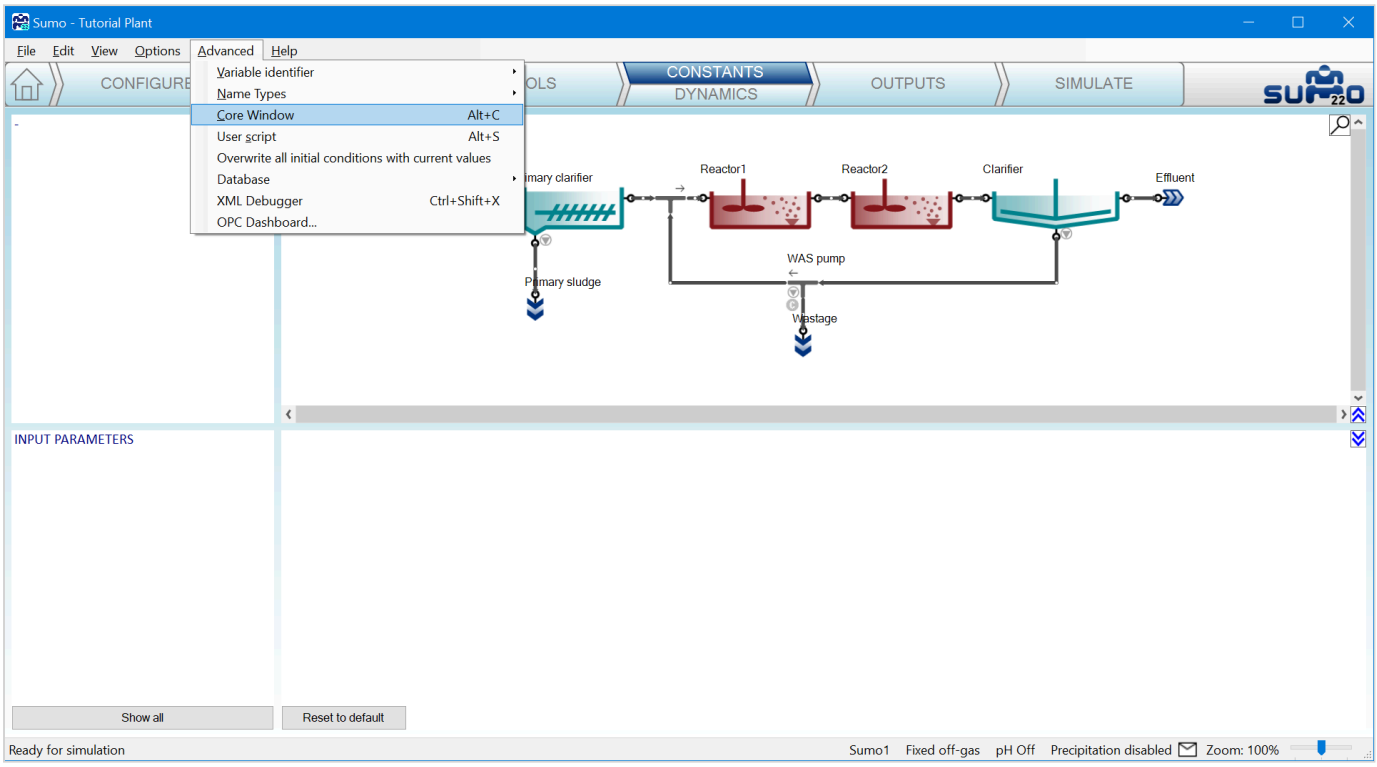


Figure ACW-1. Advanced core window from menu

As it can be seen in Figure ACW-02 the advanced core window is divided into two panels.

The left panel contains the list of all variables that are available inside the current project. The internal variable symbols (i.e. the names that are used by the Sumo system itself) follow the naming conventions detailed below:

- All variable names contain one or more namespaces and the variable name itself. The namespaces and the name are separated by double underscores ('__'). A general internal symbol has the following structure: <<Application>>__<<Project>>__<<Process unit>>__<<variable name>>.
- All variable symbols have 'Sumo__' as their application level namespace. Global variables like solver numerical parameters have their names directly after the 'Sumo__' namespace (e.g. Sumo__StopTime).

- The variables specific for a given project are organized under a project level namespace. In current Sumo versions this is called ‘Plant__’, so all variables that are project specific, have the ‘Sumo__Plant__’ classifier.
- The process unit names form the third level of namespacing, so e.g. all variables in ‘Reactor1’ of the ‘Plant’ example have ‘Sumo__Plant__Reactor1__’ as their namespace classifiers.
- According to the above, the total COD in Reactor1 has the internal symbol of ‘Sumo__Plant__Reactor1__TCOD’.
- There is a separate category of global Sumo variables that are called the Sumo constants. Atomic weights, general physico-chemical constants, etc. belong here. These variables are namespaced as ‘Sumo__Constant__’.

There is a possibility to filter the variable names appearing in the panel: at the top of the left panel a textbox accepts different filter expressions. Typing the first few characters of the internal symbols allows to show only those variables that have symbols starting with those characters. E.g. typing ‘Sumo__Plant__Reactor1’ shows those variables only that belong to the ‘Sumo__Plant__Reactor1’ process unit.

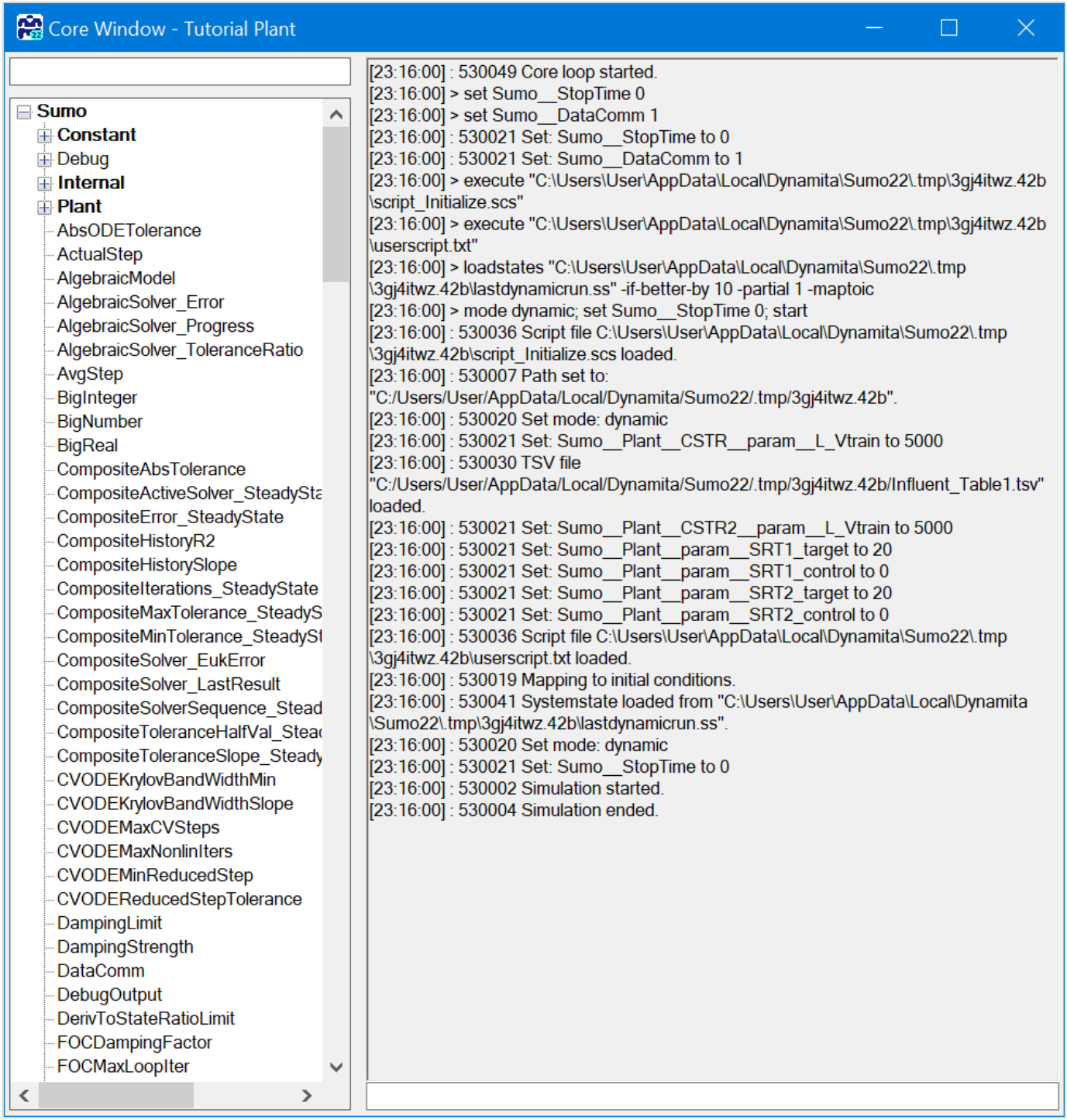


Figure AWC-02. The advanced core window

The right panel consists of a list of recently issued core commands (at the top) and a command line where Sumo core commands can be typed manually. This way the full power of the underlying core can be achieved. The commands that can be used are described in the **Sumo script commands** chapter.

Exporting variables for further processing

Sumo supports exporting any variables into tab separated (.tsv) text files. These files can be directly read by Microsoft Excel or other applications. For variable exporting the direct command interpretation capability of the advanced core window is used.

To export the results of a run, the 'writetsv' command should be used in the command line, with a file name as a parameter. The data to be exported will be saved into the file determined by that file name.

Once the writetsv command has been issued, the simulation needs to be rerun from the command line for the data export to happen.

We will use the birthday cake data from the influent tool thus add it to the Influent unit under Dynamics. It has data for a 16-day simulation. Let us assume that the data from this run needs to be exported to a file. In order to do that, let us open the advanced core window.

At the core window, type the command 'writetsv "c:\Users*username*\Documents\plant.tsv"' into the command line as it is shown in ACW-03, then press Enter (don't forget to change 'username' to your user name on your computer).

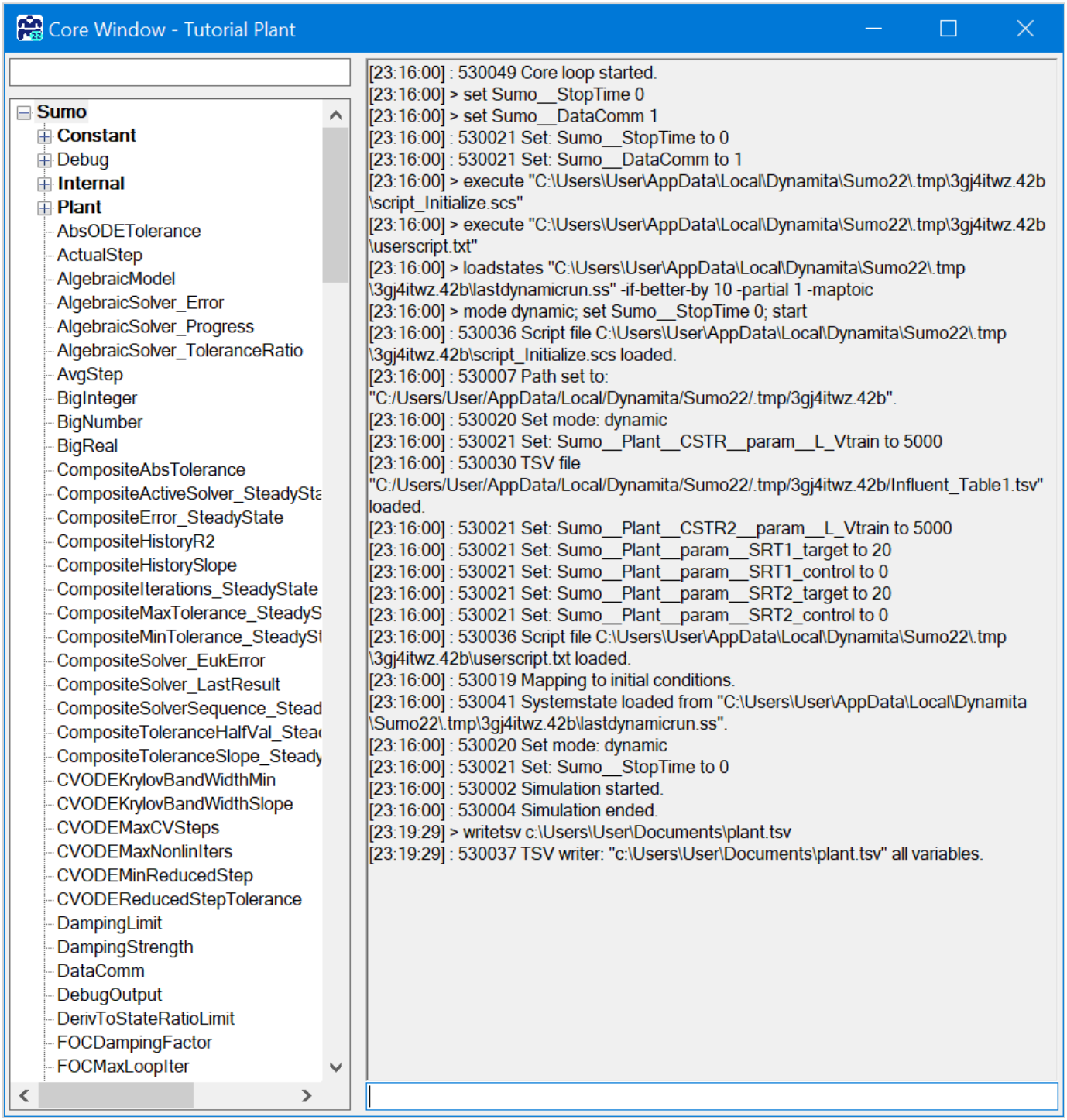


Figure ACW-03. Issuing a 'writetsv' command in advanced core window

Once Enter has been pressed, the system answers with a '530037 TSV writer: "c:\Users\username\Documents\plant.tsv" all Variables' message in the command history panel. Now start the 16-day simulation from Sumo main window. Once the simulation finished '530004 Simulation ended.' message appears followed by 'savestates' messages.

At this point you have your file at your 'Documents' folder (if you followed the filename suggestions), that can be opened by your Excel or your favourite application. The data file is a plain ASCII file where the variables are in columns with tab as the column separator. This file format can be read by Microsoft Excel.

With the previous example, we have exported all the variables that could be found in our example project. There are situations however, when we only want to do that for only a few selected variables. In such cases a second parameter can be given to the 'writetsv' command.

This second parameter is the name of the file that contains a list of the variable symbols we want to export. This file should also be a plain ASCII file that can be easily created with e.g. the Notepad software on standard windows installations.

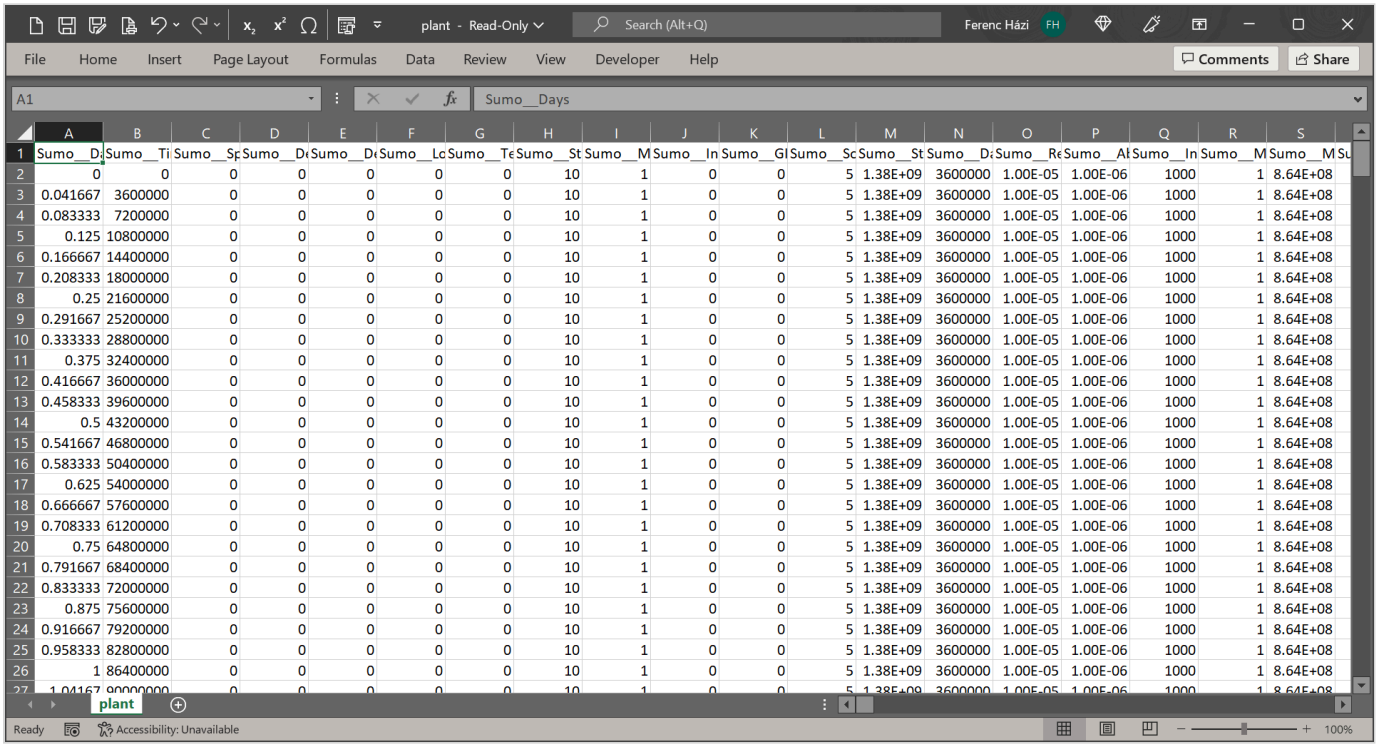


Figure ACW-04. Exported data open in Microsoft Excel

In our example let us assume that we only want to export the ammonia and nitrate concentrations in our plant effluent. According to the previous paragraph, we need to create a file that contains the list of the variables. In order to create the file, open Notepad, and type the names of the variables as in Figure ACW-05 (for information how to determine your variables' symbols, please see the Plantwide Excel file chapter) then Save the file to your 'My Documents' folder, and name it as 'variables.tsv'.

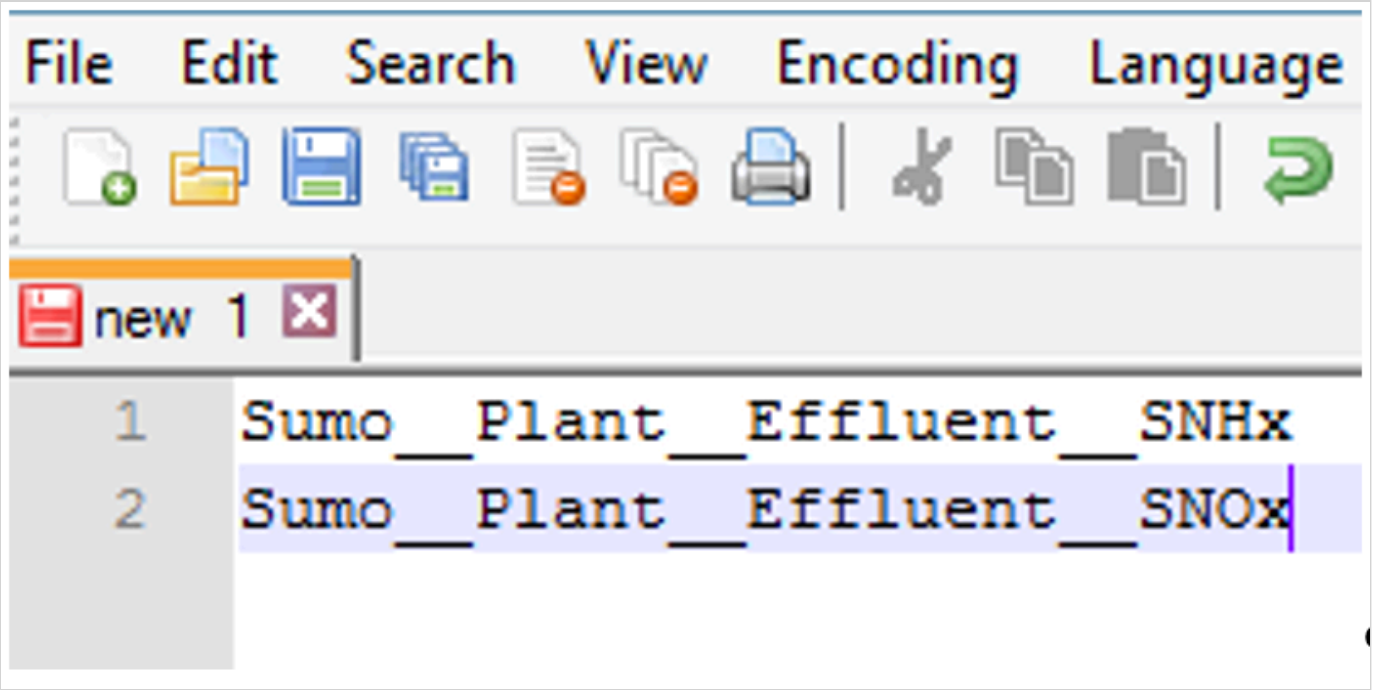


Figure ACW-05. Example export variable list

Once this is done, the command 'writetsv "c:\Users\username\Documents\plant2.tsv" "c:\Users\username\Documents\variables.tsv"' should be typed into the command line. After this, by typing 'start' into the command line and pressing Enter the simulation should be rerun again.

The newly created datafile now contains only those variables that were determined in our list as Figure ACW-06 demonstrates for the 16-day simulation.

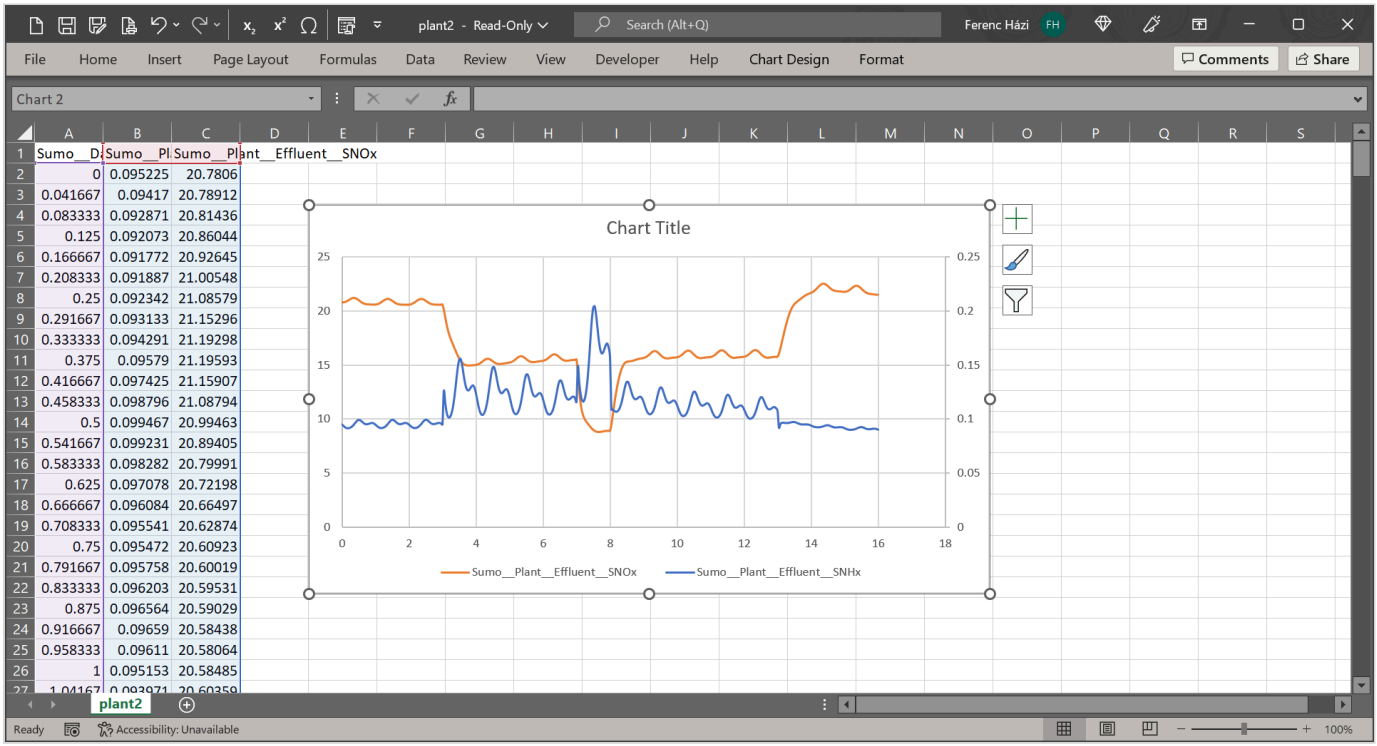


Figure ACW-06. Exported variables open in Microsoft Excel using an export variable list

XML Debugger

How to debug the inside of a simulation

Introduction

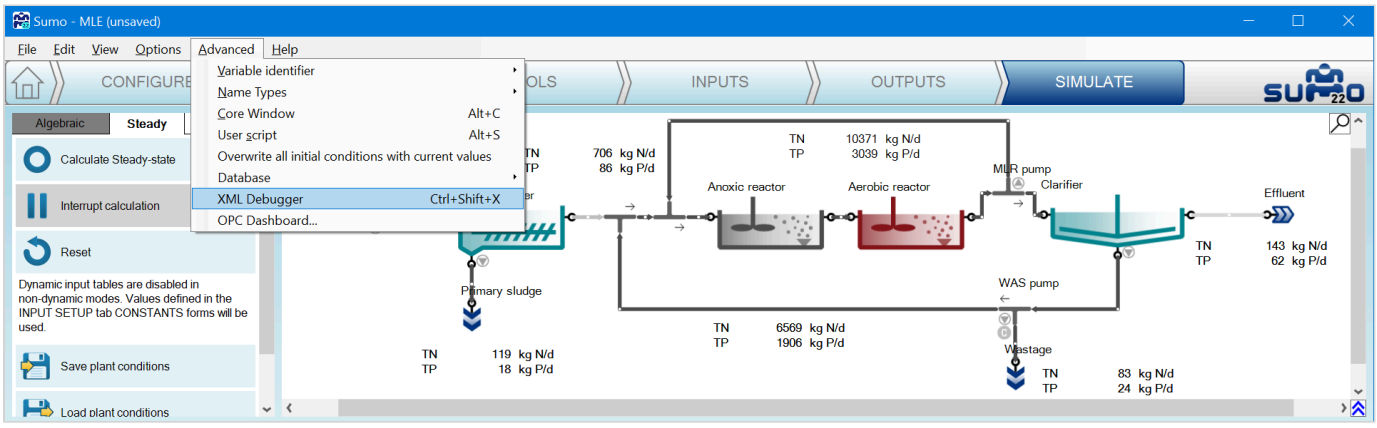
A model generally can be really complex and at a certain level it is really hard to track where the result came from. To help to understand the root of a result and provide some debugging aid Sumo has the XML debugging tool.

How to open and load a model

When the model doesn't predict the numbers it should, it's usually a good idea to check its inner workings and see how things are calculated. The XML Debugger lets you do this in a simple way. We will use the MLE plant as an example, how to use this tool.

