Getting started with BatchReactor®

Use Case 3: Simulation of mass transfer resistance

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Introduction

When simulating a vapor-liquid reactor with BatchReactor®, the gas and the liquid phases are considered, by default, at the thermodynamic equilibrium. This assumption is correct as long as the mass transfer rate is fast enough. However, in some applications (heterogeneous reactions, bioreactors...), it is necessary to refine the model by taking into account the mass transfer resistance. It is then possible to analyse the influence of the equipment (mixing device, vessel geometry...) and the operating conditions (gas flowrate, rotation speed…) on the mass transfer kinetics.

This document describes the use of the mass transfer model in BatchReactor®.

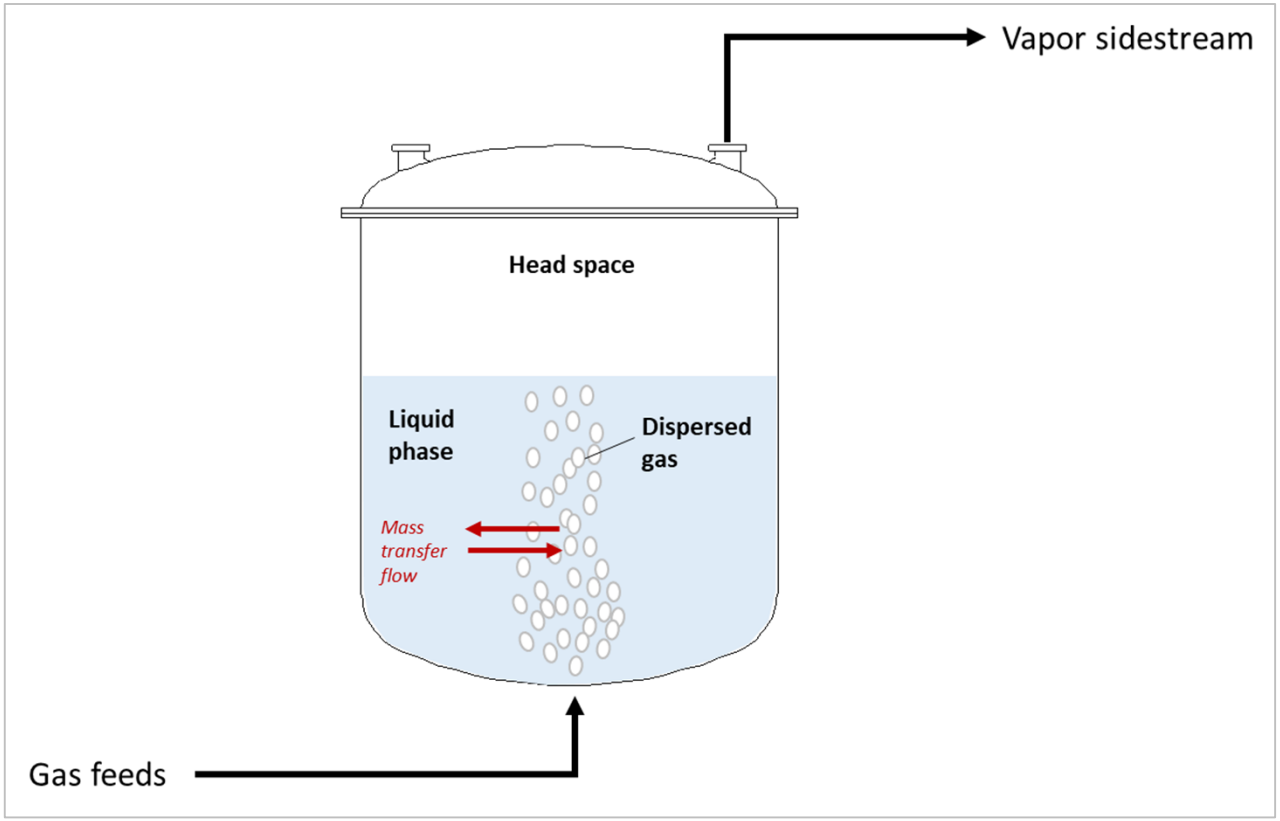
Here are the steps to follow:

- Step 1: selection of the compounds
- Step 2: configuration of the reactor topology and the mass transfer model
- Step 3: description of the operating mode
- Step 4: simulation of multiple different configurations

Before reading this document, it is recommended to consult “Getting Started with BatchReactor® - Use Case 1”

Description of the model

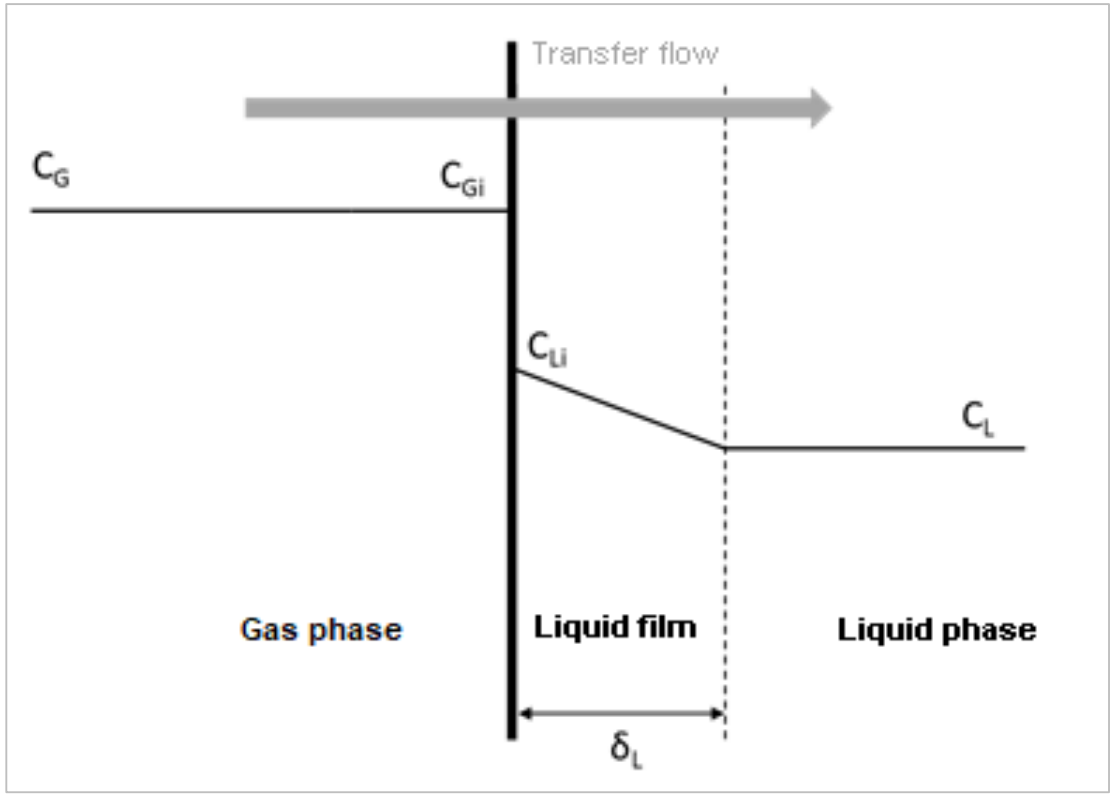
This tutorial is based on an example of a reactor that is fed with pure oxygen which creates a dispersed gas phase inside the liquid phase. The goal is to use the mass transfer model in order to analyse the influence of mass transfer kinetic on the composition of each phases.



The oxygen mass transfer flow corresponds to the molar flowrate of oxygen that is absorbed (or stripped) in the liquid phase.

Description of the model

The mass transfer model is based on the two-film theory. According to this theory, on either side of the gas-liquid interface, there is a film in which mass transfer is governed by diffusion. Assuming that the mass transfer resistance is mostly localized on the liquid side, the gas phase is considered at the thermodynamic equilibrium with the liquid film, and the mass transfer flow is calculated from the knowledge of mass transfer coefficients ($k_L a$) in the liquid phase.