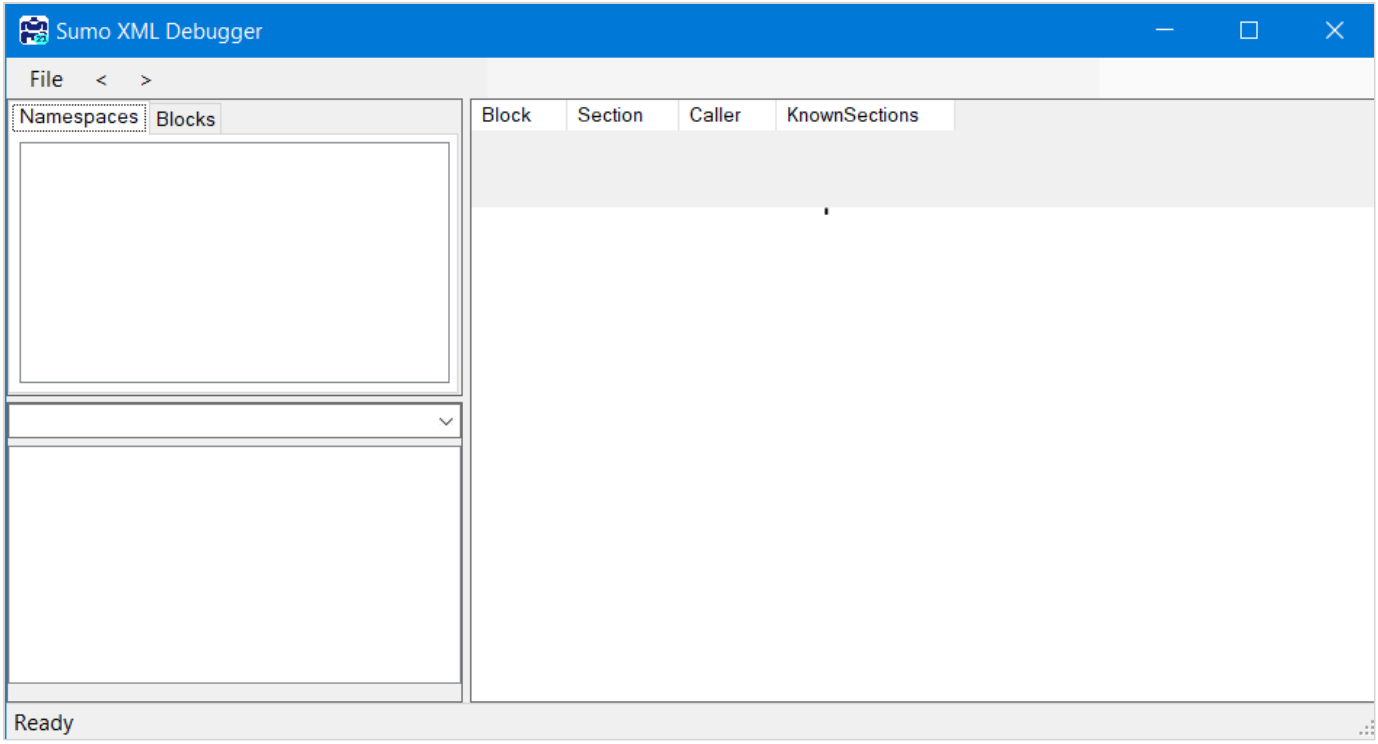
Start XML debugger

Once you've run the simulation to the state that you want to debug, click XML Debugger in the Advanced menu, or press Ctrl-Shift-X:



XML Figure 1 - Start debugger

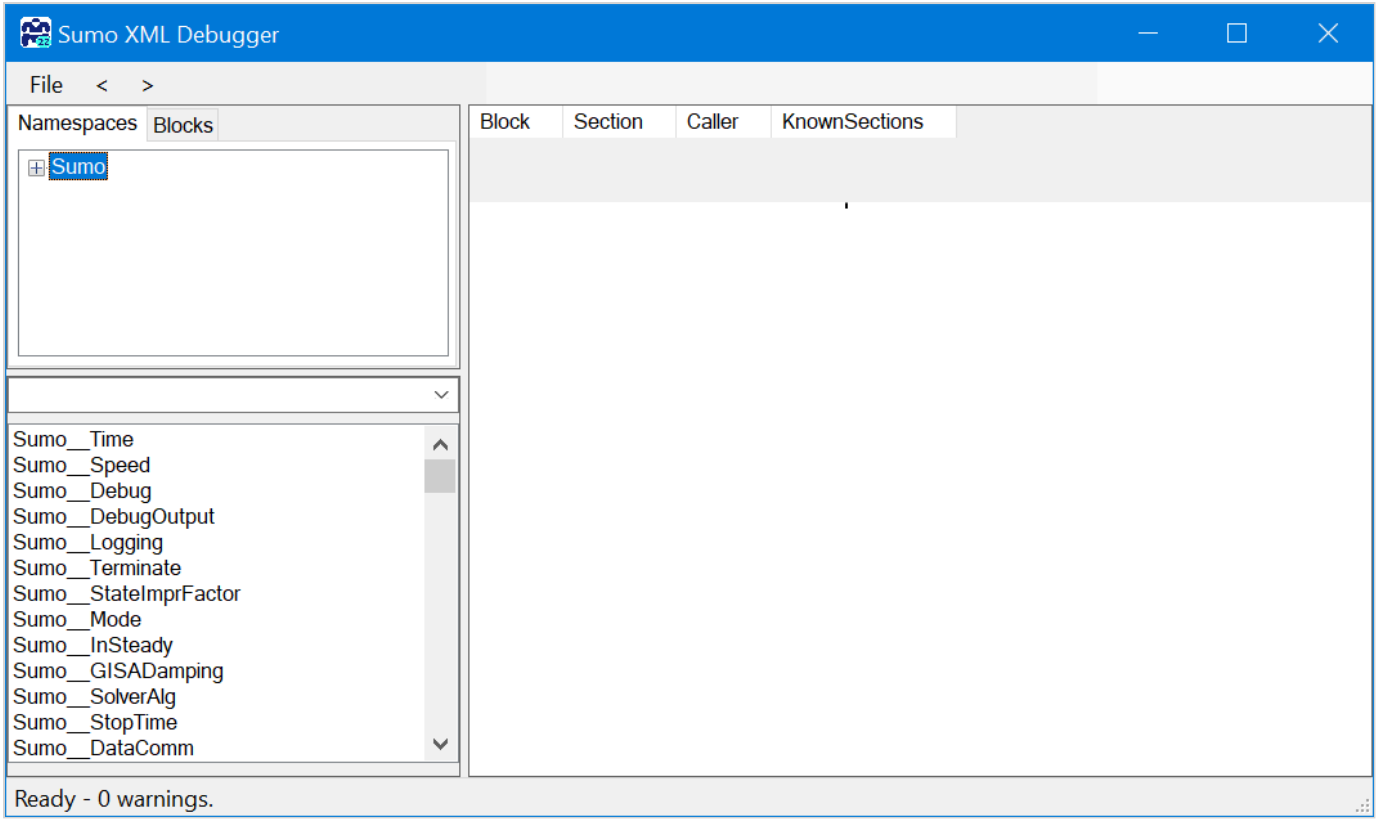
A new window will be opened called Sumo XML debugger:



XML Figure 2 - Debugger opening screen

Load the xml of current project

Click File → Load Current XML, which will load the code behind the currently running model:



XML Figure 3 - Current XML loaded

On the left hand side there are three blocks:

- Namespaces and Blocks tabs:
  - Under Namespaces the structure is identical to the setup seen in the Advanced CoreWindow and similar to Output setup bottom left panel with Raw settings). each layer is considered as a namespace and build up the Incode name of the variable (short description about these can be found in the Plantwide excel calculation chapter).
  - Under Block the structure is following the model structure differently. In this part you can follow the order of calculation blocks, as loading functions, parameters, initializing variables at ZeroTime, calculations in DataComm or the structure of Algebraic loops in the model.
- search field and
- list of variables based on search field and namespace selection.

You have the option to load and browse other XMLs or even build some, but you will only get the numbers for the current one.

Find variables

Once the xml is loaded the blocks can be opened and variables can be selected from the left side of the window (maximize window can help to see everything).

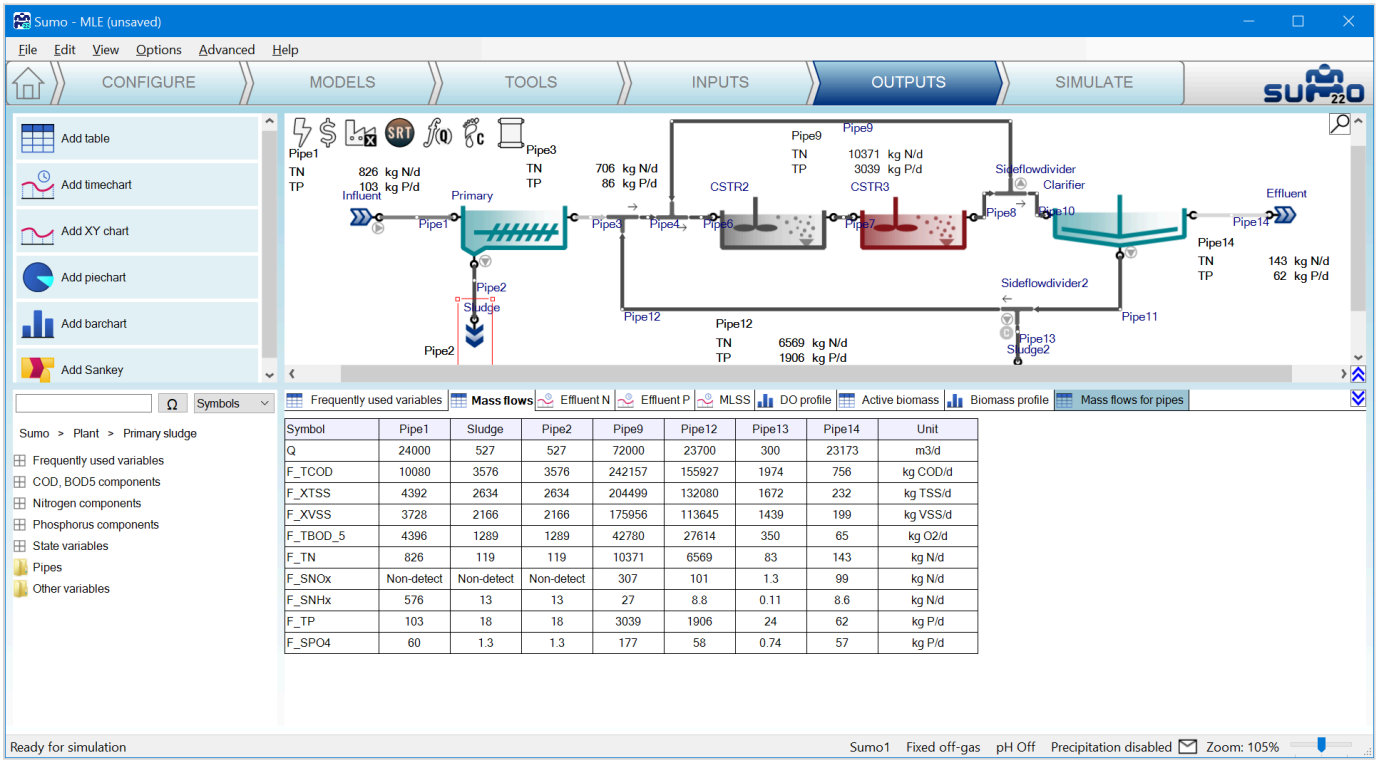
In this example we will check why the Primary sludge flow is different from the expected, thus start at the sludge flow: understand how the primary sludge flow is calculated.

How to: find the variable symbol for check

There are various ways to find the symbol of the variable we want to follow in the debugger. The easiest one is to start from Sumo Outputs tab. Go to the opened Sumo project Outputs tab and change the:

- Advanced|Variable identifier to **Symbols**
  This will change the Name column in any input or output table to Symbols and will show the relevant symbols.
- Advanced|Name types to **Incode names**
  This will change the displayed names of process units on the drawing board and in any table header or chart legend. The setting helps to navigate through the debugger plant structure.

Let us see how this translates for the primary sludge flow. On the figure below (XML Figure 4) the unit names changed as well as the variable names in the table first column. The Mass flows table starts with symbol '**Q**' which originally showed up as '**Flow rate**' (Advanced|Variable identifier|Name). However the column headers are numbered pipes and not unit names as we are looking for. By switching on the View|Show pipe names option we could identify the primary sludge pipe or simply drag and drop the Sludge unit to the table. You can move the column next to Pipe2 and see they have identical values.



Symbol	Pipe1	Sludge	Pipe2	Pipe9	Pipe12	Pipe13	Pipe14	Unit
Q	24000	527	527	72000	23700	300	23173	m3/d
F_TCOD	10080	3576	3576	242157	155927	1974	756	kg COD/d
F_XTSS	4392	2634	2634	204499	132080	1672	232	kg TSS/d
F_XVSS	3728	2166	2166	175956	113645	1439	199	kg VSS/d
F_TBOD_5	4396	1289	1289	42780	27614	350	65	kg O2/d
F_TN	826	119	119	10371	6569	83	143	kg N/d
F_SNOx	Non-detect	Non-detect	Non-detect	307	101	1.3	99	kg N/d
F_SNHx	576	13	13	27	8.8	0.11	8.6	kg N/d
F_TP	103	18	18	3039	1906	24	62	kg P/d
F_SPO4	60	1.3	1.3	177	58	0.74	57	kg P/d

XML Figure 4 - Symbols and Incode names showed

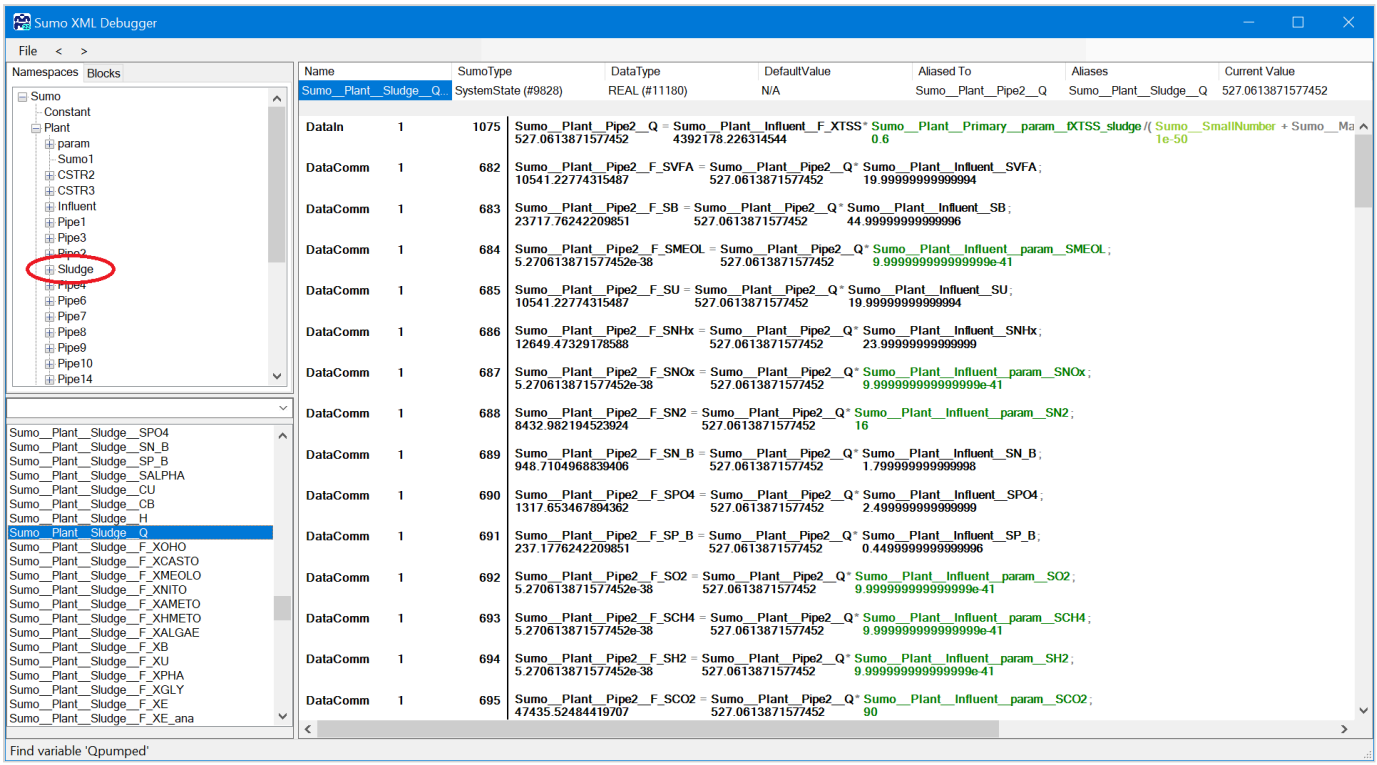
The variable symbol of the primary sludge flow rate is '**Q**' of the *Sludge* unit in this project.

Search for it in the debugger

After identifying the symbol of the variable there are various ways to find the variable.

The structure of Namespaces

Go directly to the Namespaces: Sumo|Plant|Sludge. It will list at the bottom all the variables used in the *Sludge* process unit. The list is extensive but the '**Q**' is there.

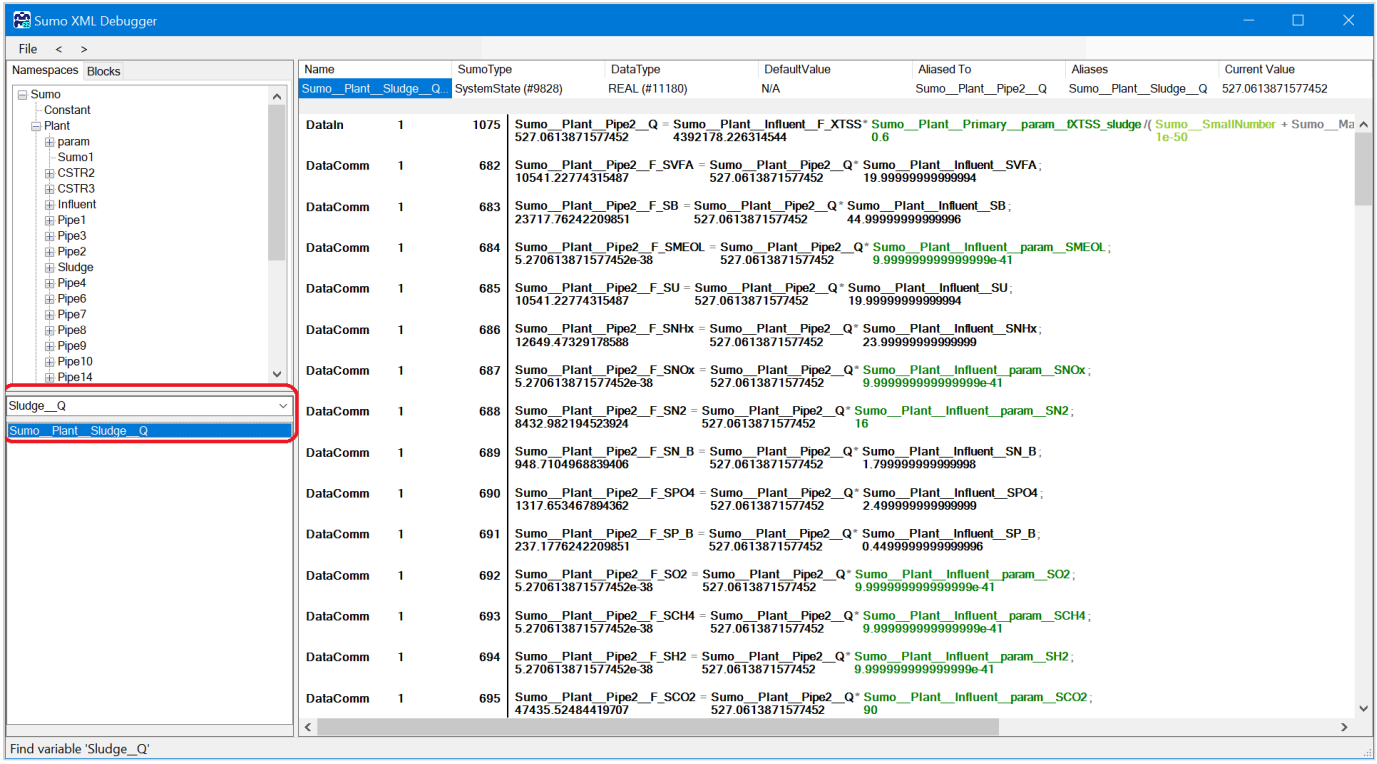


XML Figure 5 - Use Namespaces structure

Search

Type in the variable symbol as a general convention: unit name__variable name so in this case ***Sludge__Q***.

The full Incode name of the variable does not contain any special characters and the namespace levels are separated by '__' every time. The search field accepts regular expressions to easier control the list of results.



XML Figure 6 - Search by symbol

Check variable calculation

Once the variable is on the list at the bottom left panel, select it. On the right hand side the following information is available:

Variable specification

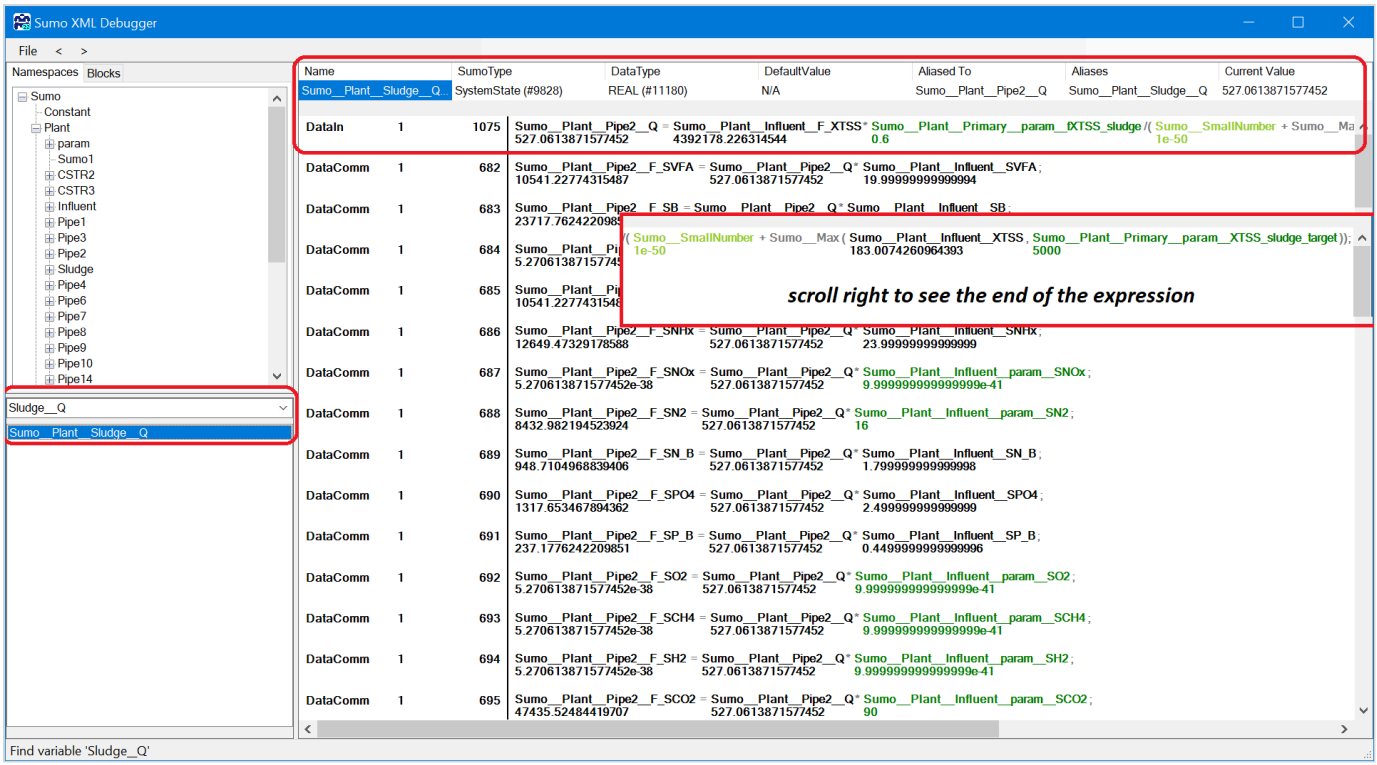
The top section shows the variable specification:

- Name: full incode name of variable
- SumoType: Parameter, Constant, StateVariable, Systemstate (any calculated variable), etc.
- DataType: Real, Integer, Boolean, Array, etc.
- DefaultValue: default value for parameters
- Aliased to: The linked variable with identical calculation logic, this the value of this variable and the 'Aliased to' variable always will be identical
- Aliases: the list of aliased variables connected to the variable indicated at 'Aliased to'
- Current value: the latest calculated value of the variable in Sumo (only available if the current XML is loaded)

Calculation of the variable

The first row below the specification is always the equation how the variable is calculated: left side is the variable and right side is the expression. It starts with the codelocation (when the calculation is performed, for

details see the Book of SumoSlang), blocksection, row and it ends with the equation as below (you have to scroll to the right to see the full equation):



XML Figure 7 - Variable specification and calculation

The equation is using full Incode names and below each variable the current value is indicated. This way the variable using wrong values in the calculation can be identified.

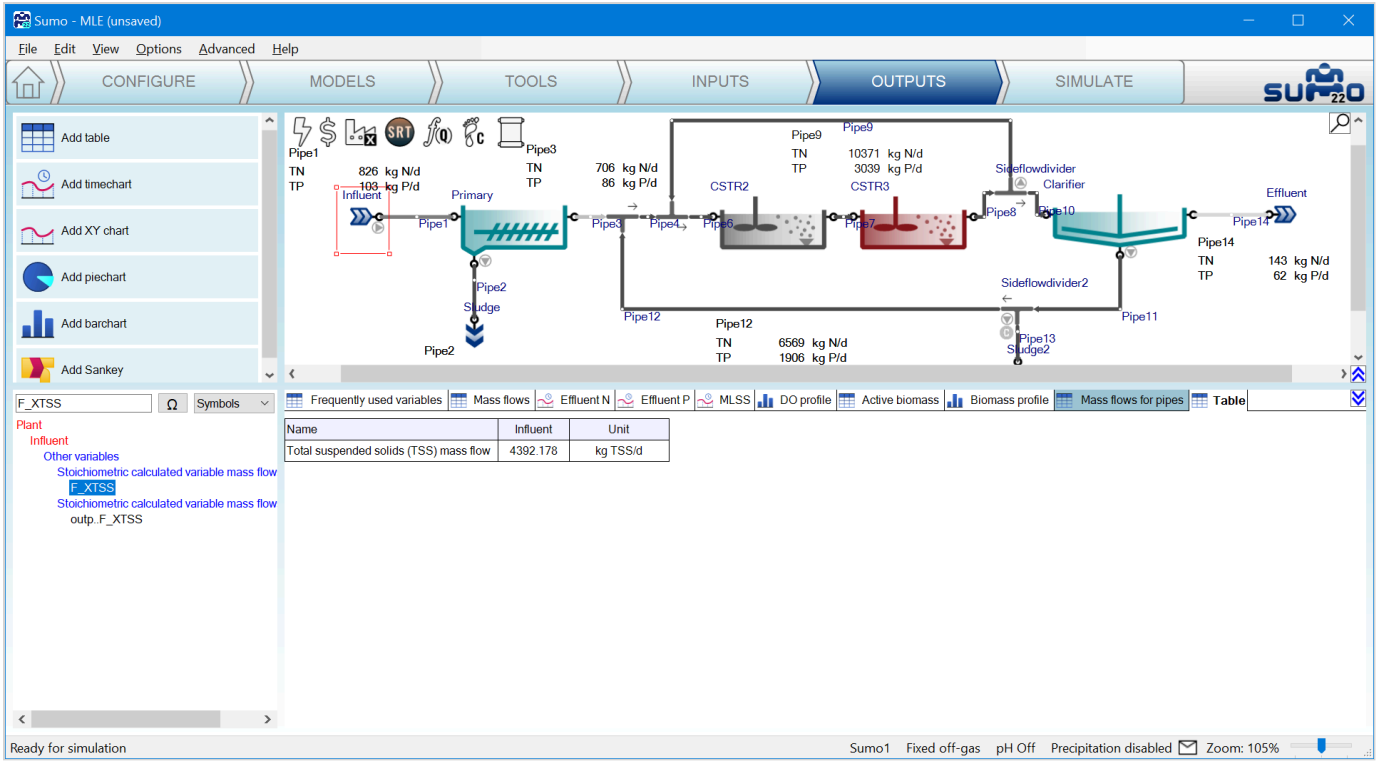
The variables used in the expressions are color coded for easier identifying them:

- red: investigated variable
- blue: state variables
- black: systemstates
- green: parameters
- light green: system constants
- grey: functions

Note: there is a glitch if the investigated variable is an alias (has an Aliased To) so the Aliased to variable has to be clicked (in this case it is Pipe2__Q).

Find the name

To find out the name of the variable used in the calculation the Sumo Outputs can be used. On the bottom left panel select the Symbols/Raw and type in the variable name after selecting the (F_XTSS and select Influent):

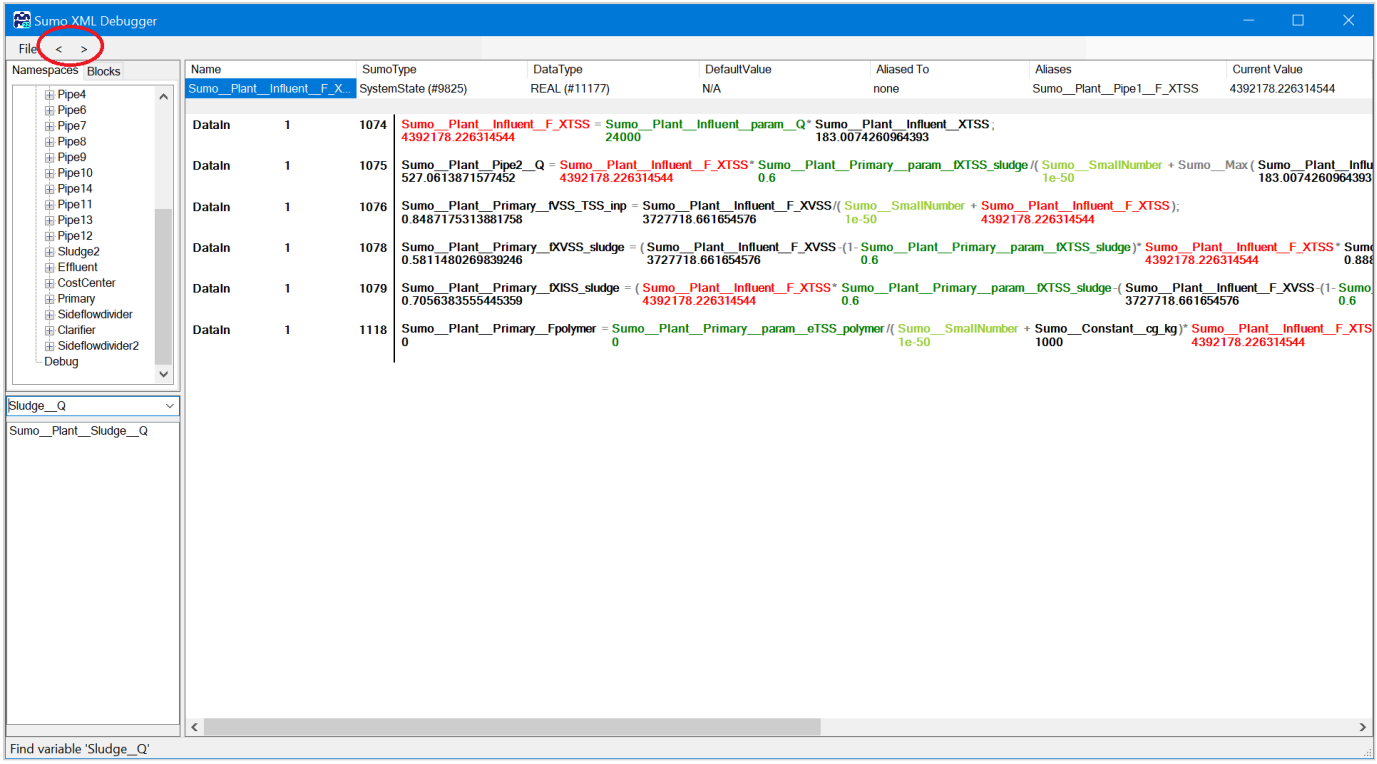


XML Figure 8 - Find out variable name

Remember to set the Advanced|Variable identifier back to **Names** to see that F_X_{TSS} stands for TSS mass flow.

Where is the issue?

If the first expression (Sludge Q = influent TSS mass flow * removal percent/sludge TSS concentration) is not helping (as the only systemstate is the Influent__F_XTSS) the tool has the feature to follow up on a variable: just click on it and you get the same information for the variable as you can see below for the Influent__F_TSS. On this page the investigated variable is highlighted with red letters. Next to the File menu there are two button for **Back** and **Forward** between the already checked variables. Using the Back menu the tool goes back to Sludge__Q variable calculation (XML Figure 9).



XML Figure 9 - Variable specification and calculation, next step

Under the calculation of the investigated variable all the equation is listed where the variable is used in the expression (highlighted with red on the right hand side).

This way on a step-by-step basis you can figure out which calculation or which input parameter is wrong.

Sumo silent installation

Install sumo in silent way

Command

Open a terminal (cmd on windows) and run the following command :

```
Sumo22.1.0-installer.exe config
"auto|install|ok|all|C:\Sumo22#;#C:\Sumo22|ok" exitonfinish
```

Description

The config string breaks down to the following parts separated by a pipe mark:

- **Language :** auto is to automatically detect the language of the system. 1 is for English, 2 is for Korean and so on in the order of flags on the first page.
- **Method :** it should be install. You could use it for uninstall too, if you wanted.
- **License agreement :** ok means you accept it. You'll need to accept the license agreement.
- **Who to install :** type all for "all" users or "tome" for just for the installing user.
- **Install path and working path :** separated by "#;#". Working path is only set for the installing user. Please use english only letters for working path, and preferably to the install location as well. Please be aware that if you do an "all" install, all users should have access to the working directory.
- **Confirmation :** ok would be needed here

Developers Topics

SumoSlang for Dummies

written by Dwight Houweling

Introduction

SumoSlang is a very powerful tool for developing your own "customized" process models. The purpose of this little document is to provide a tour through a stripped down version of the SumoSlang language. To highlight the features that will be familiar to someone with a basic understanding of process modelling and simulation and help get you started on building your own custom models so that you can "learn by doing". So SumoSlang for Dummies, or maybe SumoSlang for Doers... call it what you want.[0]

The tutorials are organized as follows:

- The first one is really the most basic use of SumoSlang to develop a model that maps flow and state variable components `SV` from an Influent element, through a basic CSTR and into an Effluent element. `SV` components are directly mapped with no reactions performed. Not very interesting but a good place to start.
- In the second tutorial we add reactions to the basic CSTR developed in the previous tutorial. Now the model starts to be useful.
- In the third one, we look at using parameters `PAR` and calculated variables `CVAR` . What do they add to the model, how are they tracked and how do they leverage *SUMO*'s `Model Base` ?
- The fourth and final tutorial will add the missing information to make our basic CSTR compatible with other flow elements in the *SUMO* process unit library.

This is by no means intended as an exhaustive treatment of what SumoSlang can do and the reader is referred to the BoSS[1] as the definitive reference on SumoSlang. Nevertheless, I hope these four tutorials are enough to provide you with the basic knowledge and confidence required to start building your own models.[2] If you prefer not to follow the steps outlined below you can also download the tutorial files and use them as templates for getting started on your own.

Tutorial 1: How to add a basic CSTR

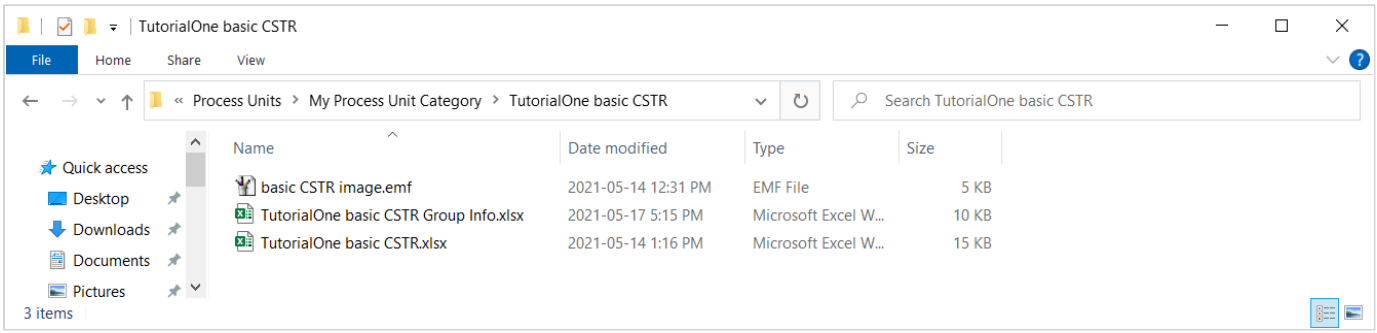
Step 1

Find the folder where you have *SUMO* installed. On my computer it is `C:\Users\cdhou\AppData\Local\Dynamita\Sumo21`. There should be a folder here named "My Process Code" and inside of that you will find "Process Units" and "My Process Unit Category". This is where we are going to work.[3]

Step 2

For a "basic CSTR" we will create a folder named `\TutorialOne basic CSTR` containing the following three files[4]:

- `basic CSTR image.emf` which is an image file to visually represent the process unit on the *SUMO* drawing board,
- `TutorialOne basic CSTR Group Info.xlsx` which is an Excel file to explain to *SUMO* the organization and use of the files in this folder.
- `TutorialOne basic CSTR.xlsx` which is the Excel file which contains the actual code describing the process unit model.

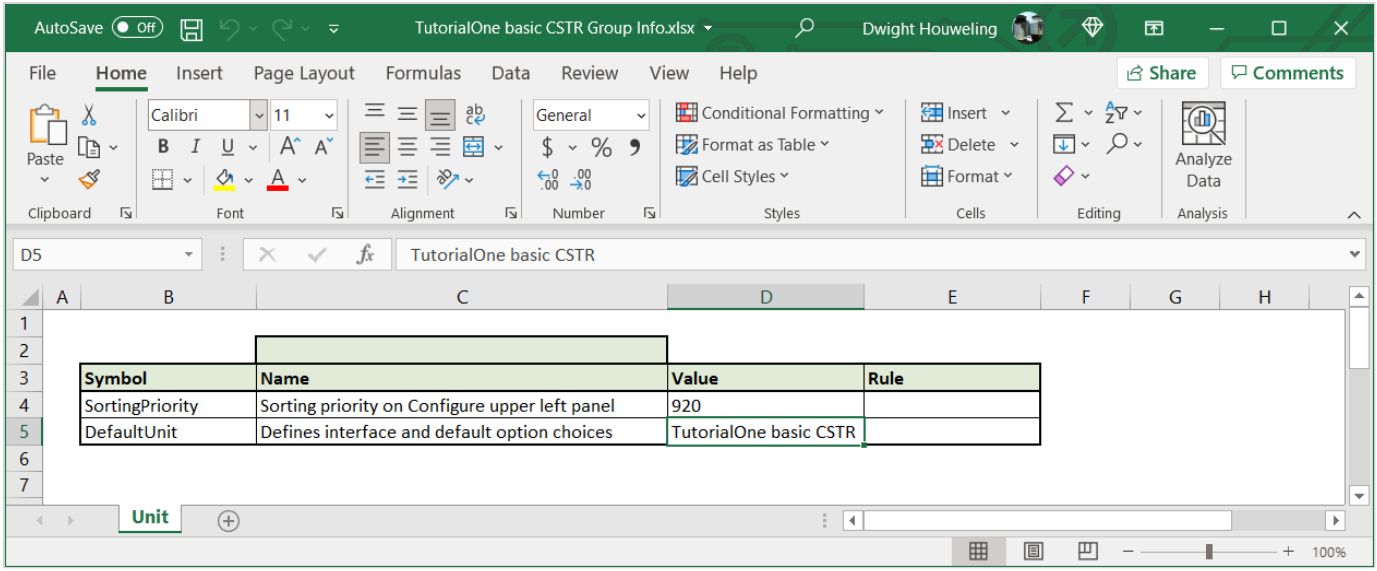


Step 3

Now we use the "Group Info" file to instruct *SUMO* on how this folder is organized. At its most basic level, `TutorialOne basic CSTR Group Info.xlsx` must be organized with the following elements:

- A worksheet named `Unit` containing a table with the column headings `Symbol`, `Name`, `Value` and `Rule`.
- Rows to identify the `SortingPriority` and `DefaultUnit`. Note that `DefaultUnit` refers to the name of the Excel file in the current folder where the Sumo Model Translator (SMT) should look for process unit model code.

SMT is pretty strict about how it wants to see this information presented. Apart from the font, coloring and style of the table, which are optional, it should look exactly like this:

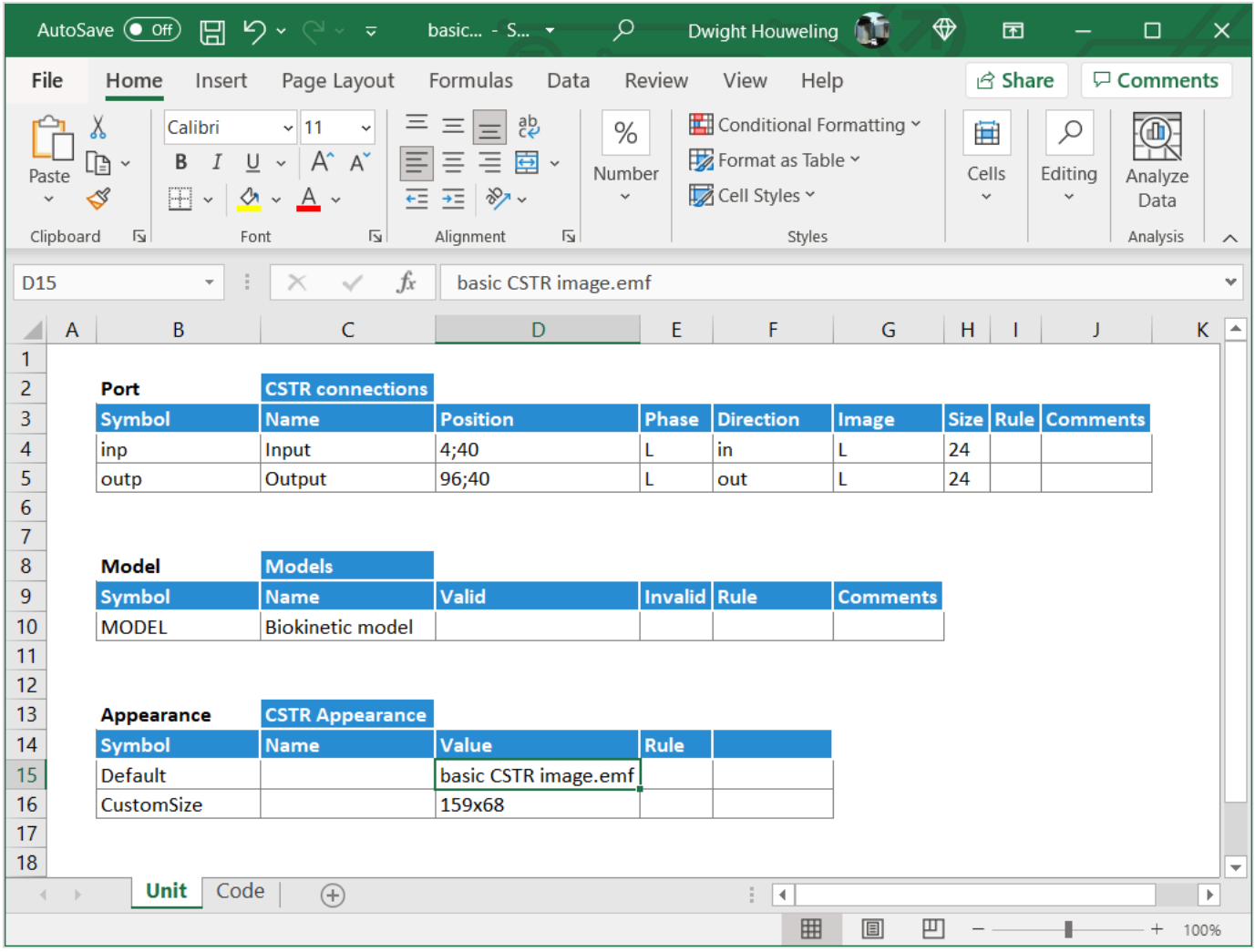


Step 4

Inside `TutorialOne basic CSTR.xlsx` we need to include two worksheets named `Unit` and `Code`. The `Unit` worksheet needs to include three tables:

- The `Port` table which explains the number of connections that can be made to the element, how they should be named, and more.
- The `Model` table which identifies which are valid and invalid biokinetic models that can be associated with this model file.
- And the `Appearance` table which identifies which image file from the working folder should be displayed on the drawing board.

Again, the SMT is strict about how it wants to see this information presented. Notably, tables need to start in column B and the column naming and structure of the tables needs to be respected. It is best to follow the example provided below or work from the template `\My Process Code\Process Units\My Process Unit Category\TutorialOne basic CSTR.xlsx` which you can download from here.



Port	CSTR connections							
Symbol	Name	Position	Phase	Direction	Image	Size	Rule	Comments
inp	Input	4;40	L	in	L	24		
outp	Output	96;40	L	out	L	24		

Model	Models				
Symbol	Name	Valid	Invalid	Rule	Comments
MODEL	Biokinetic model				

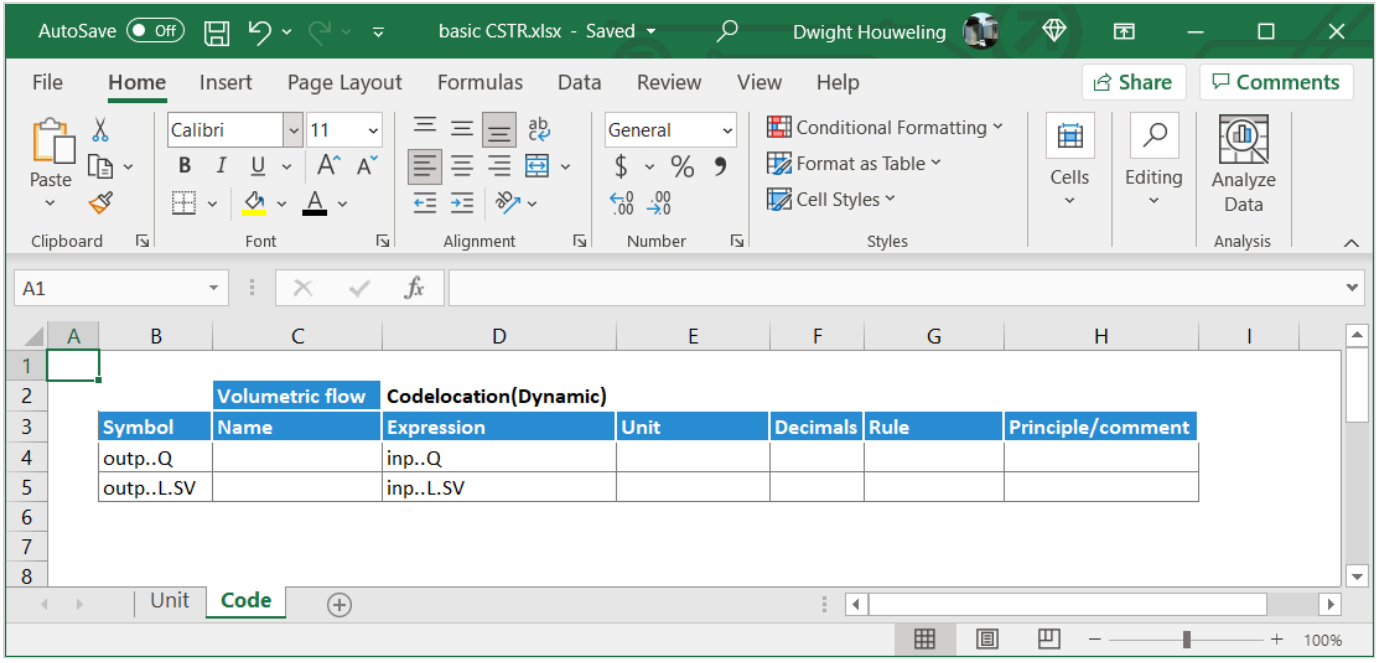
Appearance	CSTR Appearance			
Symbol	Name	Value	Rule	
Default		basic CSTR image.emf		
CustomSize		159x68		

Step 5

The `Code` worksheet can be even simpler. In this tutorial we make it a single table that includes two lines:

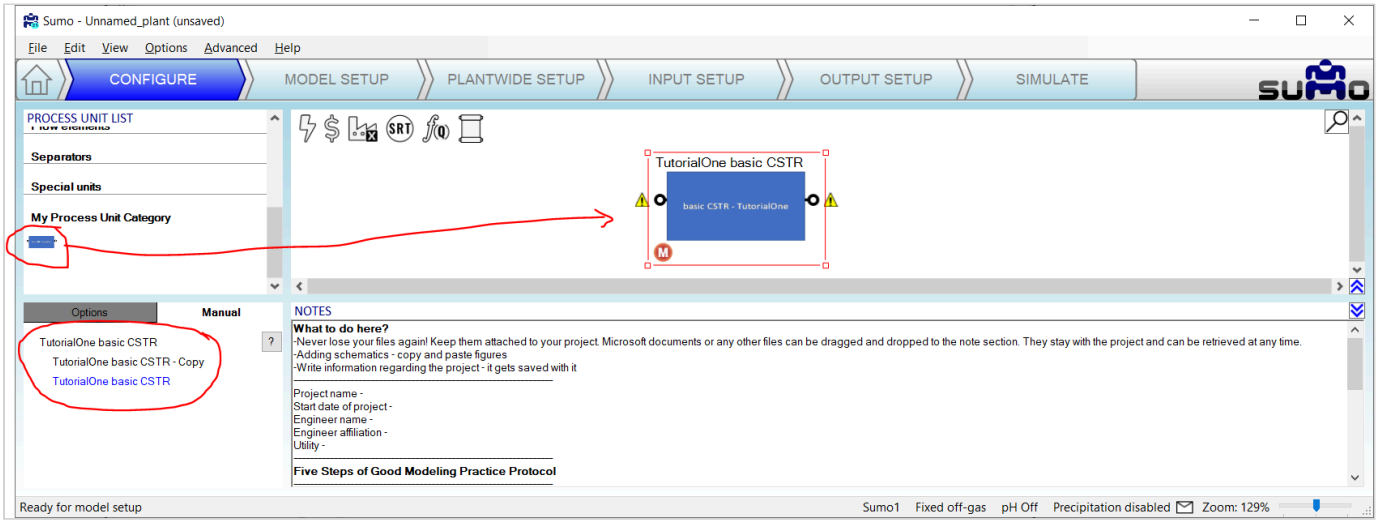
- Cells `$B$4` and `$D$4` which, respectively, assign the value of the flow in the output `outp..Q` to the value of the flow in the input `inp..Q`. Simple mapping of the inlet flow to the outlet.
- Cells `$B$5` and `$D$5` which, respectively, assign the value of the state variables in the output `outp..L.SV` to the value of the flow in the input `inp..L.SV`. Simple mapping of the inlet state variables to the outlet with no transformations or conversions. Boring, I know, but a good place to start. Patience young grasshopper!

It's worth noting here that `inp..L.SV` is SumoSlang's, well... "slang" for all of the state variables in the input stream to the "basic CSTR"[5]. And, if we are more precise, it is actually the liquid phase state variables and so excludes gas phase state variables (i.e. bubbles and headspace) which are assumed in most cases to not travel between CSTRs. And maybe one final point, the definition of the input is in fact anything connected to the port location identified in `Unit` worksheet cell `$D$5`. But it's actually not necessary to understand all of that detail. A lot can be accomplished just by carefully following and tweaking the template files.



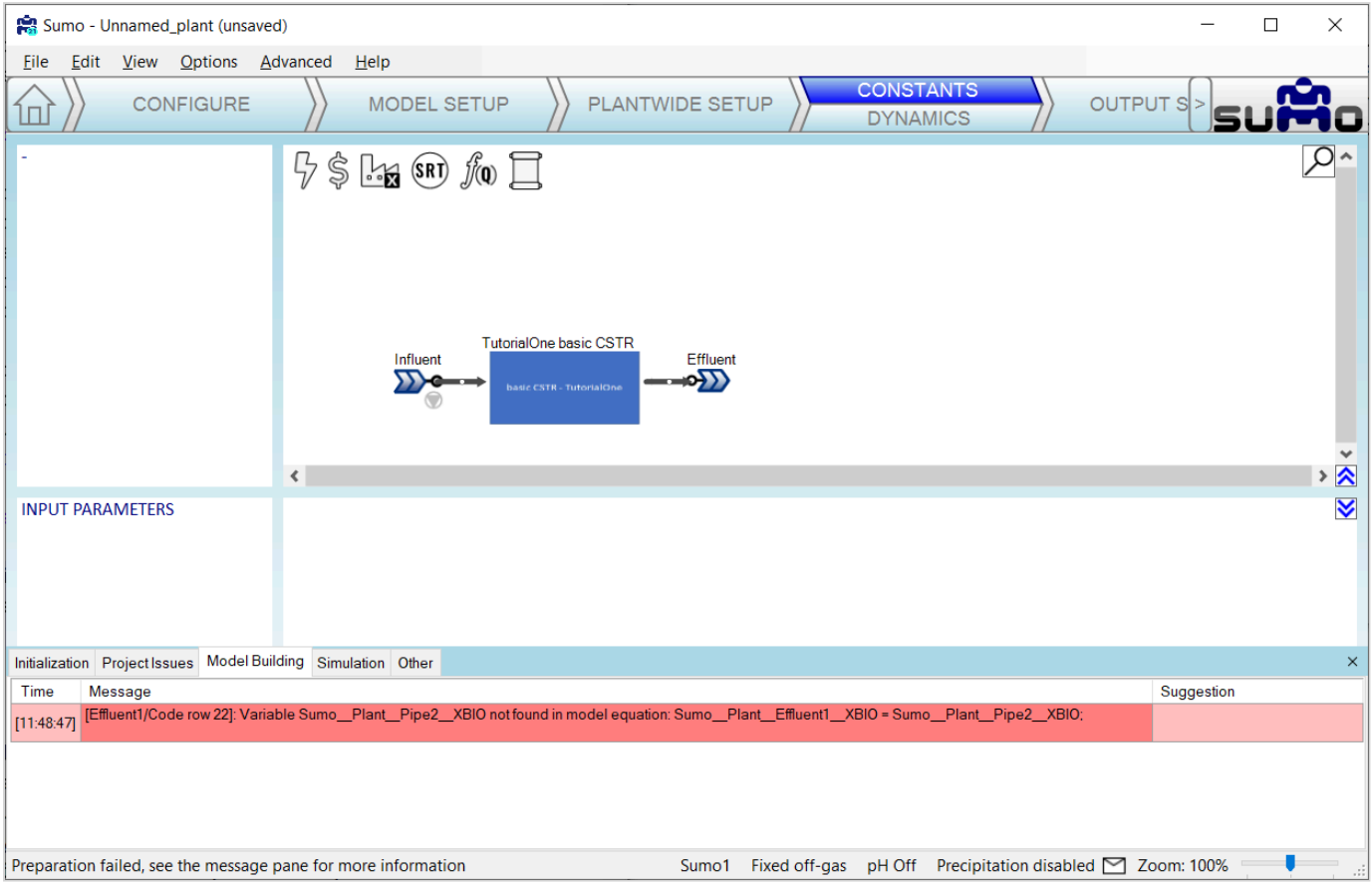
Step 6

Now we open *SUMO* to see if we have successfully created our `TutorialOne basic CSTR`. We find that our new category `My Process Unit Category` appears to the left of the *SUMO* drawing board along with the standard library of *SUMO* process units. We can drag our unit to the drawing board where it is given the name of our folder `\TutorialOne basic CSTR` and, by looking in the bottom left hand corner under `Manual`, we see that the process unit file referenced is also named `TutorialOne basic CSTR.xlsx`.[6] Note if you created a copy of `TutorialOne basic CSTR.xlsx` in the `\My Process Unit Category` folder then it would also appear in this list as shown below. This is a useful feature in cases where you want to have alternate versions of your process unit code.



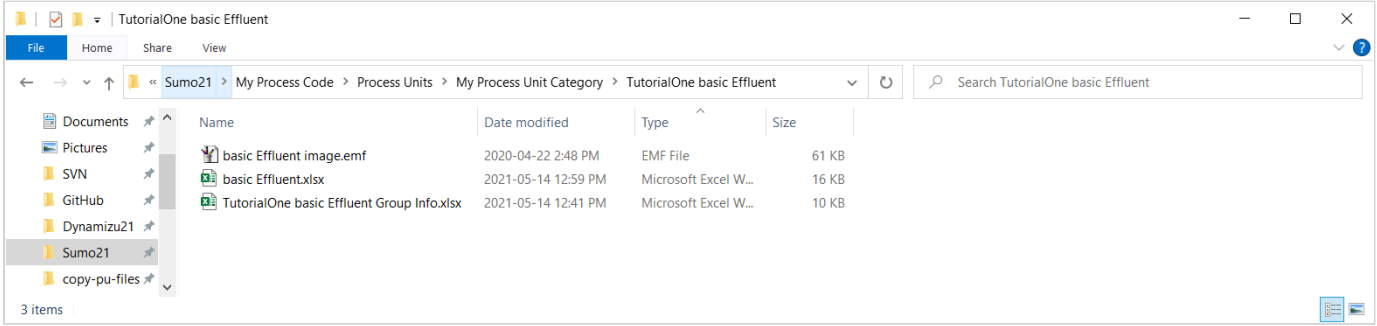
Step 7

The model above will build, but if we try to connect the influent and effluent flow elements then we get a build error related to the inability to calculate `XBIO` in the effluent object. The reason for this is that the standard library "Effluent" object in *SUMO* is looking for parameters in addition to the `Q` and `L.SV` which were mapped to the `outp..` in `TutorialOne basic CSTR.xlsx`. So for this tutorial we cannot use the standard library `Effluent` object. Instead we will create a `TutorialOne basic Effluent` element inside `\My Process Unit Category`.