With:

- C_G, C_L : concentration of gas, liquid (mol/L)
- C_{Gi}, C_{Li} : concentration of gas, liquid at the interface (mol/L)
- δ_L : thickness of the liquid film (m)

Description of the model

The transfer flow for each compound is obtained from the following relation:

$$\Phi = k_L a \, (C_{Li} - C_L)$$

With:

Φ Mass transfer flow (mol/(L.h))

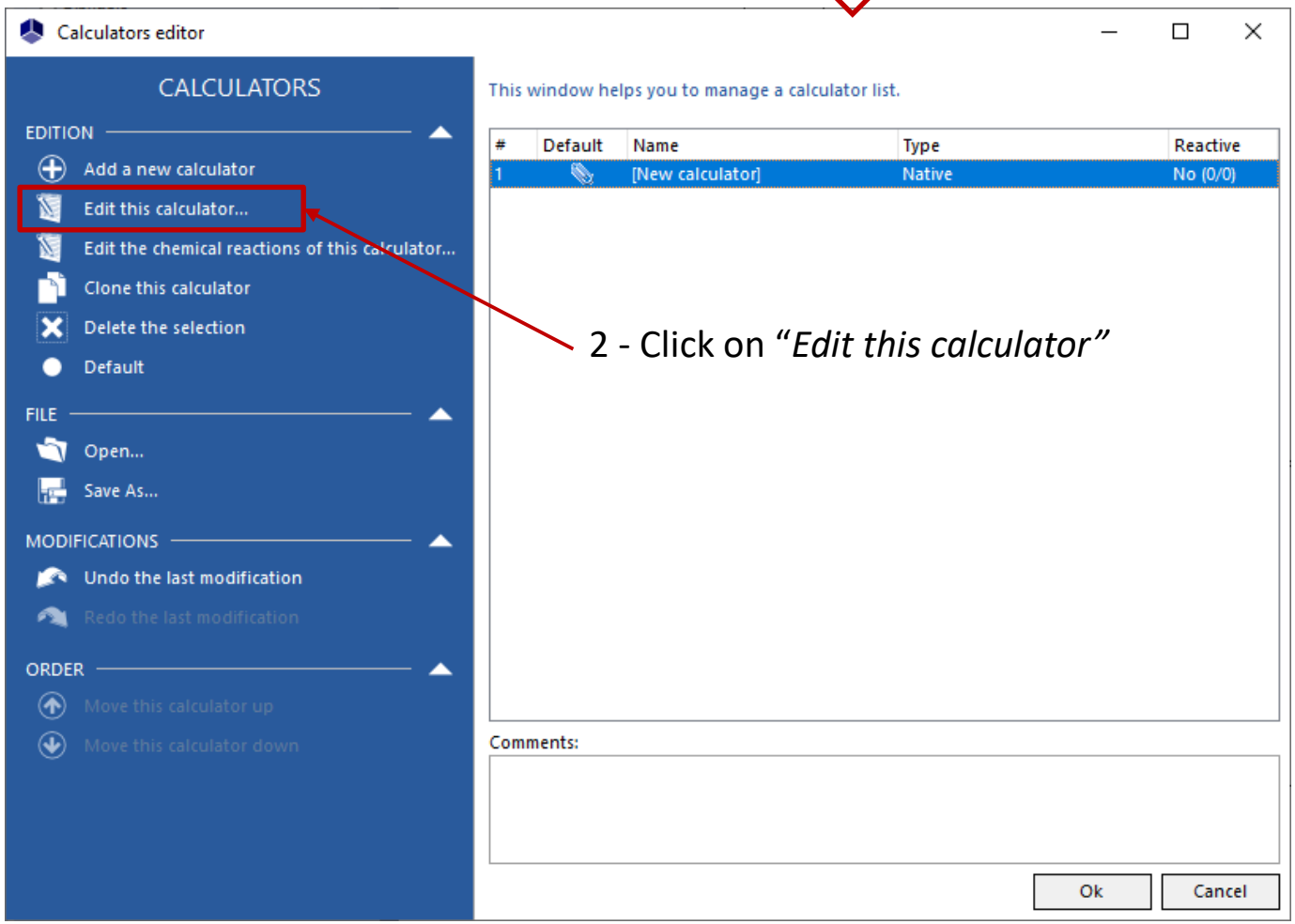
$k_L a$ Volumetric mass transfer coefficient in the liquid phase (h^{-1})

The following configurations will be simulated:

- Configuration 1: with no transfer resistance
- Configuration 2: with transfer resistance and $k_L a$ predicted by the software
- Configuration 3: with transfer resistance and $k_L a$ regressed from experimental data