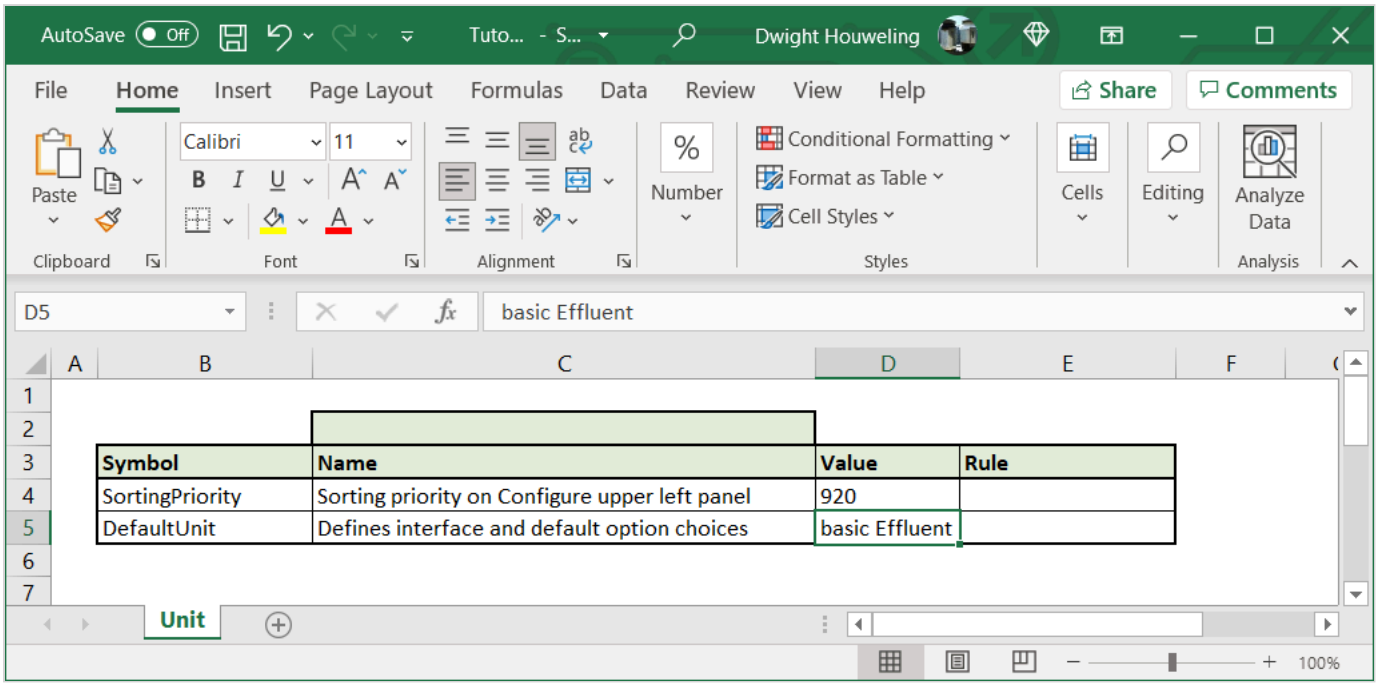
Step 8

Creating a "basic Effluent" object is very similar to creating the "basic CSTR". First we start with the folder structure as shown below:



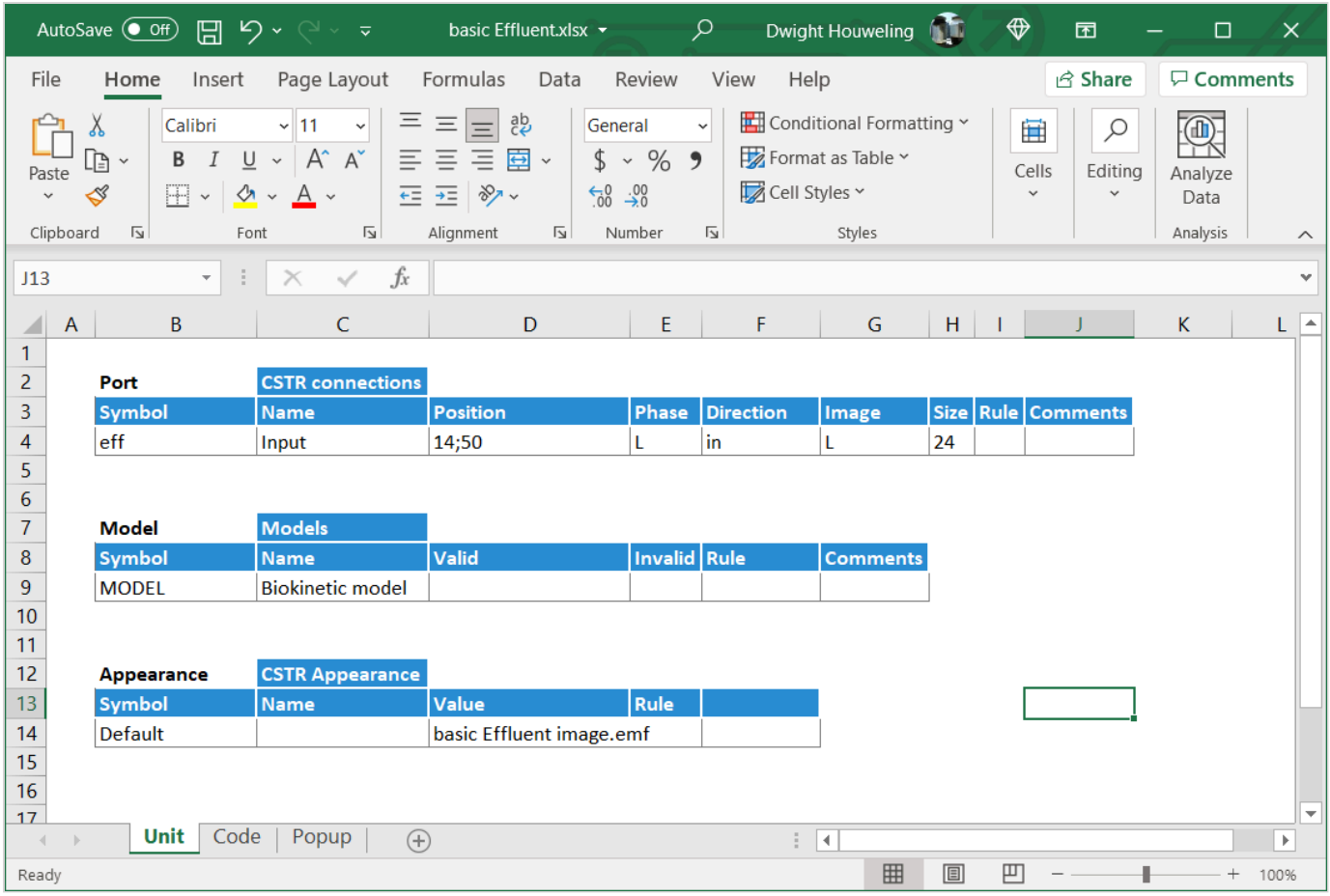
Step 9

The `Group Info` file `TutorialOne basic Effluent Group Info.xlsx` looks very similar to `TutorialOne basic CSTR Group Info.xlsx`:



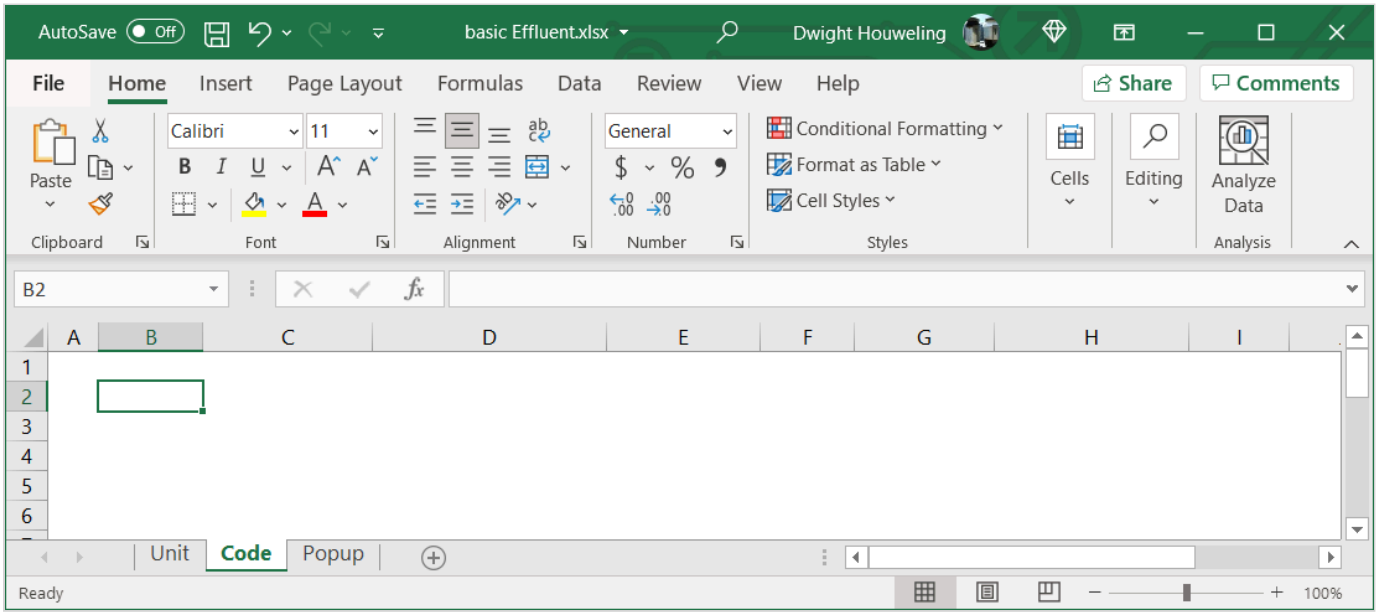
Step 10

The `Unit` worksheet in `basic Effluent.xlsx` is also very similar to `TutorialOne basic CSTR.xlsx` with the exception that there is now only an input port which, somewhat ironically, we name "eff":



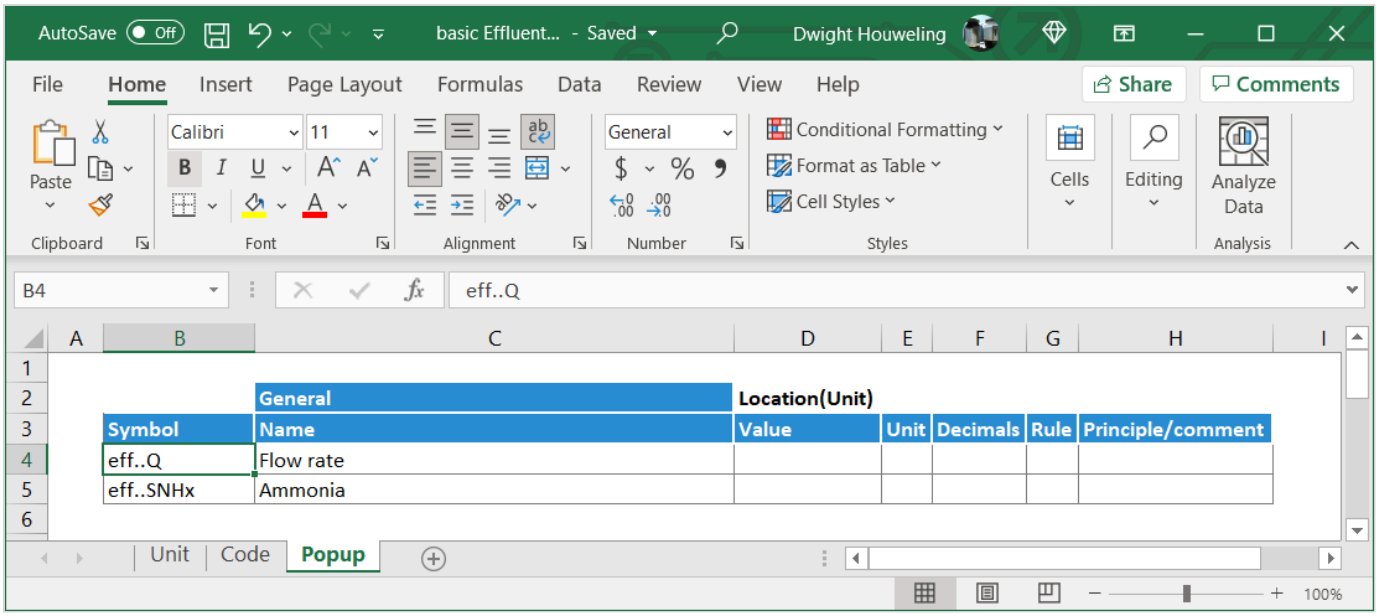
Step 11

So with only an input, and no output, the effluent object doesn't even need to map variables from one port to another. The `Code` worksheet can therefore be completely empty:



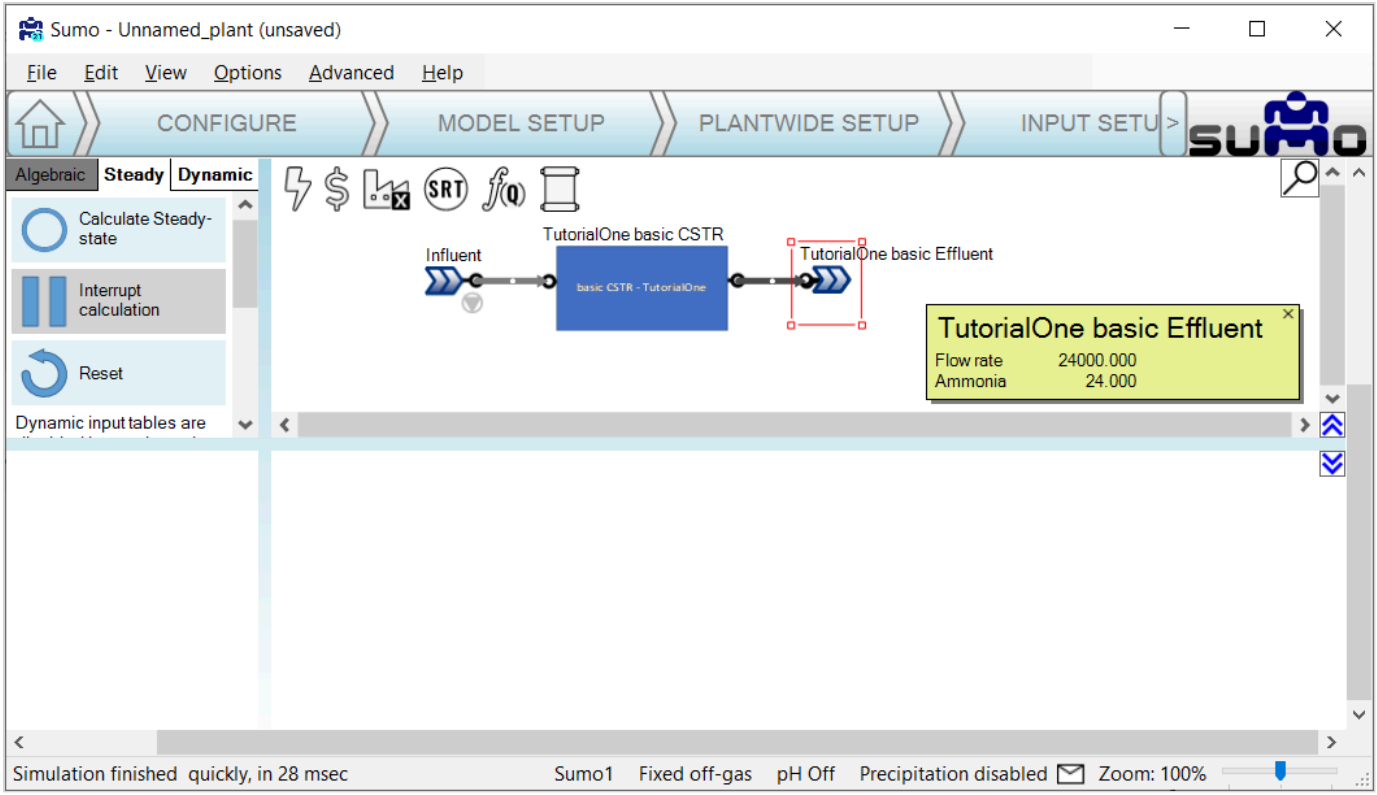
Step 12

But in this case we will add a `Popup` worksheet that will allow display of model variables. We will display flow `Q` and ammonia `SNHx`:



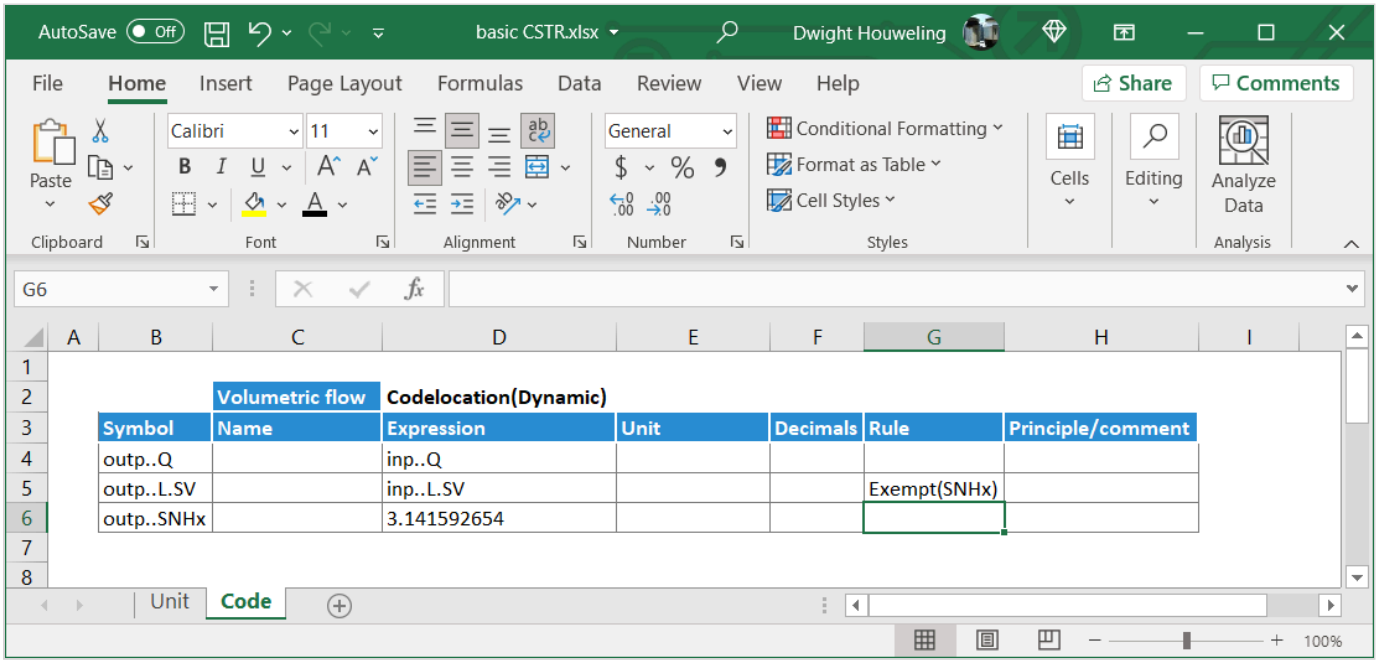
Step 13

Now we open *SUMO* again and find that when we connect an `Influent` from the `Flow elements` category together with our `TutorialOne basic CSTR` and `TutorialOne basic Effluent` from the `My Process Unit Category` then we can successfully build a model. And when we simulate in steady state and then place our cursor over the effluent element, we see from the popup that the model has successfully mapped the influent flow from the influent element, through our basic CSTR and in the effluent element.



Step 14

That's it, a new model has been created using SumoSlang to map flow and components from the inlet to the outlet of a CSTR. Maybe as one final exercise, try making the change below to the `Code` worksheet in `basic CSTR.xlsx`. Is the new value of `outp..SNHx` correctly mapped to the effluent object when you run steady state in *SUMO*? What happens if you omit the rule `Exempt(SNHx)` in cell `$G$5`?



Summary of Tutorial 1

Tutorial One demonstrated how to strip SumoSlang down to its most basic nuts and bolts. The result is a trivial model: influent flow and components are mapped across a reactor to an effluent without any reactions or transformations. Nothing more than this: In => Out. This isn't very interesting. But the power of SumoSlang will be revealed in how it scales. Any model coded once can be then be reused multiple time to build very complex models, far beyond the scale you would ever be able to program in Excel, Python, Matlab or whatever happens to be your programming tool of choice. In addition, SumoSlang leverages a `Model Base` that includes a vast library of components with associated biokinetic, water chemistry, and gas transfer processes. We will explore how SumoSlang interacts and leverages the `Model Base` in the next tutorial.

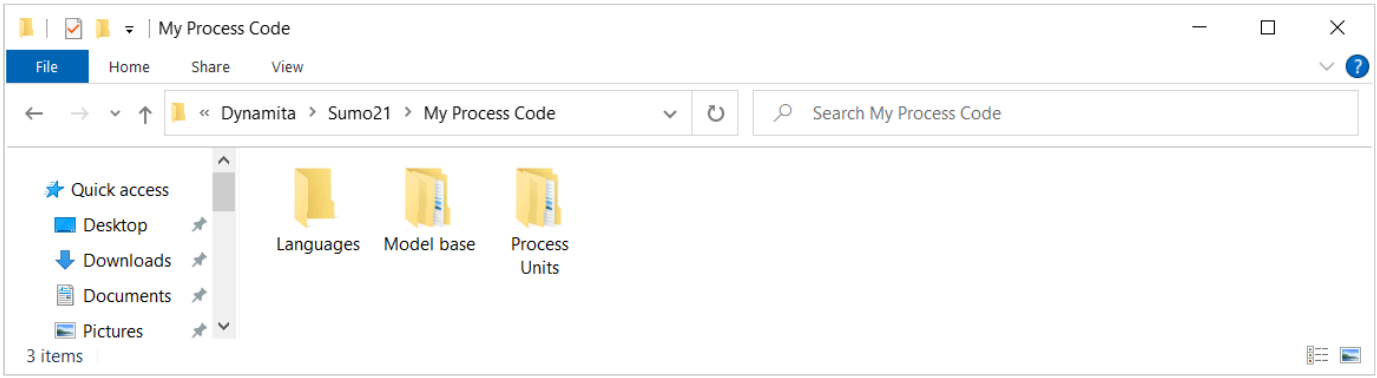
Tutorial 2: Introducing Conversions

At its heart, process simulation is about solving the following mass balance across the `Process Units`:

Change in Mass of Component X with respect to time = Mass Flow of X in - Mass Flow of X out + Conversion rate of X

The *Conversion rate of X* in the above equation is what we think about when we talk about "ASM" or "Activated Sludge Models". In many cases, it is the most interesting part of the model and where most of the complexity lies. But even though it is possible to directly code ASM process equations in the `Code` worksheet of the `Process Units` ,in our case the `basic CSTR.xlsx`, this would not be the best way to use SumoSlang. In SumoSlang, the code for the ASM-type models are referred to as the `Model Base` and kept separately from the code for the `Process Units`. One way to think about this is that the *Conversion rate of X* in the mass balance described above is coded in the `Model Base` whereas the rest of the mass balance equation is coded in the `Process Units`.

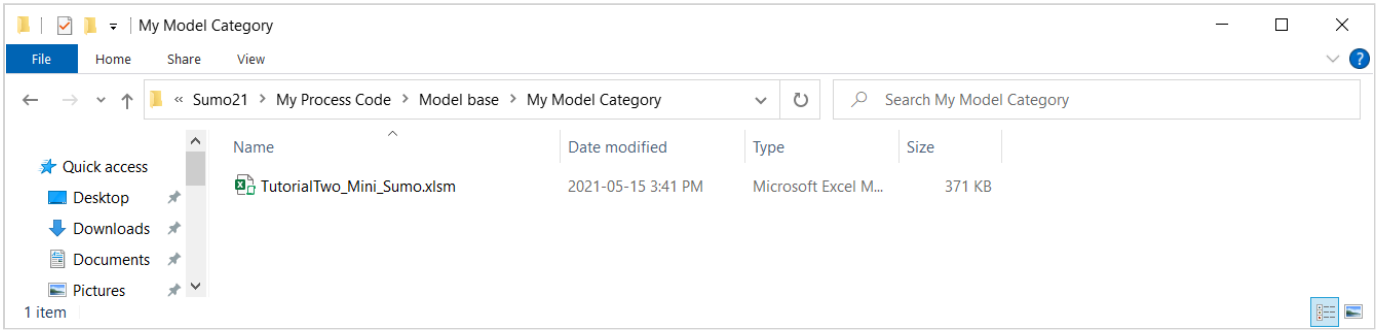
The separation of code for the `Model Base` and `Process Units` is shown in the folder structure below.



The advantage of this separation is that the `Process Units` code can be used with different `Model Base` codes. And new constituents added to the `Model Base`, one might for example want to add PFAS, are automatically pulled into and compatible with the `Process Units` code. There is no need to update the code for each of the 30+ models coded in the `Process Units` folder structure. What a relief! So let's get started building reactions into our basic CSTR.

Step 1

In the standard *SUMO* "Process code" folder, locate the "Mini_Sumo.xlsm" file. On my computer it is located at `C:\Users\cdhou\AppData\Local\Dynamita\Sumo21\Process code\Model base\Full plant models`. Copy this file into the "Model base" folder in the parallel "My Process code" folder structure and rename it `TutorialTwo_Mini_Sumo.xlsx`. In my computer it is `C:\Users\cdhou\AppData\Local\Dynamita\Sumo21\My Process Code\Model base\My Model Category` and looks as follows:



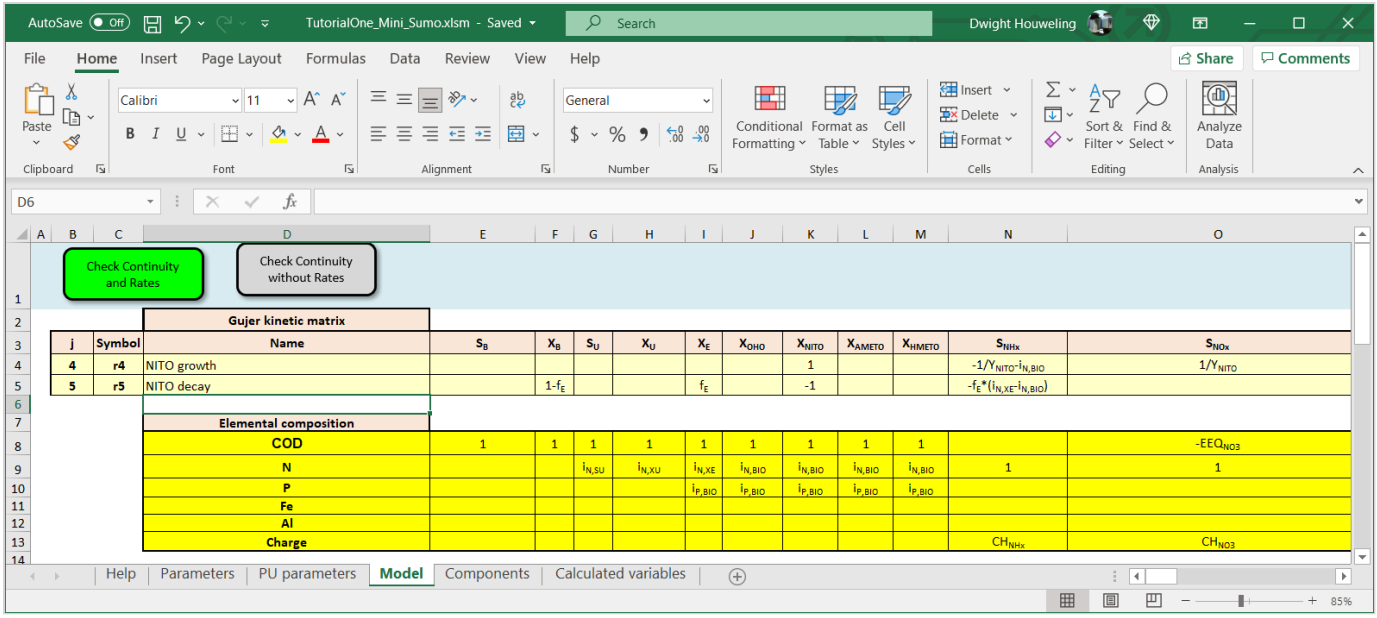
Step 2

This model file contains all of the biokinetic processes, stoichiometry and parameters required to describe the conversion rates of our model components. But to start, in the spirit of making things as simple as possible, we are going to reduce the complexity of this model to that of a simple nitrification model. In the `Model` worksheet, delete rows 4-6 (corresponding to r1, r2 and r3) as well as rows 9-29 (corresponding to r6 to r26). This should leave you with only r4 and r5, which represent the growth and decay of nitrifying organisms `XNITO`.

Step 3

Correct the numbering in columns B and C so that these two processes are identified as "1", "2", "r1" and "r2". Then edit the cells of the stoichiometric matrix so that instead of showing symbolic parameters, only hardcoded numeric values are shown. By doing this we are "deparametizing" the model[7]:

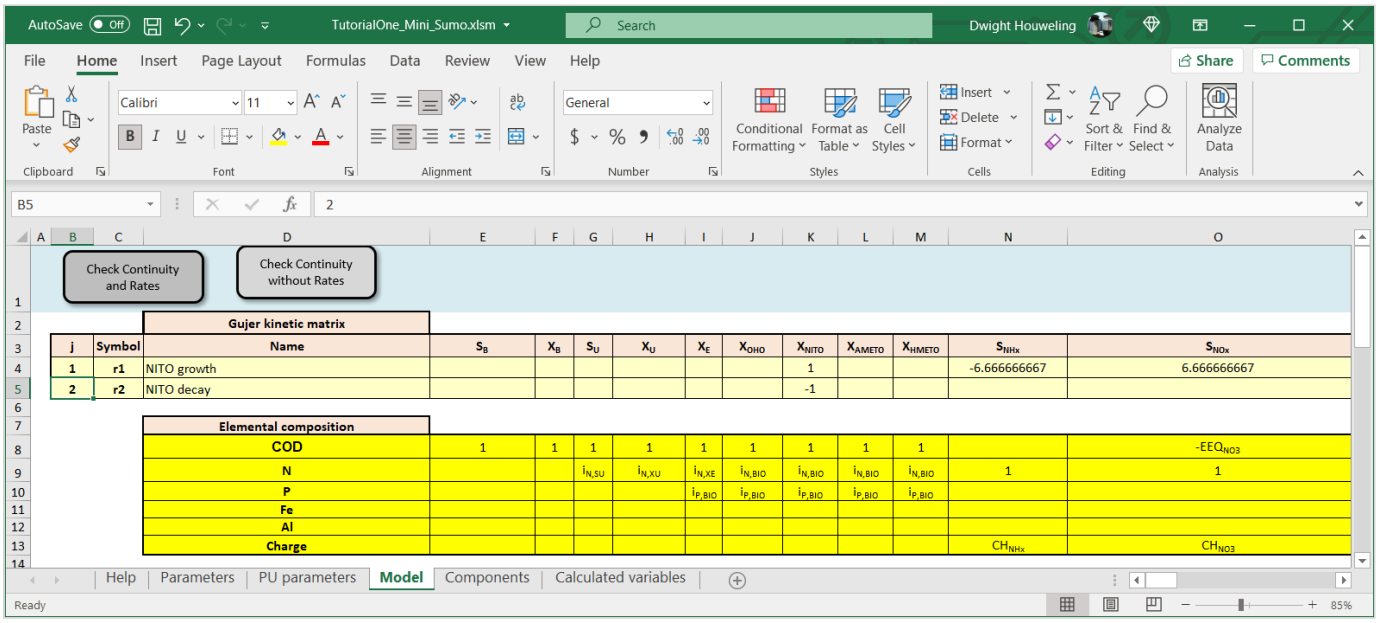
- Below is the `TutorialTwo_Mini_Sumo.xlsx` with all process deleted except NITO Growth and Decay. The stoichiometric matrix contains symbolic or "parametized" terms like `1/YNITO` which we want to "deparametize":



j	Symbol	Name	S_B	X_B	S_U	X_U	X_E	X_{OHO}	X_{NITO}	X_{AMETO}	X_{HMETO}	S_{NHx}	S_{NOx}
4	r4	NITO growth							1			$-1/Y_{NITO}$-$i_{N,BIO}$	$1/Y_{NITO}$
5	r5	NITO decay		1-f_E			f_E		-1			-f_E*($i_{N,XE}$-$i_{N,BIO}$)	

Elemental composition											
COD	1	1	1	1	1	1	1	1	1		-EEQ_{NO3}
N			$i_{N,SU}$	$i_{N,XU}$	$i_{N,XE}$	$i_{N,BIO}$	$i_{N,BIO}$	$i_{N,BIO}$	$i_{N,BIO}$	1	1
P					$i_{P,BIO}$	$i_{P,BIO}$	$i_{P,BIO}$	$i_{P,BIO}$	$i_{P,BIO}$		
Fe											
Al											
Charge										CH_{NHx}	CH_{NO3}

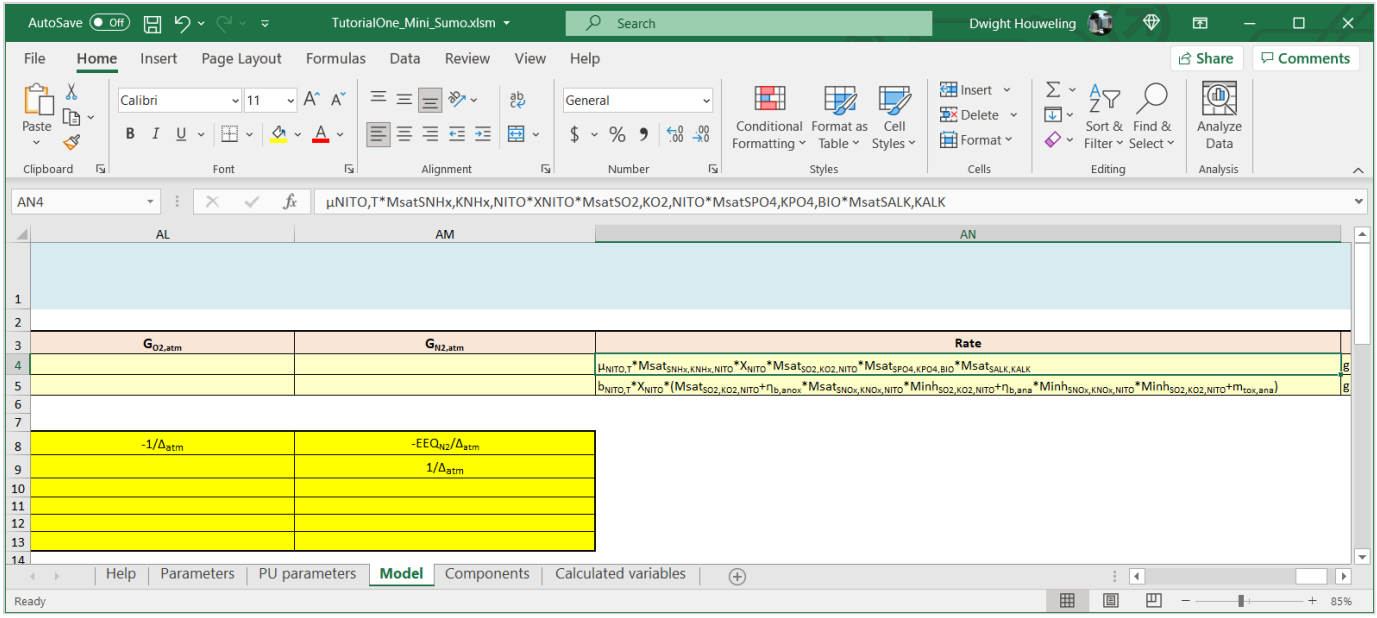
- The "deparametized" version is shown below with only four stoichiometric terms remaining to describe growth (+1) and decay (-1) of nitrifiers `XNITO` and the utilization of ammonia `SNHx` (-6.667) and generation of nitrate `SNOx` (+6.667) associated with growth of nitrifiers[8]. We will ignore all other stoichiometric terms like `XB`, `XE`, `SALK` or even dissolved oxygen `SO2` for this simplified case:



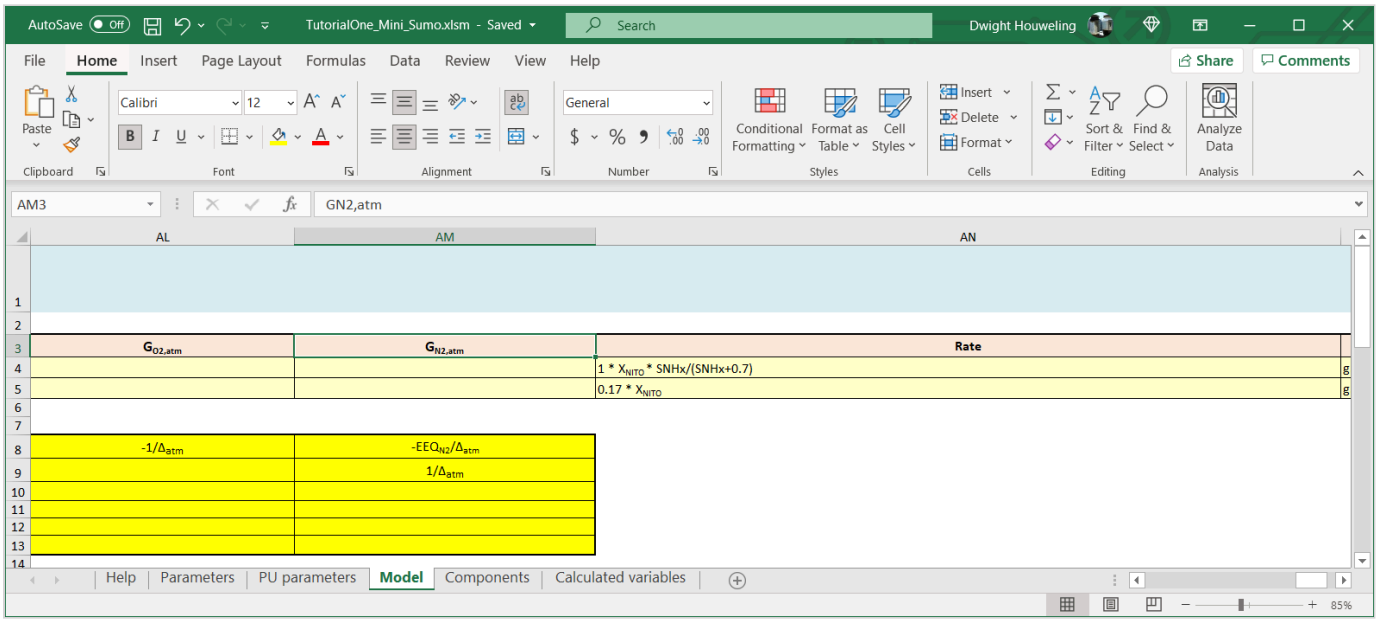
j	Symbol	Name	S_B	X_B	S_U	X_U	X_E	X_{OHO}	X_{NITO}	X_{AMETO}	X_{HMETO}	S_{NHx}	S_{NOx}
1	r1	NITO growth							1			-6.666666667	6.666666667
2	r2	NITO decay							-1				

Elemental composition											
COD	1	1	1	1	1	1	1	1	1		-EEQ_{NO3}
N			$i_{N,SU}$	$i_{N,XU}$	$i_{N,XE}$	$i_{N,BIO}$	$i_{N,BIO}$	$i_{N,BIO}$	$i_{N,BIO}$	1	1
P					$i_{P,BIO}$	$i_{P,BIO}$	$i_{P,BIO}$	$i_{P,BIO}$	$i_{P,BIO}$		
Fe											
Al											
Charge										CH_{NHx}	CH_{NO3}

- Finally we simplify the process rate equations from:



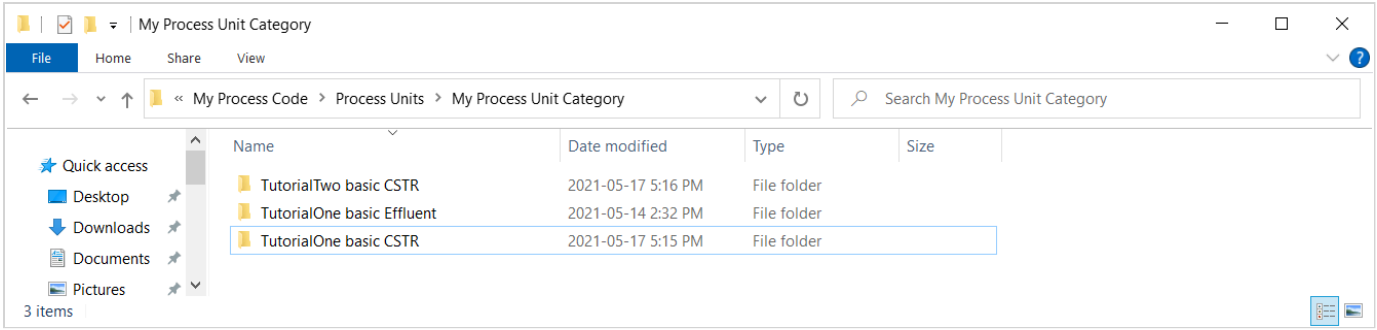
- To the following which only relies on definitions of State Variables `XNITO` and `SNHx` but otherwise does not contain any symbolic parameters:



- There is a second stoichiometric matrix below the one we have been manipulating that contains "evaluated" terms for the stoichiometric matrix and reaction terms, i.e. numbers not letters. You can update this second matrix by clicking on the "Check Continuity and Rates" button. However, it is not necessary to do this. The *SUMO* Model Translator (SMT) will ignore this second matrix.

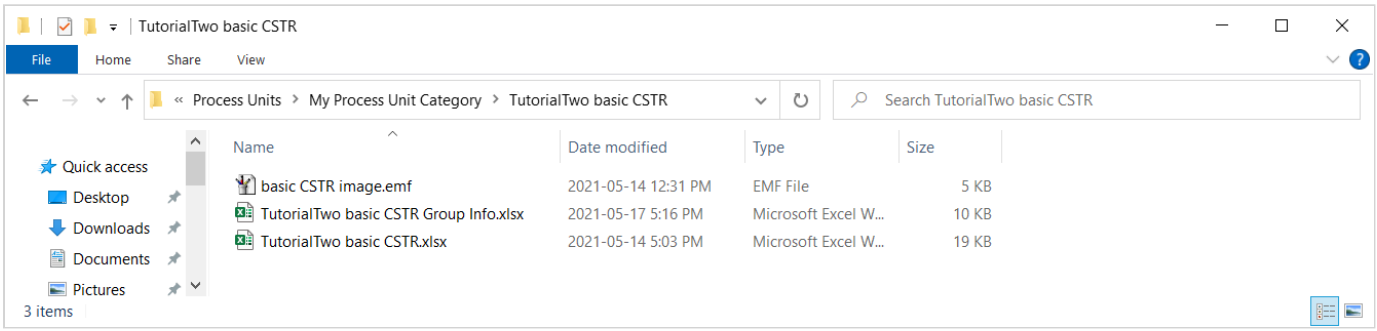
Step 4

We now create a new folder where we will develop the `TutorialTwo basic CSTR`:



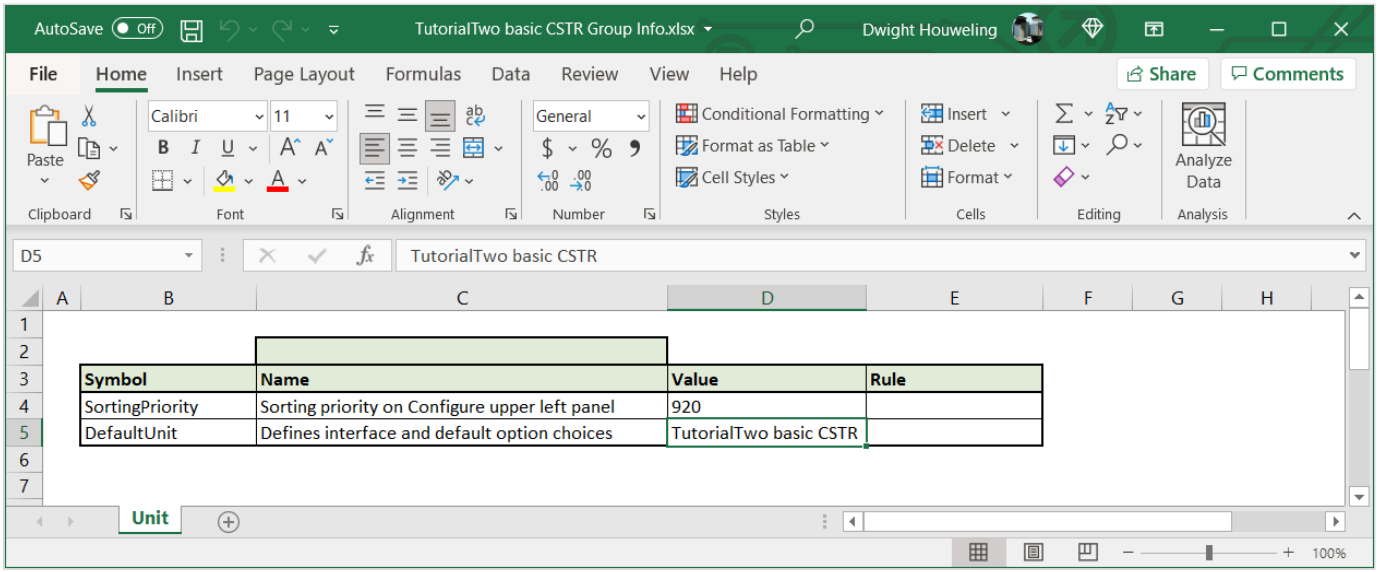
Step 5

We can copy the three files from the `\Tutorial One basic CSTR` into `\Tutorial Two basic CSTR` but we need to update the names of the Excel files as follows:



Step 6

The update to the "Group Info" file is to update the name of the file where the process code is located:

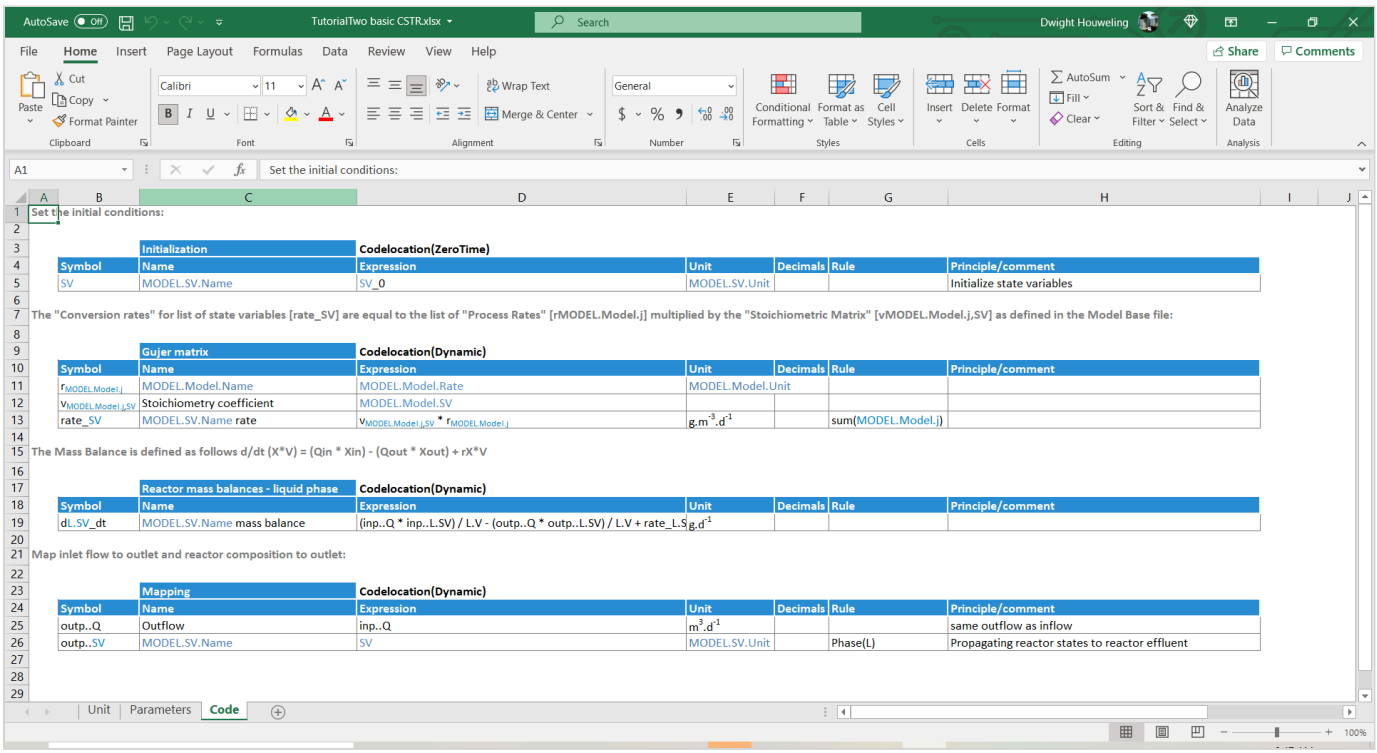


Step 7

The `Code` worksheet is updated to include four tables.

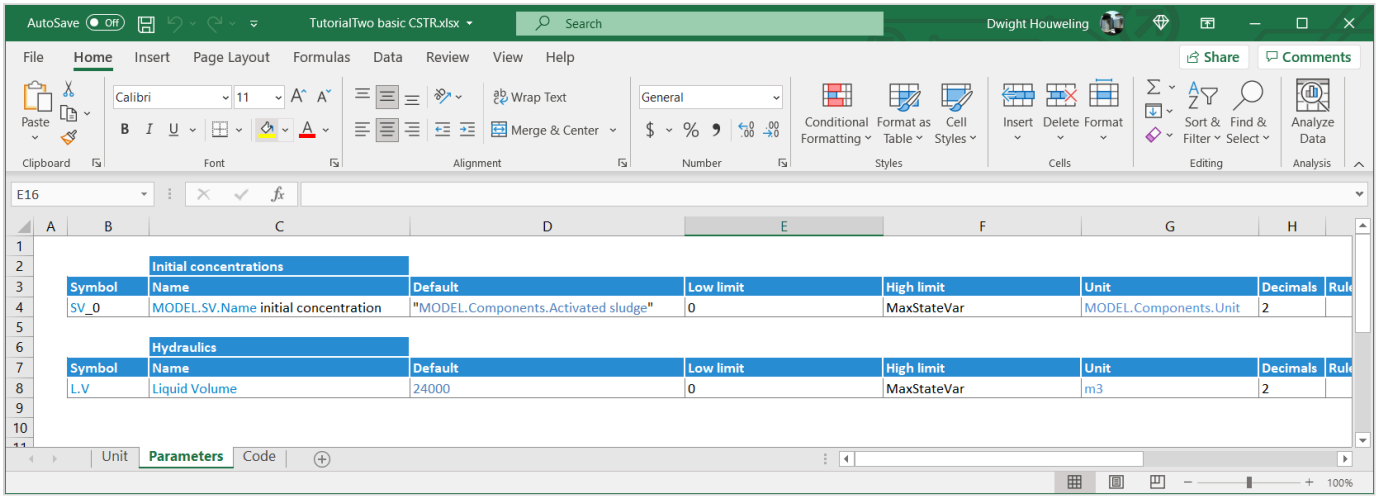
- The first table in rows 3 to 5 assigns the state variable components `SV` in the CSTR compartment to their initial conditions `SV_0`. Note that the heading to this table cell `$D$3` specifies that this assignment is only to be made once, in the `Codelocation(ZeroTime)`. That means initial conditions are assigned only at the very beginning of the simulation.
- The second table in rows 9 to 13 defines the conversion rates of each of the state variable components `rate_SV` as the matrix multiplication of the individual process rates `rMODEL.Model.j` and the stoichiometric matrix `vMODEL.Model.j,SV`. `rMODEL.Model.j` is a reference to the rate expressions of the `Model Base` following SumoSlang's "triplet notation". More on this notation can be found in the BoSS.[9] For the `TutorialTwo_Mini_Sumo.xlsm` file we developed, it refers to the expressions defined in cells `$AN$4` and `$AN$5` of the `Model` worksheet. Similarly, `vMODEL.Model.j,SV` is SumoSlang's triplet notation for the stoichiometric matrix described in cells `$E$4:$AM$5` of this same worksheet.
- The third table in rows 17 to 19 uses the conversion rates `rate_SV` as part of the mass balance to define the change with respect to time of the concentration of liquid[10] state variables `dL.SV_dt`. This is the so called differential equation that the *SUMO* numeric engine will integrate during a model simulation. Note that this mass balance introduces a new parameter `L.V` to represent the liquid volume of the `basic CSTR`. We will define `L.V` in a new worksheet named `Parameters`. More about the `Parameters` worksheet below.
- The fourth table in rows 23 to 26 provides mapping of the influent flow `inp..Q` to the reactor effluent `outp..Q` as well as the concentration of state variables in the reactor compartment `SV` to the reactor effluent `outp..SV`.

The four tables are shown below:



Step 8

The `Parameters` worksheet is used by SumoSlang to define any user defined parameters or pull them in from the `Model Base`. In this case we define the liquid volume `L.V` to 24000 and the initial conditions for the state variables `SV_0` to `"MODEL.Components.Activated sludge"`. The expression `"MODEL.Components.Activated sludge"` refers to the column labelled `Activated sludge` in the `Components` worksheet of the `Model Base`. In our file `TutorialTwo_Mini_Sumo.xlsm` it is found in column F.

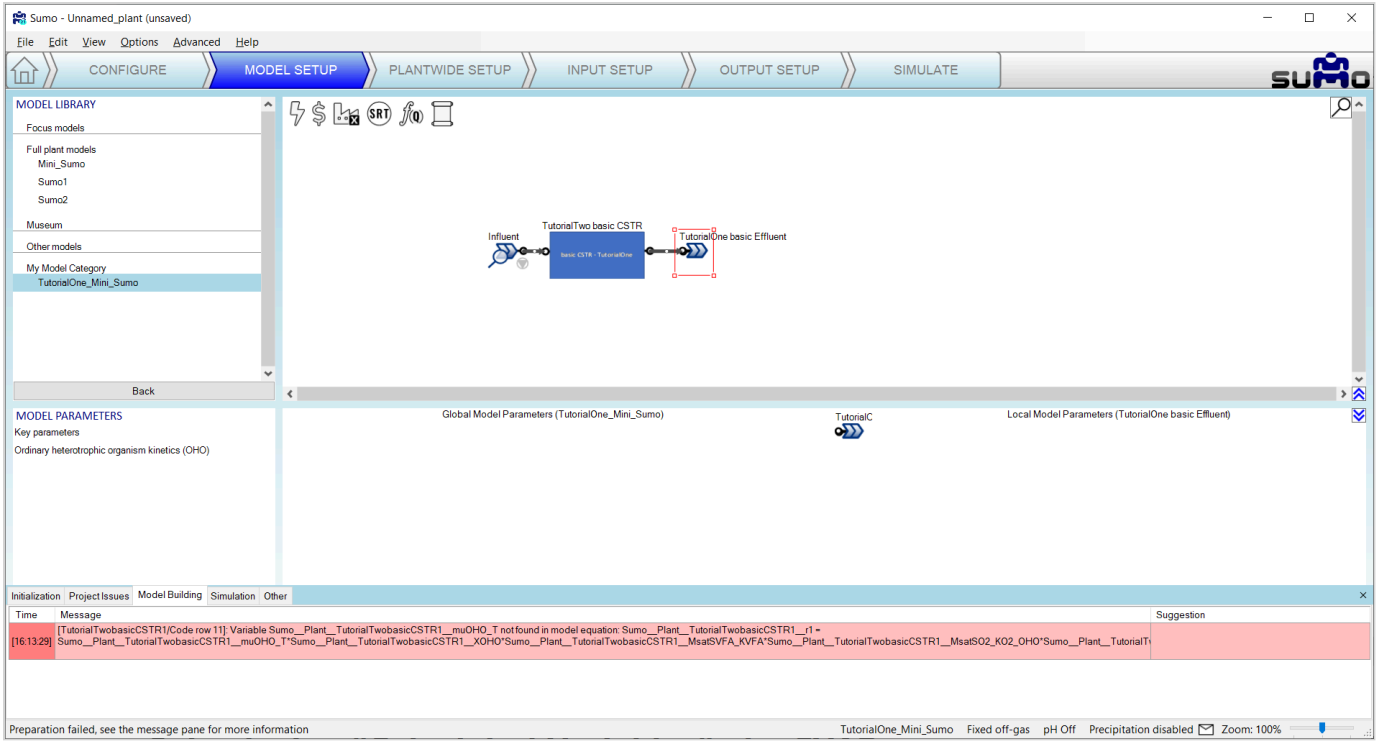


Step 9

The `Unit` worksheet does not require any updating.