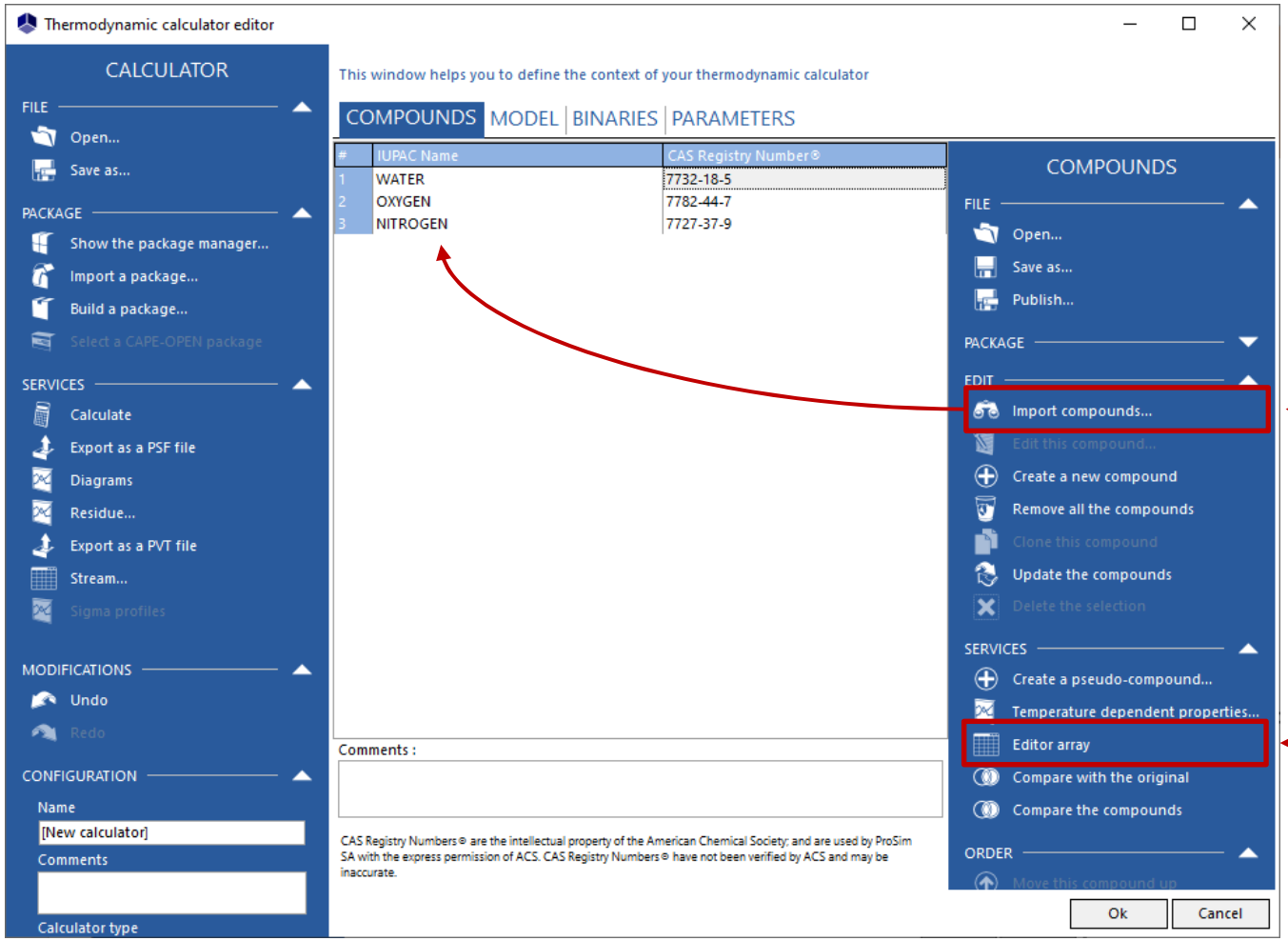
Step 1: Selection of the compounds

1 - Click on the "*Edit the thermodynamics and compounds*" icon to access the "*Calculators editor*" window