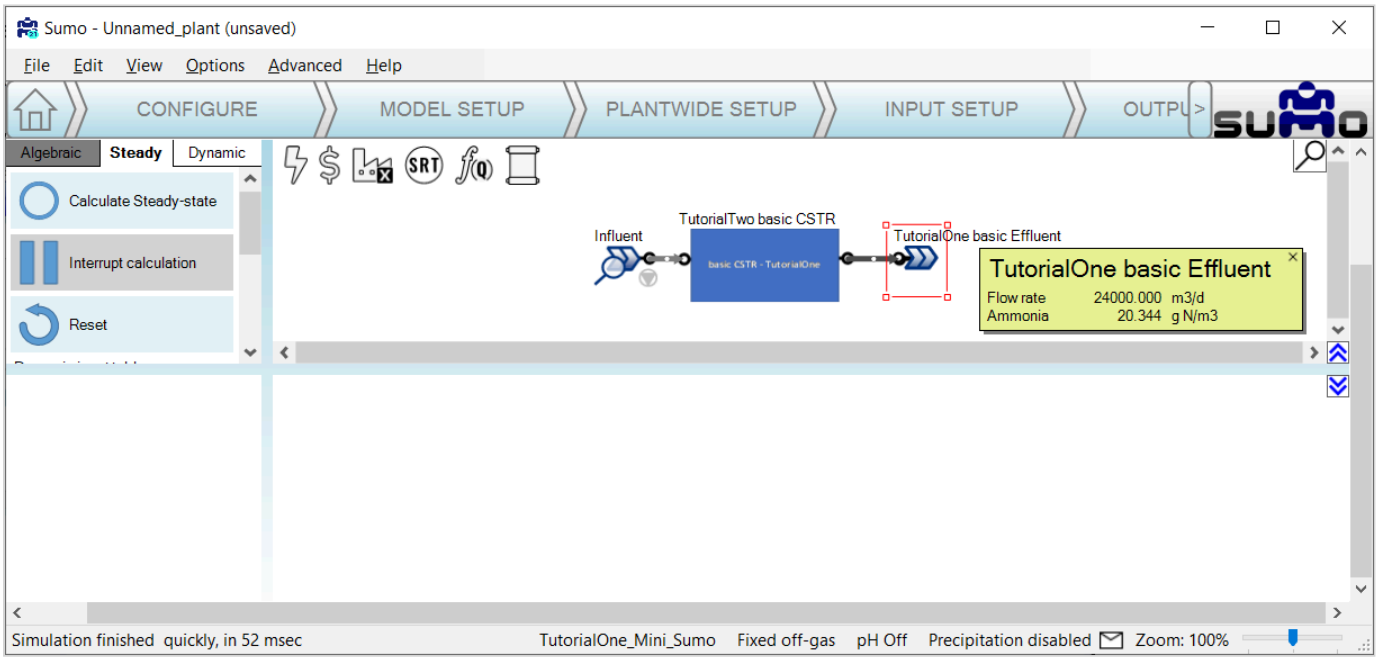
Step 10

When we open *SUMO*, we create flowsheet and select "TutorialTwo_Mini_Sumo" from Model Base:



Step 11

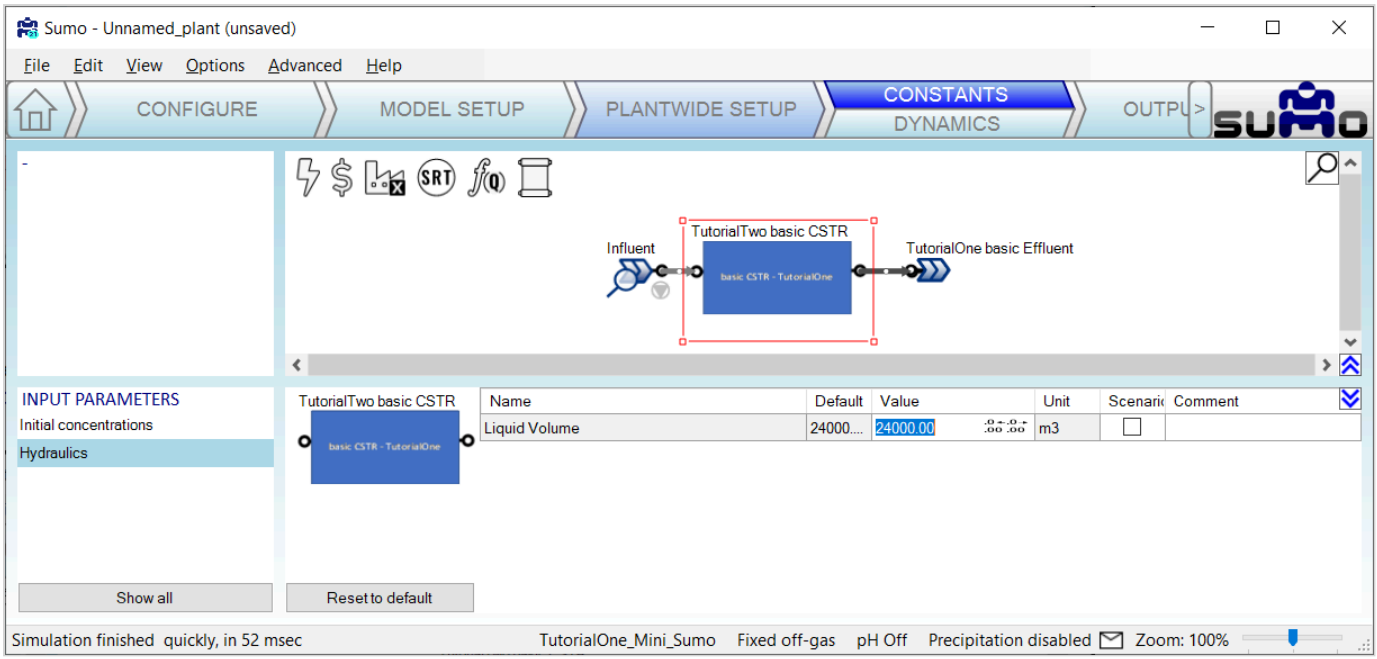
After changing the Model Base to "TutorialTwo_Mini_Sumo" we are able to build the model and steady state simulations show an effluent ammonia concentration as follows:



Step 12

The liquid volume `L.V` that we defined in the `Parameters` worksheet of `basicTwo CSTR.xlsx` can be changed by the user in `INPUT SETUP` tab. How does the predicted effluent ammonia change if

double the reactor volume to 48000 m^3?



Summary of Tutorial 2

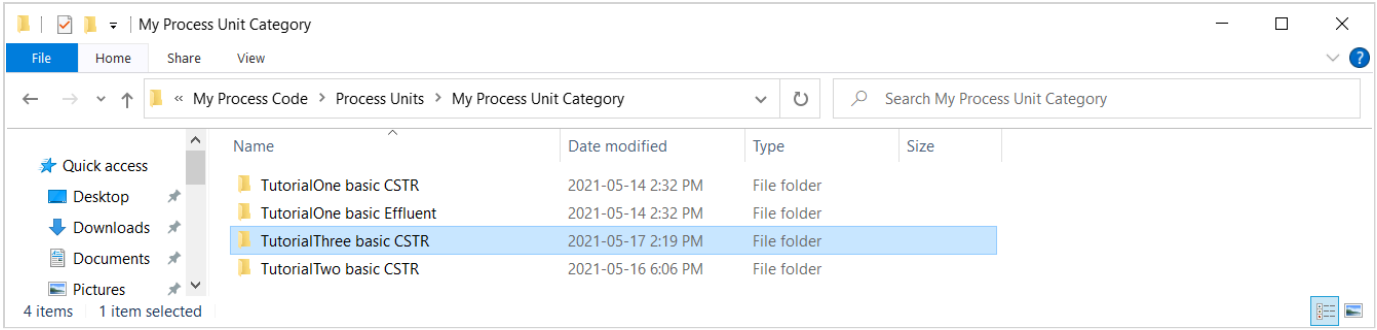
Tutorial Two demonstrated how to introduce reactions to our basic CSTR. In technical speak: a mass balance differential equation for the *SUMO* numeric engine to integrate during simulation runs. Instead of coding reactions directly into the `Process Units`, we learned how to leverage the `Model Base` which we pulled into the `Process Units` using "triplet notation". Unfortunately, the process unit file `basicTwo CSTR.xlsx` is not compatible with the standard library of *SUMO* `Process Units` and `Model Base`. The reason for this is that it is missing the code to import the `Model Base` parameters `PAR`. Also it does not calculate and map certain calculated variables `CVAR` that other process units expect to be mapped to the `..outp` port of our basic CSTR. These shortcomings will be addressed in the remaining two tutorials.

Tutorial 3: Introducing Calculated Variables

The purpose of this tutorial is to make our `basic CSTR` compatible with the `Mini_Sumo` from *SUMO*'s standard `Model Base`.

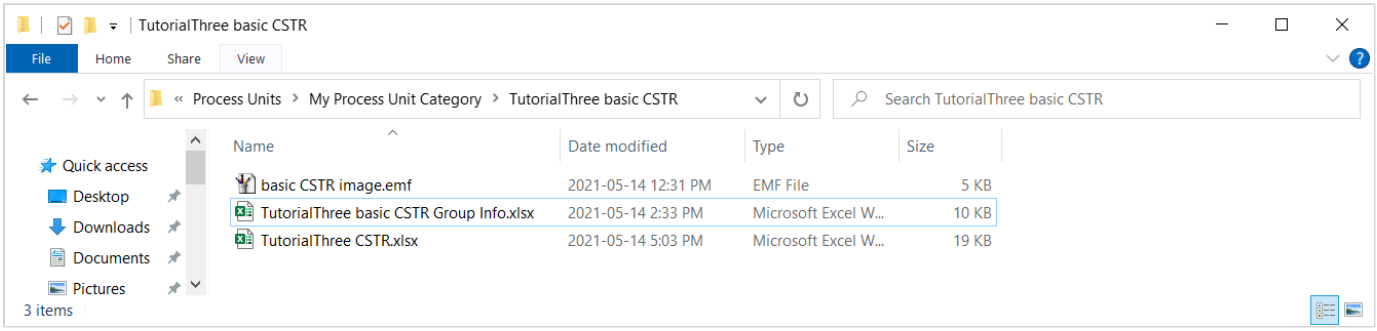
Step 1

First, let's create a copy of `Tutorial Two basic CSTR` inside the `My Process Unit Category` and call it `TutorialThree basic CSTR`:



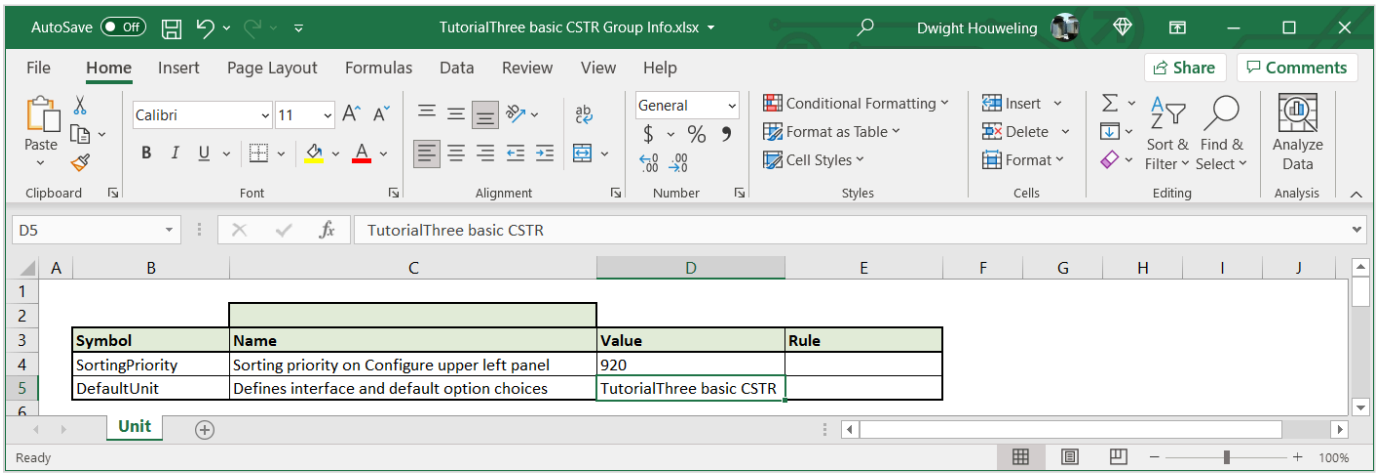
Step 2

Next, we update the file names in `\TutorialThree basic CSTR` as follows:



Step 3

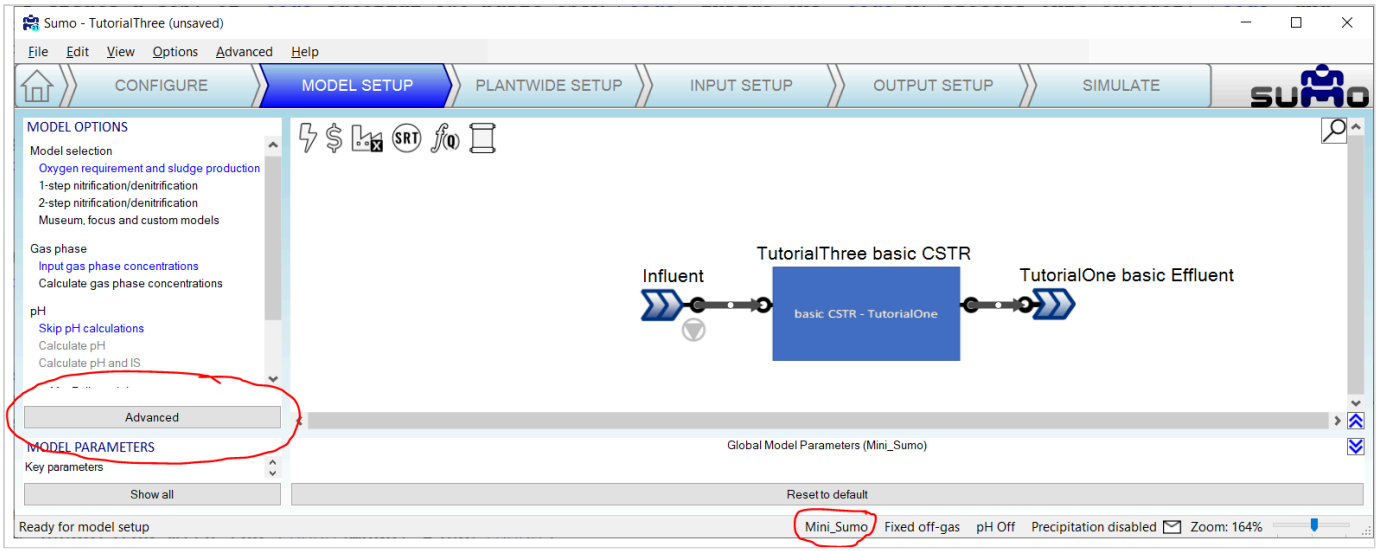
Make sure the `Group Info` file references the `TutorialThree basic CSTR.xlsx`:



Step 4

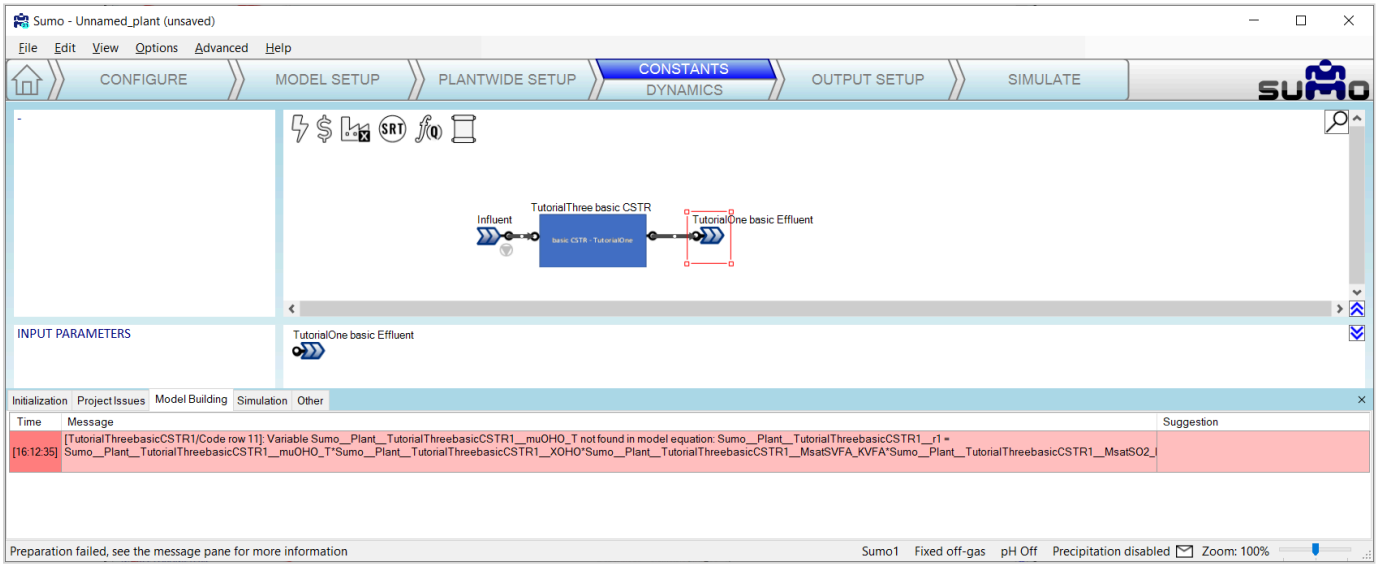
Now let's build a simple model in *SUMO* using `Influent` from the `Flow elements` and `TutorialThree basic CSTR` and `TutorialOne basic Effluent` from the `My`

`Process Unit Category`. Also, let's select `Mini_Sumo` from the `Advanced` option in the `MODEL SETUP` step. *SUMO* should then display `Mini_Sumo` at the bottom of the drawing board window:



Step 5

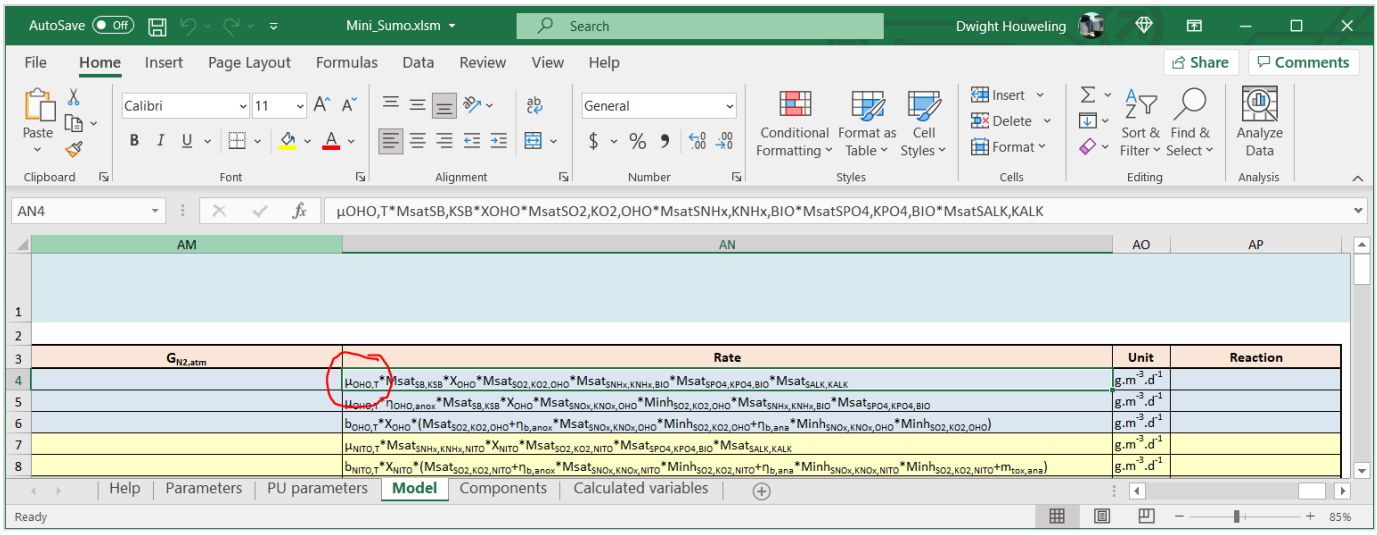
When we attempt to build the model we get the error highlighted below that *SUMO* cannot find `muOHO_T`. This is a parameter associated with the `Model Base`.



Step 6

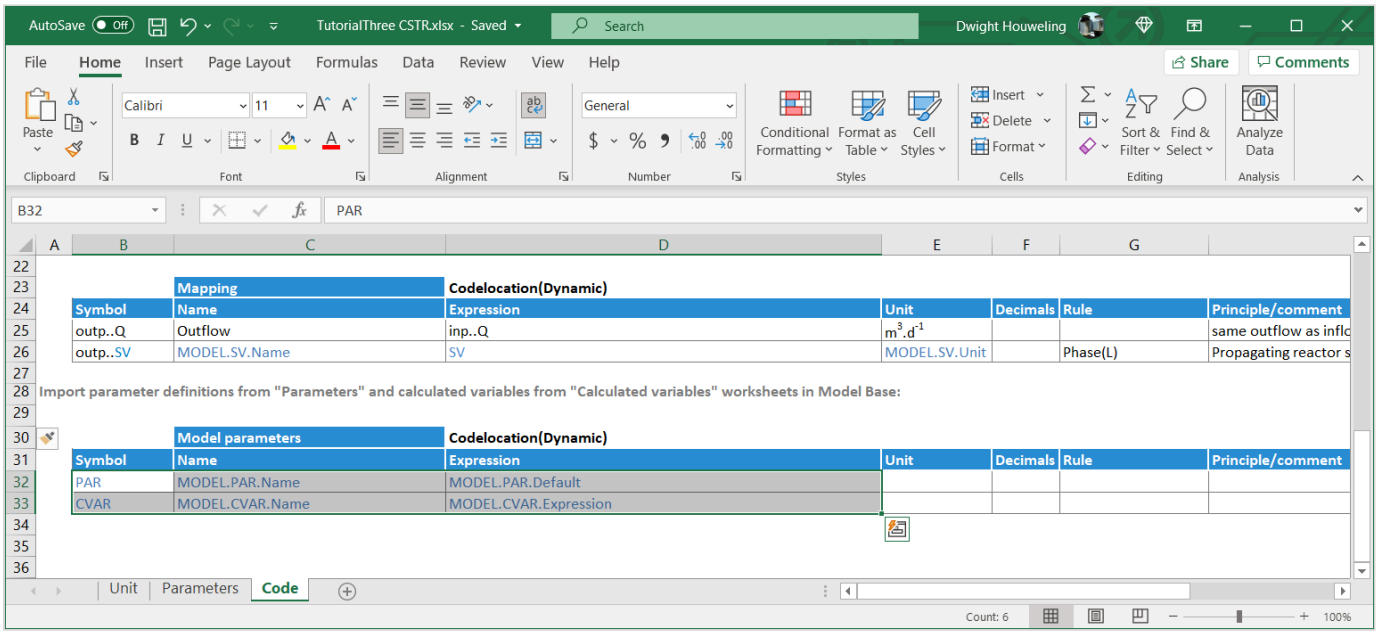
When we search `Mini_Sumo.xlsx` [11] for this `muOHO_T`, we find that it is used in the very first process rate equation of the `Model` worksheet. In addition, a search throughout this file `CTRL+F` reveals that it is calculated in the `Calculated variables` worksheet based on parameters like `muOHO` and `Tbase` which are defined in the `Parameters` worksheet. Notice how Greek letters in Excel are translated into their

latin equivalent in *SUMO* and commas are replaced with underscores. So what is referred to as `muOHO_T` in *SUMO* is actually $\mu_{OHO,T}$ in the Excel file.



Step 7

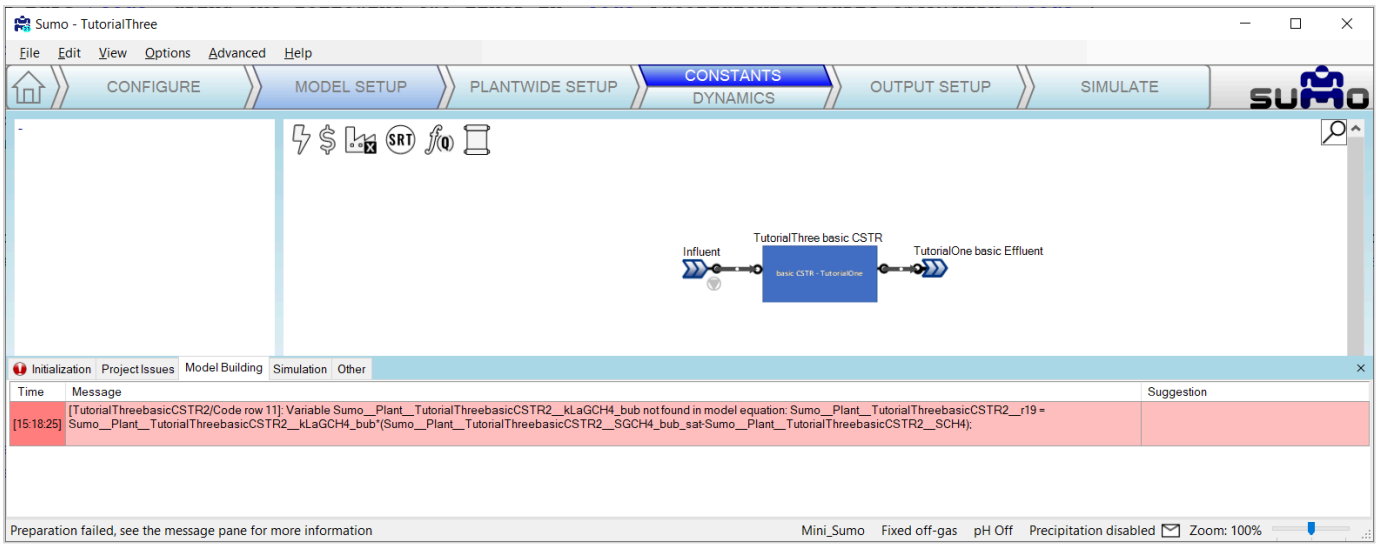
To correct this error, we will import the parameters `PAR` and calculated variables `CVAR` from the `Model Base` using the following two lines in `TutorialThree basic CSTR.xlsxMini_Sumo.xlsx` [12]:



Step 8

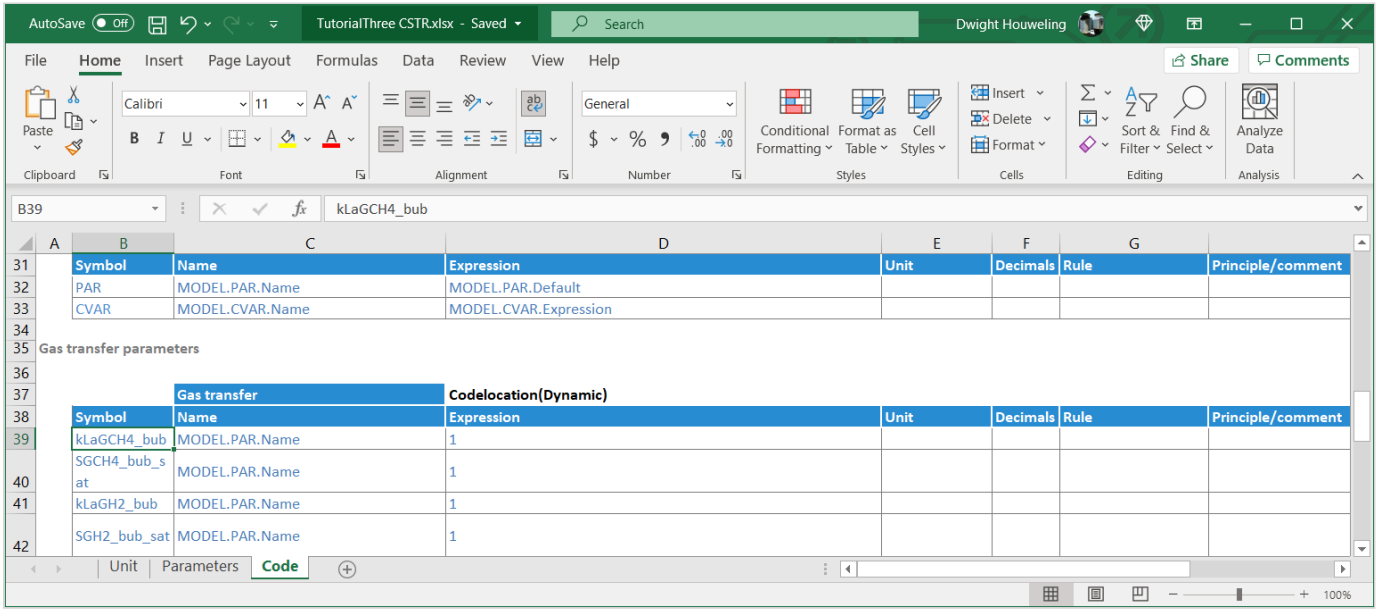
Now, we reopen *SUMO* and when we try to build our simple flowsheet, the error related to `muOHO_T` no longer appears. But instead we have a new error related to `kLaGCH4_bub`. After searching the `Mini_Sumo.xlsx` we find it in the `Methane gas transfer - bubbles` rate in the `Model` worksheet. Interestingly, it does not appear in the `Parameters` or `Calculated variables`

worksheets. Actually, SumoSlang is looking for this to be calculated directly in the process unit file. For example in the standard library CSTR process units[13], this parameter would be calculated in `Code` worksheet as `kLaG.SV,bub` where `G.SV` is expanded by SumoSlang to include all gas phase state variables including `CH4`.



Step 9

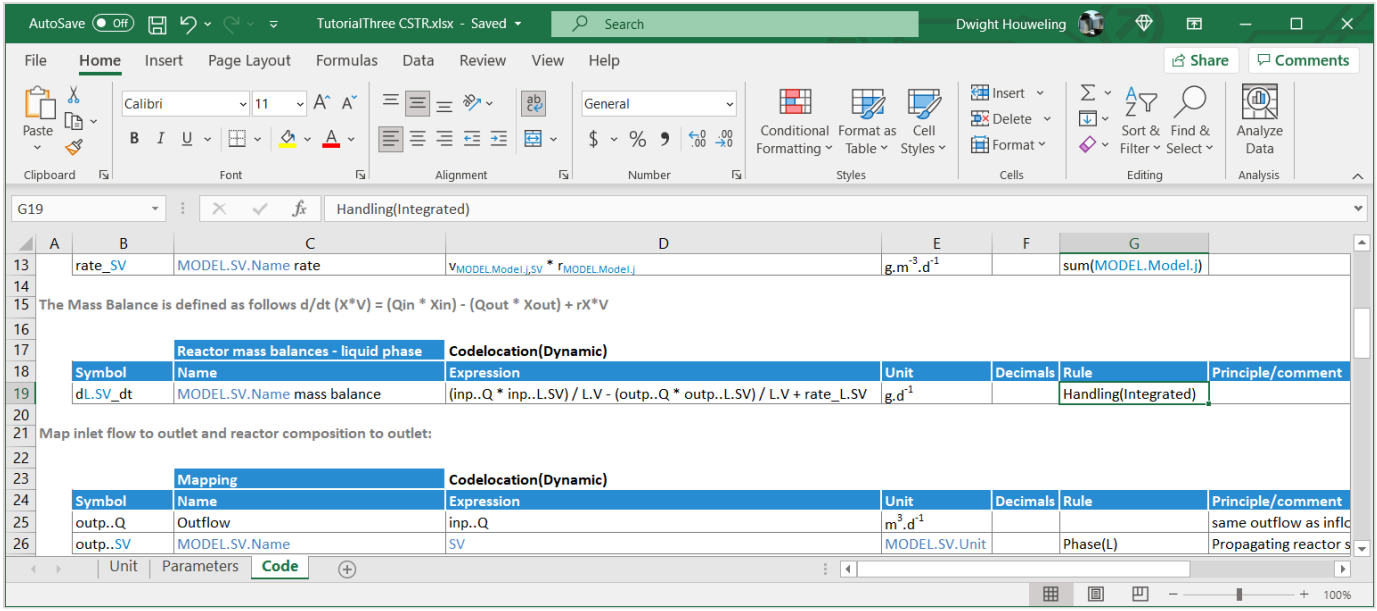
So we will provide *SUMO* with the gas transfer parameters it is looking for by coding them into the `Code` worksheet and assigning them placeholder values of `1`.



Step 10

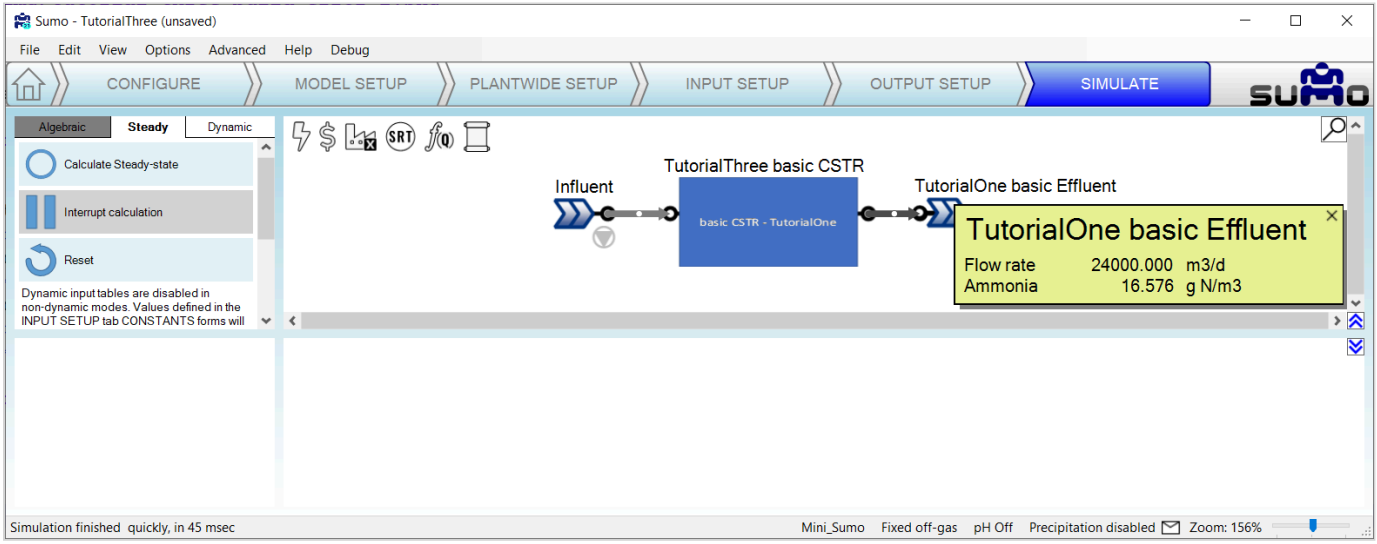
But in fact, we don't want *SUMO* to calculate gas transfer rates since we have only have placeholder values for the gas transfer `kLa` coefficients. SumoSlang provides a nice way to handle this by adding a `Rule` to the

calculation of mass balance. This `Rule` specifies that the mass balance will only be calculated for state variables `SV` which have been identified in `Model Base` to have `Handling(Integrated)`. The handling of each of the state variables is identified in the `Components` worksheet table heading `Handling`. For `Mini_Sumo.xlsx` you will find that most state variables are `Integrated` but gases are `Set`.



Step 11

Once again we reopen *SUMO* and try to build our basic CSTR model. And this time there are no errors. Success!



Summary of Tutorial 3

Tutorial Three demonstrated how to import parameters `PAR` and calculated variables `CVAR` from the `Model Base`. In addition, the reliance of the *SUMO* standard model library on calculation of gas transfer `kLa` coefficients in the `Process Code` was demonstrated. The updates to the `basic CSTR` process unit code in this tutorial makes it compatible with the standard *SUMO* `Model Base`. However, there is still one more step required to make it compatible with the standard *SUMO* `Process Units`. This final change is demonstrated in Tutorial Four.

Tutorial 4: Compatibility with the *SUMO* Process Unit Library

Step 1

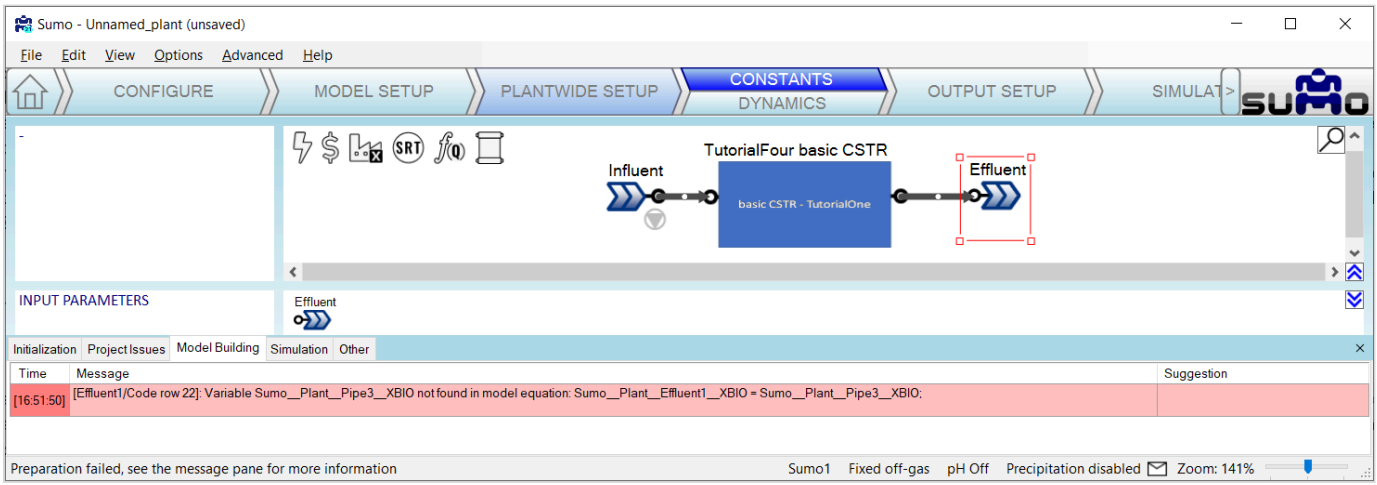
Make a copy of the `TutorialThree basic CSTR` folder and rename it `TutorialFour basic CSTR`. Update the names of the files in this folder to make it consistent with the folder name and also remember to change the name of the process unit file referenced inside the `Group Info` file.

Step 2

Double check that you can successfully build and simulate a model using the `Mini_Sumo` model as described in Tutorial Three but using the `TutorialFour basic CSTR`.

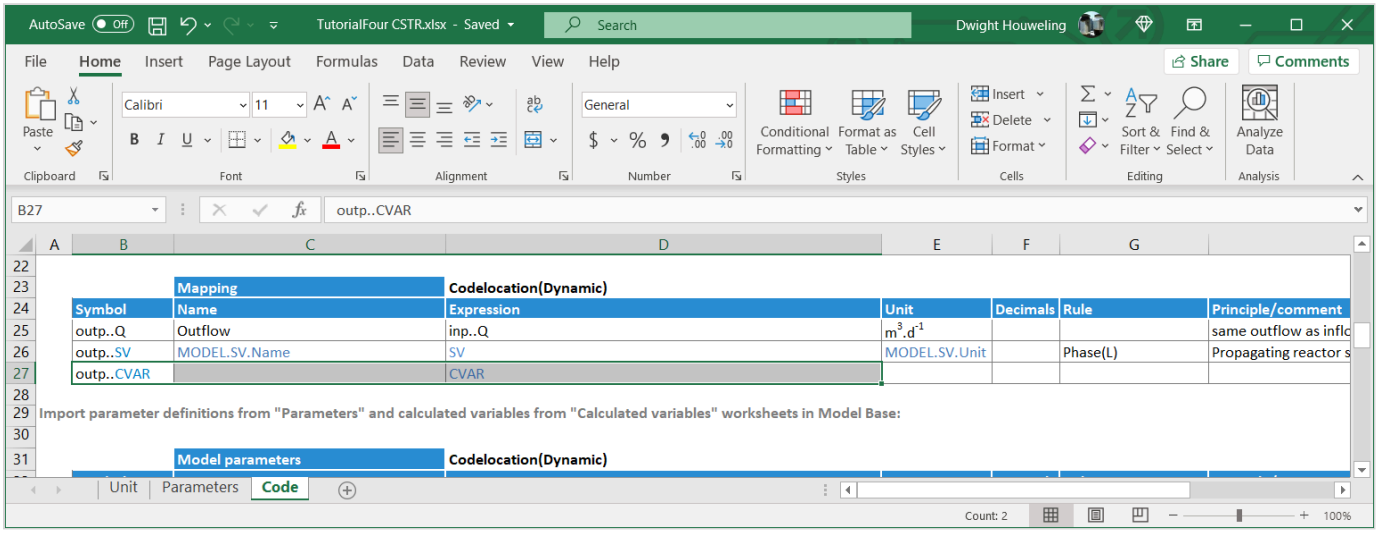
Step 3

Next we will delete the `TutorialOne basic Effluent` and replace it with the `Effluent` element from the standard *SUMO* `Flow elements`. When we try to build this model we get the following error:



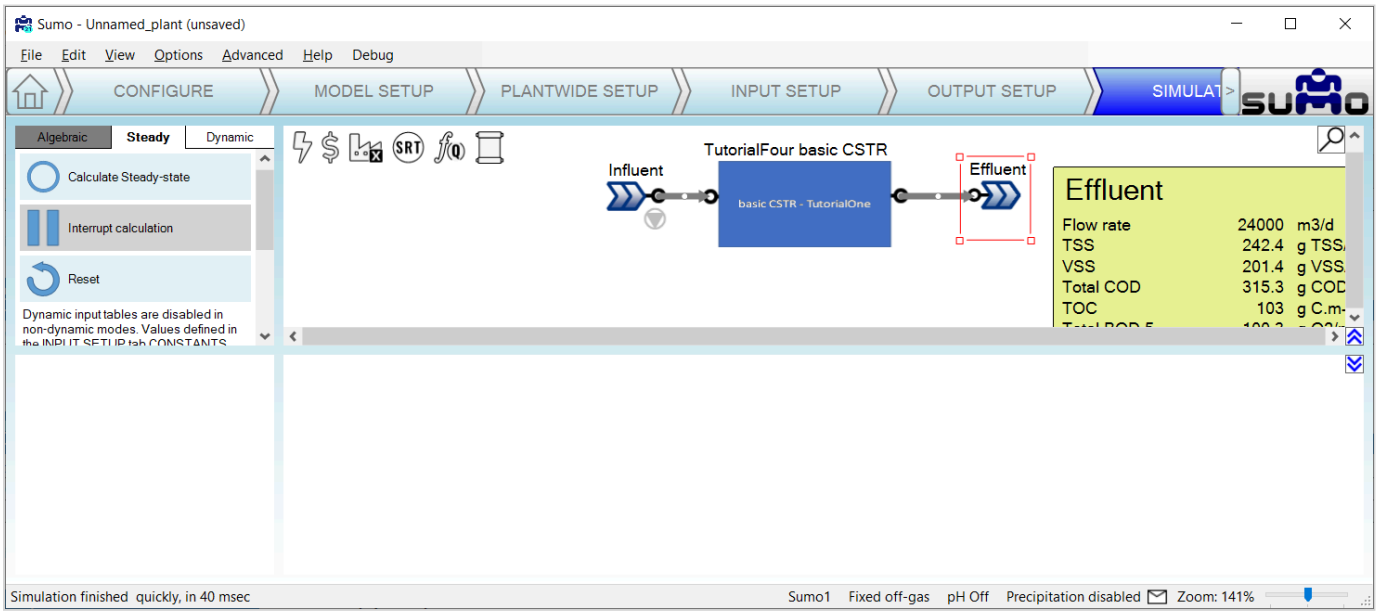
Step 4

In short, *SUMO* is looking to assign `XBIO` in the `Effluent` to the value in the effluent of the `basic CSTR`. A review of the `Model Base` indicates that `XBIO` is a calculated variable `CVAR` and so we conclude that our code is not mapping `CVAR` to the `..outp` of the reactor. We can add the following line to the `Code` worksheet of `TutorialFour basic CSTR.xlsx` to rectify this:



Step 5

We reopen *SUMO* and try to build the model with the standard library `Effluent` element. Success! And when we mouseover the `Effluent` element we see the calculated variables from the `Model Base` displayed on the screen:



Summary of Tutorial 4

Tutorial Four demonstrated how to map `CVAR` to the effluent of our `basic CSTR` process unit. This is important because it makes our process unit compatible with the standard library of *SUMO* process units. Many of these process units are very simple like splitter and mixer element that do need to not interface with the `Model Base`. They therefore rely on the mapping of both `SV` and `CVAR` from upstream process units. Based on these four tutorials you have the fundamental tools to build custom process unit models that can leverage the `Model Base` and interface with the rest of the *SUMO* standard library of `Process Units`. So have fun! For further tips on style I suggest the BoSS as well as studying some of the standard library `Process Units`.

Next steps

The previous tutorials provided an overview of how to get started building customized process models in SumoSlang. What are some good next steps? How about the following:

- Think about a unique process that you want to develop a customized model for. For example, maybe one where inlet flow is split evenly between two outlet streams but particulate `SV` are preferentially directed to one outlet at the expense of the other. Looking at how this is coded for a hydrocyclone in the standard *SUMO* library `C:\Dynamita\Sumo21\Process code\Process units\Separators\Cyclone` might be a good place before getting started with your own customized version.
- Explore the use of "complex" models as a powerful way to further use SumoSlang to build process unit models from other process unit models. As an example, the standard *SUMO* library model for a pond `\Dynamita\Sumo21\Process code\Process units\Bioreactors\Pond` uses the code for an equalization basin `\Dynamita\Sumo21\Process code\Process units\Flow elements\Equalization basin` to model the interaction between a pond water column and its sediment layer. Note how the `Pond` model includes an additional worksheet named `Structure` which invokes several process units from the standard library including the `Variable volume equalization basin`.
- Explore the use of "array" notation to specify multiple compartments within a single process unit. A good example of the use of array notation is provided in the plug flow bioreactor `\Dynamita\Sumo21\Process code\Process units\Bioreactors\PFR`.

Footnotes

[0]

SumoSlang can be a little intimidating to the uninitiated, even for an experienced modeller. These tutorials are written for you if you are already familiar with how process models work, the Gujer matrix, systems of differential equations, maybe you have even done some coding on your own, but nothing as a sophisticated as

what's "under the hood" of a commercial simulation software package like *SUMO*. Imagine Orville Wright transported in time into the cockpit of a 747. Arguably he would know as much as anyone about airplanes and how to fly them. But in a 747 cockpit there are so many buttons, so many little lights, he would have no idea what does what! No question of "learning by doing". Common sense dictates he should not touch anything without supervision and hours of training. You think this example too dramatic? After all, no one ever died crashing their computer. True, but the fact is that it is easier to learn when complexity is stripped away. And this is just as true for modelling as it is for learning to fly an airplane. After all if Orville Wright had been forced to learn to fly in a Boeing 747, then the history of aviation might have turned out very differently.

back

[1]

The BoSS aka Book of SumoSlang

back

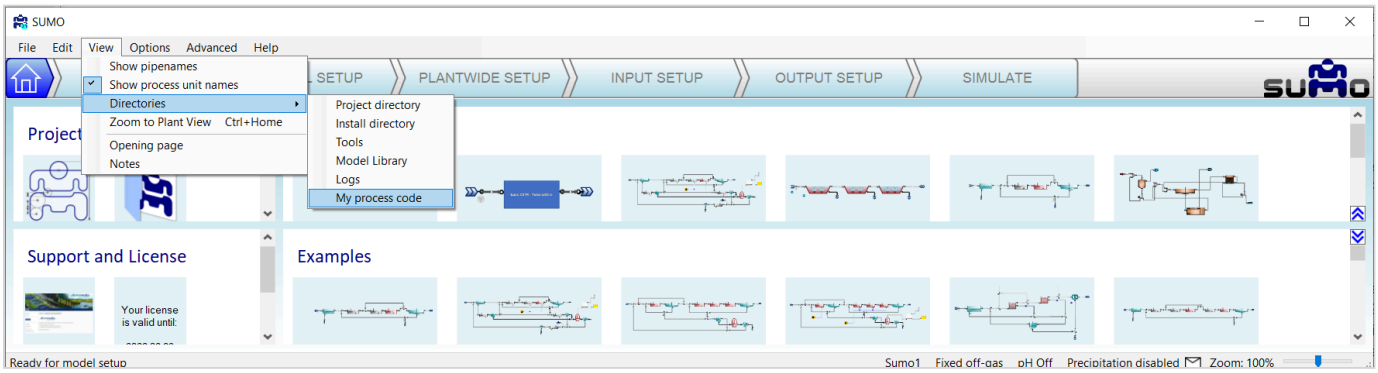
[2]

When do we need to code SumoSlang? Can't we create models directly in *SUMO*? In fact, for most cases, creating models doesn't require any coding at all. A novel BNR process may be unique and different from any other BNR process in the world, but it is still just a combination of aerated and unaerated bioreactors. So no need for SumoSlang, just drag and drop bioreactor elements into the *SUMO* drawing board and away you go, happy modelling! But suppose the model involves a hybrid reactor with unique interactions between suspended and attached growth, maybe even something interesting happening with the gas phase too. And perhaps there is no process unit in the standard *SUMO* library that adequately captures the unique behavior in this reactor. This is a more complex case and in most commercial software you would be stuck. But in *SUMO* it's not a problem because you can just code it yourself.... in SumoSlang!

back

[3]

Note that if you find a directory named "Process Code" but not "My Process Code" then you chose separate locations for the "Install" and "Working" directories on installation of *SUMO*. Another way to find the location of "My Process Code" is from the main menu of the *SUMO* "View | Directories | My process code".



back

[4]

The names of these files is important. First, it is critical that the "Group Info" file include the same name as the folder in which it is found. For example, if the folder name is "Industrial DAF" then the "Group Info" file would need to be "Industrial DAF Group Info.xlsx". Or, since in this case the folder name is "TutorialOne basic CSTR" then the file name is "TutorialOne basic CSTR Group Info.xlsx". There are no constraints on the image file and other ".xlsx" files names other than no special characters, that includes hyphens! The names of the image file(s) will be referenced in the process unit excel file(s) and in a similar manner the names of the process unit excel file(s) will be referenced in the Group Info file. I use "(s)" in "file(s)" to indicate that there can be one or several of these. There can, however, be only one "Group Info" file.

back

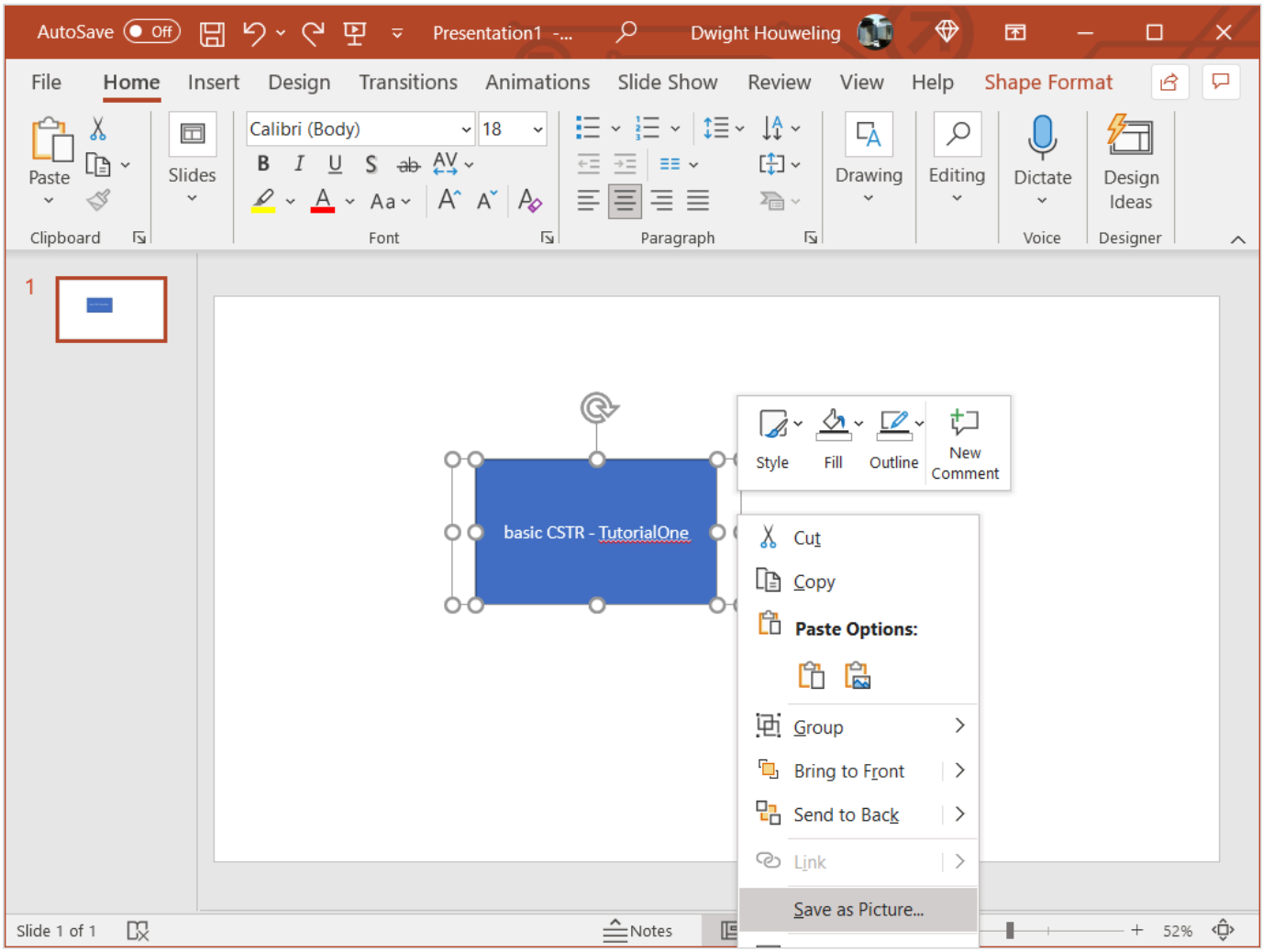
[5]

You might ask "Which state variables?" "I haven't defined any state variables yet!" The state variables refer will be the ones associated with the Model Base file that is activated in the *SUMO* flowsheet. When you open *SUMO*, the default Model Base is the Sumo1 model. This model includes some X state variables and so `inp..L.SV` and `outp..L.SV` refer to the entire list of liquid state variables associated with the input and output streams to our process unit, the basic CSTR. If you were to change the Model Base file to something different, Sumo2 or maybe your own custom Model Base, then `L.SV` would refer to state variables in that Model Base file.

back

[6]

What is the best way to create images for the drawing board? In this case I have used Powerpoint to create a rectangle with some text inside it. Then I select the image, right click and select "Save as Picture" from the drop down menu. In order to create some space in the image for the ports to appear, create a second rectangle behind the blue one. The second rectangle should have no fill and no outline. But it will define the boundaries of the image file slightly larger than the blue rectangle. This will create space for the ports to appear.



back

[7]

The purpose of deparametizing the model in Tutorial Two is so that we do not need to include code to import the `Model Base` "parameters" or "PARAM" in `basic CSTR.xlsx`. There are different ways to import "parameters" from the `Model Base` into the `Process Units` code and so it is preferable to treat this in a separate tutorial.

back

[8]