Step 1: Selection of the compounds

1 - Import the following compounds: water, oxygen, nitrogen

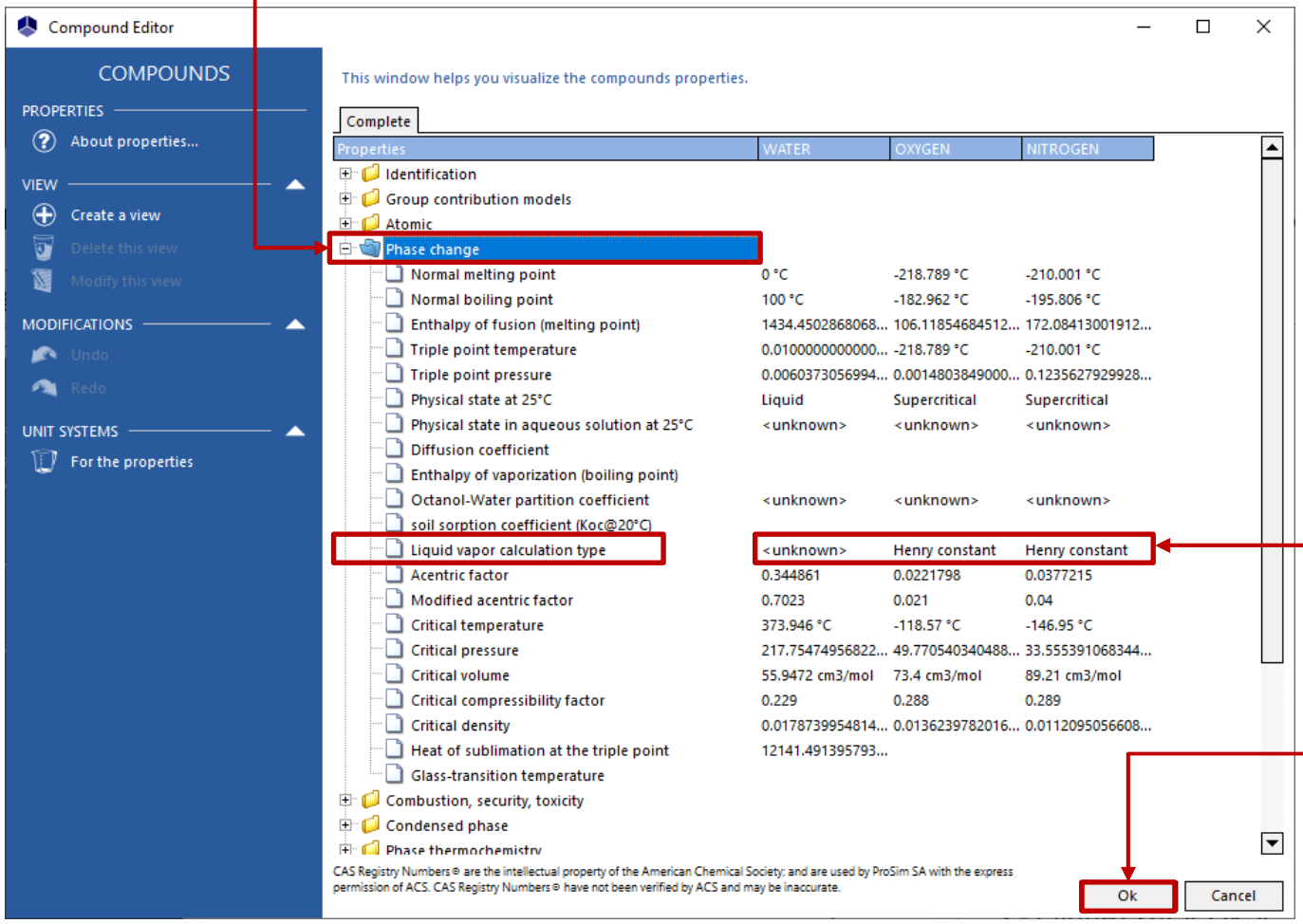


2 - Click here to edit the physical properties

For more information about compounds selection, please refer to *"Getting started with Simulis Thermodynamics - Use case 1"*

Step 1: Selection of the compounds

1 - The Henry's law is used to compute the solubility of oxygen and nitrogen in water. It requires to modify the field « *Liquid vapor calculation type* » in the « *Phase change* » category