The stoichiometry of the growth of nitrifiers is presented at its simplest here. The utilization of 1 g NH4-N generates Y g of nitrifying organisms `XNITO`. Therefore to generate 1 g of `XNITO` we require 1/Y g of NH4-N. Assuming Y=0.15 explains the hardcoded values of -6.667 and +6.667 for ammonia and nitrate, respectively.

back

[9]

Don't forget to check out the BoSS aka Book of SumoSlang!

back

[10]

SumoSlang allows you to identify and perform calculations on the liquid state variables `L.SV` separately from the longer list of all state variables `SV` which also includes gaseous components `G.SV` associated with bubbles and head space. This is a useful distinction because `L.SV` travel from reactor to reactor whereas `G.SV` do not. How does SumoSlang know whether `SV` is an `L.SV`? SumoSlang looks for these definitions in in the `Phase` column of the `Components` worksheet of the `Model Base`. Take a look in our `TutorialTwo_Mini_Sumo.xlsm` or any other of the files in the *SUMO* `Model Base`.

back

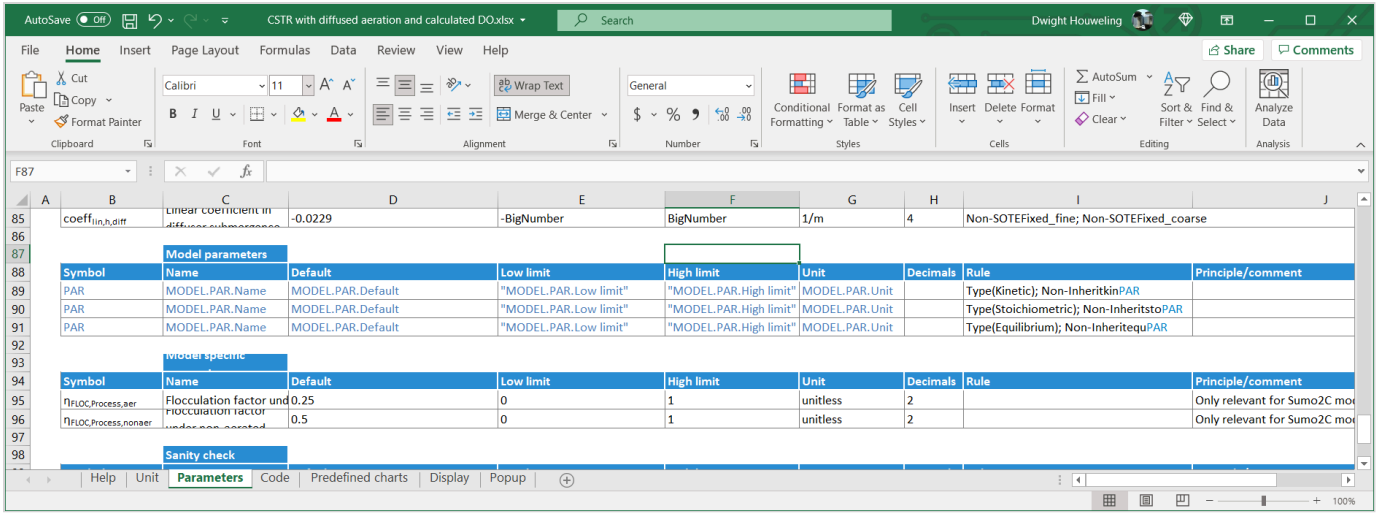
[11]

On my computer this file is located in `C:\Users\cdhou\AppData\Local\Dynamita\Sumo21\Process code\Model base\Full plant models`.

back

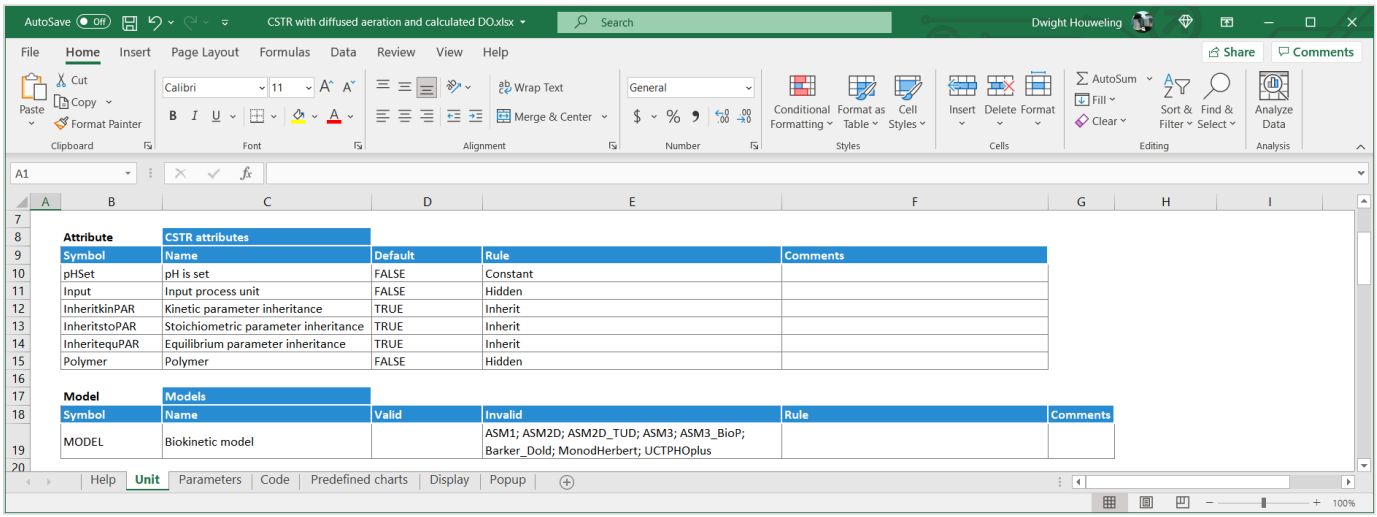
[12]

On inspecting coding of `CSTR with diffused aeration and calculated DO.xlsx` from the standard *SUMO* process unit library we find `PAR` defined three times in the `Parameters` worksheet and then another three times in the `Code` worksheet. What's going on? Do understand this we need to look at the `Rule` column. First, in the both worksheets, the three definitions of `PAR` apply, respectively, to `Type(Kinetic)`, `Type(Stoichiometric)` and `Type(Equilibrium)`. So the first thing to understand about these definitions is that they import parameters from the `Model Base` depending on whether the table heading in the `Parameters` worksheet includes `Type(Kinetic)`, `Type(Stoichiometric)` or `Type(Equilibrium)`. Secondly, in the `Parameters` worksheet these definitions are only applied if `Non-InheritkinPAR`, `Non-InheritstoPAR` and `Non-InheritequPAR`.



Symbol	Name	Default	Low limit	High limit	Unit	Decimals	Rule	Principle/comment
PAR	MODEL.PAR.Name	MODEL.PAR.Default	"MODEL.PAR.Low limit"	"MODEL.PAR.High limit"	MODEL.PAR.Unit		Type(Kinetic); Non-InheritkinPAR	
PAR	MODEL.PAR.Name	MODEL.PAR.Default	"MODEL.PAR.Low limit"	"MODEL.PAR.High limit"	MODEL.PAR.Unit		Type(Stoichiometric); Non-InheritstoPAR	
PAR	MODEL.PAR.Name	MODEL.PAR.Default	"MODEL.PAR.Low limit"	"MODEL.PAR.High limit"	MODEL.PAR.Unit		Type(Equilibrium); Non-InheritequPAR	

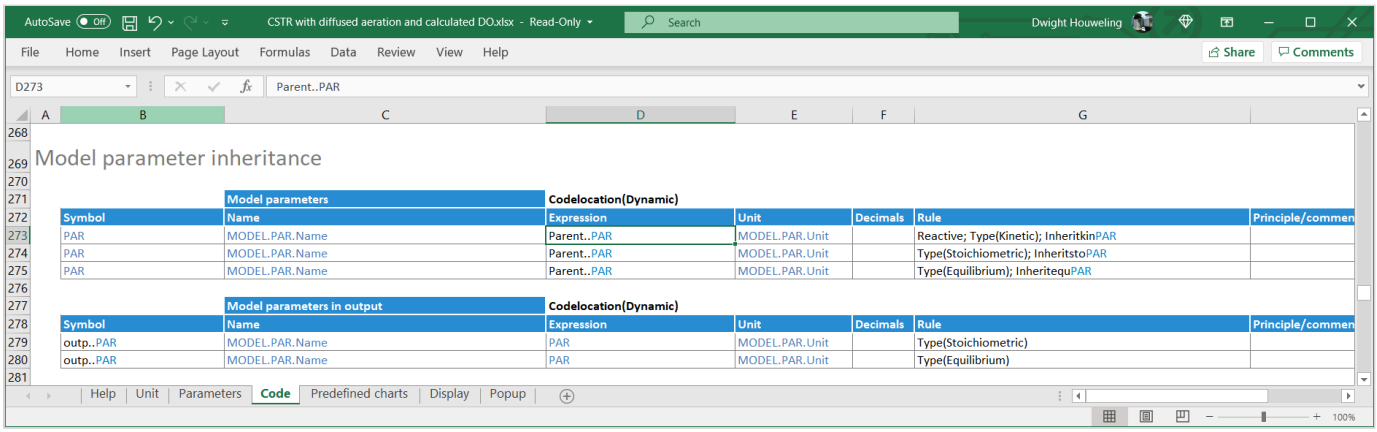
In contrast, in the `Code` worksheet, the rules are opposite: `InheritkinPAR`, `InheritstoPAR` and `InheritequPAR`. Which will prevail? The answer lies in the definitions for these inheritances which are found in the `Unit` worksheet. Since these inheritance parameters are assigned to `TRUE`, only the definitions of `PAR` from the `Code` worksheet apply.



Symbol	Name	Default	Rule	Comments
pHSet	pH is set	FALSE	Constant	
Input	Input process unit	FALSE	Hidden	
InheritkinPAR	Kinetic parameter inheritance	TRUE	Inherit	
InheritstoPAR	Stoichiometric parameter inheritance	TRUE	Inherit	
InheritequPAR	Equilibrium parameter inheritance	TRUE	Inherit	
Polymer	Polymer	FALSE	Hidden	

Symbol	Name	Valid	Invalid	Rule	Comments
MODEL	Biokinetic model		ASM1; ASM2D; ASM2D_TUD; ASM3; ASM3_BioP; Barker_Dold; MonodHerbert; UCTPHOplus		

And `PAR` is defined in the `Code` in terms of the parent unit `Parent..PAR`:

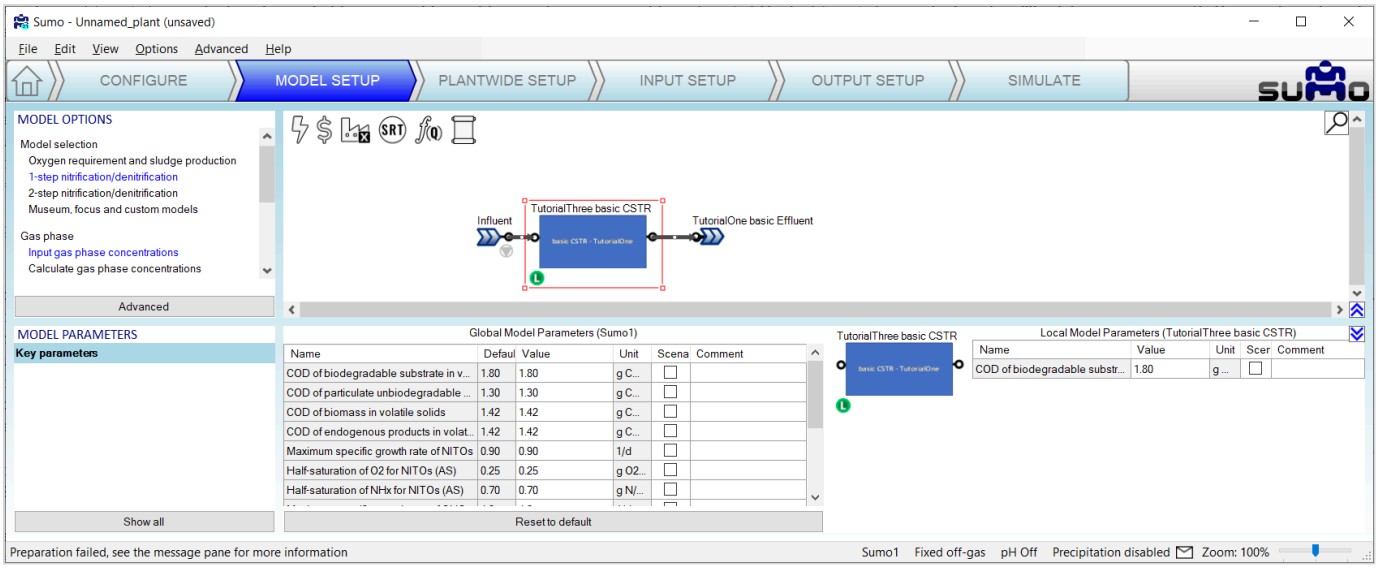


Model parameter inheritance

Symbol	Name	Expression	Unit	Decimals	Rule	Principle/commen
PAR	MODEL.PAR.Name	Parent..PAR	MODEL.PAR.Unit		Reactive; Type(Kinetic); InheritkinPAR	
PAR	MODEL.PAR.Name	Parent..PAR	MODEL.PAR.Unit		Type(Stoichiometric); InheritstoPAR	
PAR	MODEL.PAR.Name	Parent..PAR	MODEL.PAR.Unit		Type(Equilibrium); InheritequPAR	

Symbol	Name	Expression	Unit	Decimals	Rule	Principle/commen
outp..PAR	MODEL.PAR.Name	PAR	MODEL.PAR.Unit		Type(Stoichiometric)	
outp..PAR	MODEL.PAR.Name	PAR	MODEL.PAR.Unit		Type(Equilibrium)	

So what does this mean? What is the parent unit? In short, `Parent..PAR` can be thought of as a set of "Global parameters" that are applied to all process units in the *SUMO* flowsheet. "Local parameters" only apply if the user makes "local" changes to the `Key parameters` as shown below. If local changes are made, then the relevant inheritance parameters (`InheritkinPAR`, `InheritstoPAR` and/or `InheritequPAR`) for this process unit will switch to `FALSE`.



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[13]

Located on my computer at `C:\Users\cdhou\AppData\Local\Dynamita\Sumo21\Process code\Process units\Bioreactors\CSTR\CSTR with diffused aeration and calculated DO.xlsx`

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Digital Twin Toolkit

Sumo Python API setup

Various ways to install the Python API of Sumo

Sumo Python API setup

Sumo comes with a Python interface to its numerical engine. It is located under the installation folder (after installing the DTT addon):

```
<Sumo install path>/PythonAPI/dynamita
```

There are various ways to use the Python interface or API in custom Python applications.

Copying the API folder

The easiest way to use the interface is to copy the `dynamita` folder from the installation folder to the location of the custom Python application.

Let's say, the custom project is in the `C:/Users/username/My Sumo simulation` folder. Simply copy the `dynamita` folder from the Sumo install folder to this custom application folder; it will look like:

```
C:/Users/username/My Sumo simulation/dynamita
```

Every Python script located in the custom folder will be able to import the API like this:

```
import dynamita.scheduler as ds
import dynamita.tool as dtool
```

One drawback of this method is that if there are multiple Python projects in different folders, we must copy the API into each project. If the API changes we need to update all custom projects using the API.

This also can be an advantage if different projects need different versions of the API.

Setting the `PYTHONPATH` environment variable

We describe the simplest case of setting the environment varable in a command prompt window. Various editors or integrated development environments (IDE) may have other ways to set this variable.

Open a command prompt window by pressing the Windows button on the keyboard then type `cmd` and Enter. In the command window type:

```
set PYTHONPATH=<Sumo install path>/PythonAPI
```

where `<Sumo install path>` needs to be replaced to the actual path. Running scripts in this window they can access the API from the Sumo install folder; no need to copy. One drawback, or for some users advantage, is that every Python project is tied to one version of the API.

Creating a virtual Python environment

This is the safest, but most tedious way to set up the Sumo Python interface. The Python documentation contains examples how to create virtual environments .

In a virtual environment we can install the interface package with the usual `pip install` command. We can create multiple virtual environments for various Python and Sumo API versions and work safely in these environments.

In this scenario the Sumo Python interface is packaged in a so called Python Wheel file, e.g. `dynamita-22.1.0-py3-none-any.whl`, which can be installed with `pip` like:

```
pip install dynamita-22.1.0-py3-none-any.whl
```

At the moment the package should be requested from Dynamita S.A.R.L. separately. The `whl` file may be named as `dynamita-22-py3-none-any.whl`, just refering to the main Sumo version.

Hybrid virtual environment

On Linux systems Python is part of the operating system and we may not want to modify anything in that Python version. We can create a virtual Python environment following the Python documentation, to separate our workspace from the default OS Python.
After activating the virtual environment we can set the PYTHONPATH variable with the following command:

- Windows: `set PYTHONPATH=<Sumo Install path>/PythonAPI`
- Linux: `export PYTHONPATH=<Python API path>`
  In case of Linux the PythonAPI should be requested from Dynamita S.A.R.L.

Python Scheduler.py documentation

Python Scheduler documentation

How to set up your project

In order to use the Scheduler with your project, you'll need to do a few steps, before you start.

1. Make sure you have a Sumo DTT license from Dynamita! If you're unsure, keep ds.sumo.setLogDetails(6) in your script for feedback.
2. Open your project in the Sumo GUI and compile it, by clicking Simulate and waiting for the "Ready for simulation" message on the bottom left.
3. Make sure your project is in the state you want to run your code from. If you want to do multiple simulations from steady-state it might worth the effort to run steady-state here.

You have two options here. This is the easier method:

1. Import the dynamita.tool module. Documentation
2. In Python call extract_dll_from_project(project : str, path_to : str)
3. In Python call def extract_parameters_from_project(project : str, tsvdir : str, script_to : str, scenario : str = "") -> bool:
4. In your call to schedule, replace load "state.xml" with execute "script.scs" (the script you set in script_to)

If you want to keep you're environment as light as possible:

1. Open the Core window from the Advanced menu.
2. Send the *maptoic; save "state.xml"* commands from the bottom right textbox of the window to the sumocore. You can consult the SumoCore command documentation about these commands.
3. Open the project directory from the menu. View -> Directories -> Project directory.
4. Copy sumoproject.dll and state.xml to a location where you'll run your script from. It's a good idea to rename them to a custom name, so you remember later what's in them. The A2O example expects these to be renamed a2oplant.dll and a2ostate.xml. These files will be important when calling the schedule function.
5. You can close the Sumo GUI at this point or keep it open if you wish.

Setup

Function	`def setParallelJobs(self, jobs)`
Description	Sets the number of simulations to run at once. All other scheduled simulations will wait for these simulations to finish before they can start running. If this function is not called, the default is 1.
Arguments	**jobs** the number of jobs to run at once **returns** -

Function	`def setMaxJobReuse(self, reuse)`
Description	Sets the number of simulations to run in one process before restarting it. The process is only reused if multiple simulations are scheduled with the same model. The default value is 10. You should not change this value, unless you know what you're doing.

Arguments

reuse	the maximum number of jobs to run in one process
returns	-

Function `def setLogDetails(self, level)`

Description Decides what gets printed to the console by the scheduler.

Arguments

level	1 - all unknown messages from jobs are logged 2 - messages are logged from jobs 4 - all messages to jobs are logged 6 - all messages from and to jobs are logged
returns	-

Variable `message_callback`

Description Holds the handle to your message handler. The message callback gets the job id as integer and the message as string.

Example

```
ds.sumo.message_callback = msg_callback
def msg_callback(job, msg):
    print("MSG #" + str(job) + ": '" + msg + "'")
    if (ds.sumo.isSimFinishedMsg(msg)):
        ds.sumo.finish(job)
```

Variable `datacomm_callback`

Description Holds the handle to your data handler. The datacomm callback gets the job id as integer and the data as dictionary.

Example

```
ds.sumo.datacomm_callback = data_callback
def data_callback(job, data):
    print(f"DC #{job} - {data['Sumo__Time']}")
```

Simulation

Function `def schedule (self, model, commands, variables, blockDatacomm=False, jobData=None)`

Description Schedules a new simulation. Simulations will not run immediately, they use defined callbacks to communicate.

Arguments

model	Path to the model .dll file extracted from Sumo (sumoproject.dll in the .sumo file)
commands	List of commands to the simulation engine. Consult the SumoCore command documentation for availabe commands.

variables	List of variables to listen to. Variable names can be copied from Sumo's Advanced -> Core Window.
blockDatacomm	Should the simulation wait while python decides what to do? Set this to true, if you wish to control the simulation, but keep it false otherwise for faster results.
jobData	Extra information (dictionary) stored with the job, you might access later. You may set the sumo.persistent flag to keep the data once the simulation is finished.
returns	This function returns the JobID that you can reference to identify the simulation.

Example

```
job1 = ds.sumo.schedule(
                        "sumoproject.dll"
        commands      = [
                         f"load state.xml",
                         f"set Sumo__StopTime {10*ds.sumo.dur.day};",
                         f"set Sumo__DataComm {1*ds.sumo.dur.hour};",
                         f"set Sumo__Plant__Influent__param__frSNHx_TKN 2;",
                         "mode dynamic;",
                         "start;"],

        variables     = ["Sumo__Time",
                        "Sumo__Plant__Effluent__SNOx",
                        "Sumo__Plant__Effluent__SPO4"],

        jobData       = {
                            ds.sumo.persistent: True,
                            "results" : { }
                        },
        );
```

Function `def sendCommand(self, job, command)`

Description Sends a command to a job. If you send commands to a simulation that hasn't started yet, it'll get executed when it starts.

Arguments

job	Id of the target job
command	Command to the simulation engine. Consult the SumoCore command documentation for availabe commands.
returns	-

Example

```
ds.sumo.sendCommand(job1, "pause")
```

Function `def sendCommands(self, job, commands)`

Description Sends a list of commands to a job. If you send commands to a simulation that hasn't started yet, it'll get executed when it starts.

Arguments

job	Id of the target job

commands	A list of commands to the simulation engine. Consult the SumoCore command documentation for availabe commands.
returns	-

Example
```
ds.sumo.sendCommands(job1, ["set Sumo__StopTime 86400000", "set Sumo__DataComm 3600000", "start"])
```

Notes No need for closing semicolon character.

Function
```
def getJobData(self, jobId):
```

Description Gets the data you assigned to the job when you scheduled it. You may modify it and it will keep the changes.

Arguments

jobId	Id of the target job
returns	The dictionary you defined when you called schedule function. If you didn't define any job data there, this function returns null

Example
```
jobData = ds.sumo.getJobData(job)
```

Function
```
def finish(self, job)
```

Description Finish the job with the given job id, so other jobs may run. You may only finish jobs that have started running. You may not finish jobs that were scheduled but not ran yet. Often you'll want to finish a job when its simulation is finished. When a job is finished, its jobData is cleared unless sumo.persistent flag was set.

Note Usually it's better to only do one simulation per job. The scheduler optimizes jobs to run in the some process if possible to reduce overhead, but if you overuse a single job, it can cause slowdown on that job. You may impact other jobs as well, if they never get to run.

Arguments

job	the id of the job that you want to finish
returns	-

Example
```
def msg_callback(job, msg):
    if (ds.sumo.isSimFinishedMsg(msg)):
        ds.sumo.finish(job)
```

Cleanup

Function
```
def cleanup(self)
```

Description Releases all resources claimed by SumoScheduler and unloads it. Run it ONLY at the end of the Python script. You may encounter issues, if you schedule simulations after cleanup. Also cleans up any job data even if its marked persistent

Arguments	**returns** -

Utility

Function	`def isSimFinishedMsg(self, msg)`
Description	Decides if a message marks the end of a simulation.
Arguments	**returns** true, if its a simulation finished message, false otherwise

Example	`def msg_callback(job, msg):`
	`  if (ds.sumo.isSimFinishedMsg(msg)):`
	`  ds.sumo.finish(job)`

Python Tool.py Documentation

dynamita.tool.py documentation

This module provides a number of utilities to use with scripts written for Sumo.

How to import

Setup Make sure that either:

- Dynamita's Python modules are installed to your Python *or*
- The dynamita folder containing Dynamita's Python modules are copied under your project directory

Code

```
import dynamita.tool.py as dtool
```

Constants

Note	Python doesn't stop you from giving new value to constants, but doing it may cause several unexpected bugs.
dtool.msec	1 millisecond of simulation time
dtool.sec	1 second of simulation time
dtool.minute	1 minute of simulation time
dtool.hour	1 hour of simulation time
dtool.day	1 day of simulation time
dtool.week	1 week of simulation time

Structures

VariableEntry	
sumo_name	Fully namespaced name of the variable
sumo_type	Type of the variable. It can be REAL, INT, STRING, BOOL, REALARRAY
dimensions	Dimensions of the variable. It's empty if the variable is a scalar
value	Value of the variable. You don't need to call convert_to_data on this

Functions

Function

```
def convert_to_data(s: str):
```

Description Converts a string into the proper type of data based on Sumo standards

Arguments

s	the string that contains the data
returns	integer, float, string or array with the converted data

Example

```
print(dtool.convert_to_data("4.0;3.2;8.0"))
# prints [4.0, 3.2, 8.0]
print(dtool.convert_to_data("5.1"))
# prints 5.1
```

Function `def read_sumocore_xml(file_name: str) -> dict:`

Description Reads an xml state produced by the SumoCore's "save" command

Arguments

file_name	full path to the file to be loaded
returns	string -> VariableEntry dictionary, where the key is variable name

---

Function `def write_sumocore_xml(file_name: str, data: dict):`

Description Writes a xml state that can be read to the SumoCore by the "load" command. When using this function you should read an existing state with read_sumocore_xml, modify it and write it back, to ensure that all variables exist that is present in the model.

Arguments

file_name	full path to the file to be saved
data	string -> VariableEntry dictionary, where the key is variable name
returns	-

Function `write_sumocore_script(file_name: str, data: dict):`

Description Writes a SumoCore Script (.*scs) that can be used in the SumoCore with the "execute" command.

Arguments

file_name	full path to the file to be saved
data	string -> value dictionary, where the key is variable name
returns	-

Function `def create_array(begin, end = None, step = None, count = None, includeEnd = True)`

Description Generates an array based on the arguments given. You must define begin, and two out of the three other controlling arguments (end, step, count).

Arguments

begin	the first element of the array
end	the ending value of the array. If **includeEnd** is true, this value is included, otherwise its excluded.
step	the difference between two consecutive elements
count	the number of elements in the array
includeEnd	decide if **end** should be part of the array or not. If **end** is not defined, this argument has no meaning
returns	generated array

Example

```
dtool.create_array(begin = 1, end = 3, step = 1, includeEnd = True)
[1,2,3]
dtool.create_array(begin = 1, end = 3, count = 2, includeEnd = False)
[1,2]
dtool.create_array(begin = 1, end = 3, count = 2, includeEnd = True)
[1,3]
dtool.create_array(begin = 1, step = 2, count = 3, includeEnd = False)
[1,3,5]
```

Function `extract_dll_from_project(project : str, path_to : str):`

Description Extracts the dll file from a .sumo project that can be loaded into SumoCore in order to run simulations

Arguments

project	path to the .sumo file (including filename and extension)
path_to	path to the output .dll file (including filename and extension)
returns	-

Function `def extract_misc_from_project(project : str, what : str, path_to : str):`

Description Extract any file from the .sumo project. You can use this function to extract saved state.xml files from the project

Arguments

project	path to the .sumo file (including filename and extension)
what	name of the file that needs to be extracted
path_to	path to the output file (including filename and extension)
returns	-

Function `def extract_parameters_from_project(project : str, tsvdir : str, script_to : str, scenario : str = "") -> bool:`

Description Extract a script from the project that sets up the parameters as you would see in the Sumo GUI. It also includes dynamic tables. You can use the "execute" command to run this script in the SumoCore.

Arguments

project	path to the .sumo file (including filename and extension)
tsvdir	path to a folder that the module can use to save additional files
script_to	path to the output script file (including filename and extension)
scenario	scenario to be loaded. If omitted or incorrect, the module will only consider input setup values
returns	-

Function `def create_temp_folder(base : str):`

Description Creates a random, 8 character long folder. Can be used to save extracted Sumo project artifacts, like project dll, initialization scripts etc. These folders can be safely deleted to clean up the Python application folder.

Arguments

base	The random name folder will be created in this folder. Usually it is "." which means the current folder.
returns	The folder name.