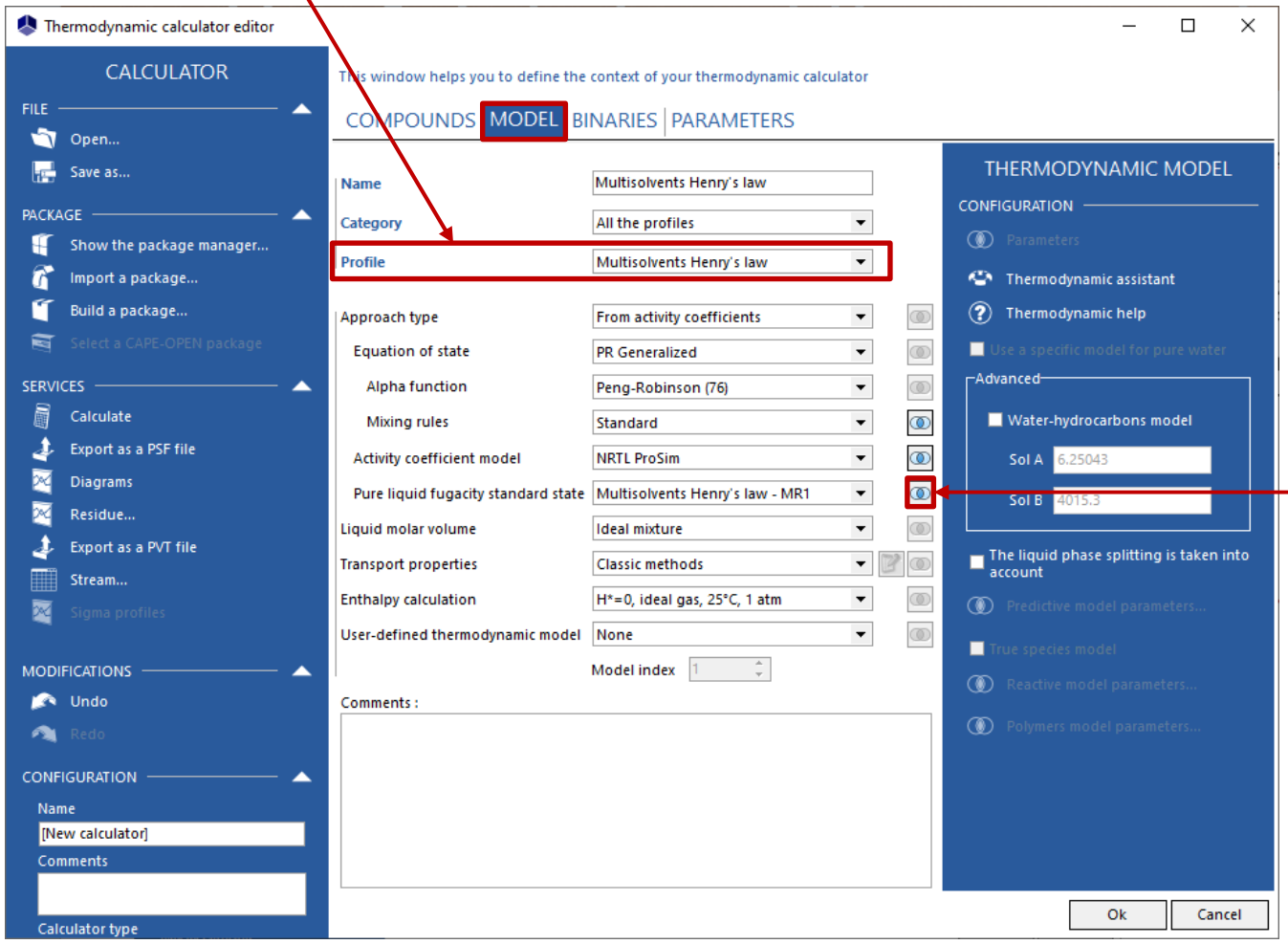


2 - For oxygen and nitrogen, select « *Henry* constant »

3 - Click on « *OK* »

Step 1: Selection of the compounds

1 - In the « *Model* » tab, select the « *Multisolvents Henry's law* » thermodynamic profile

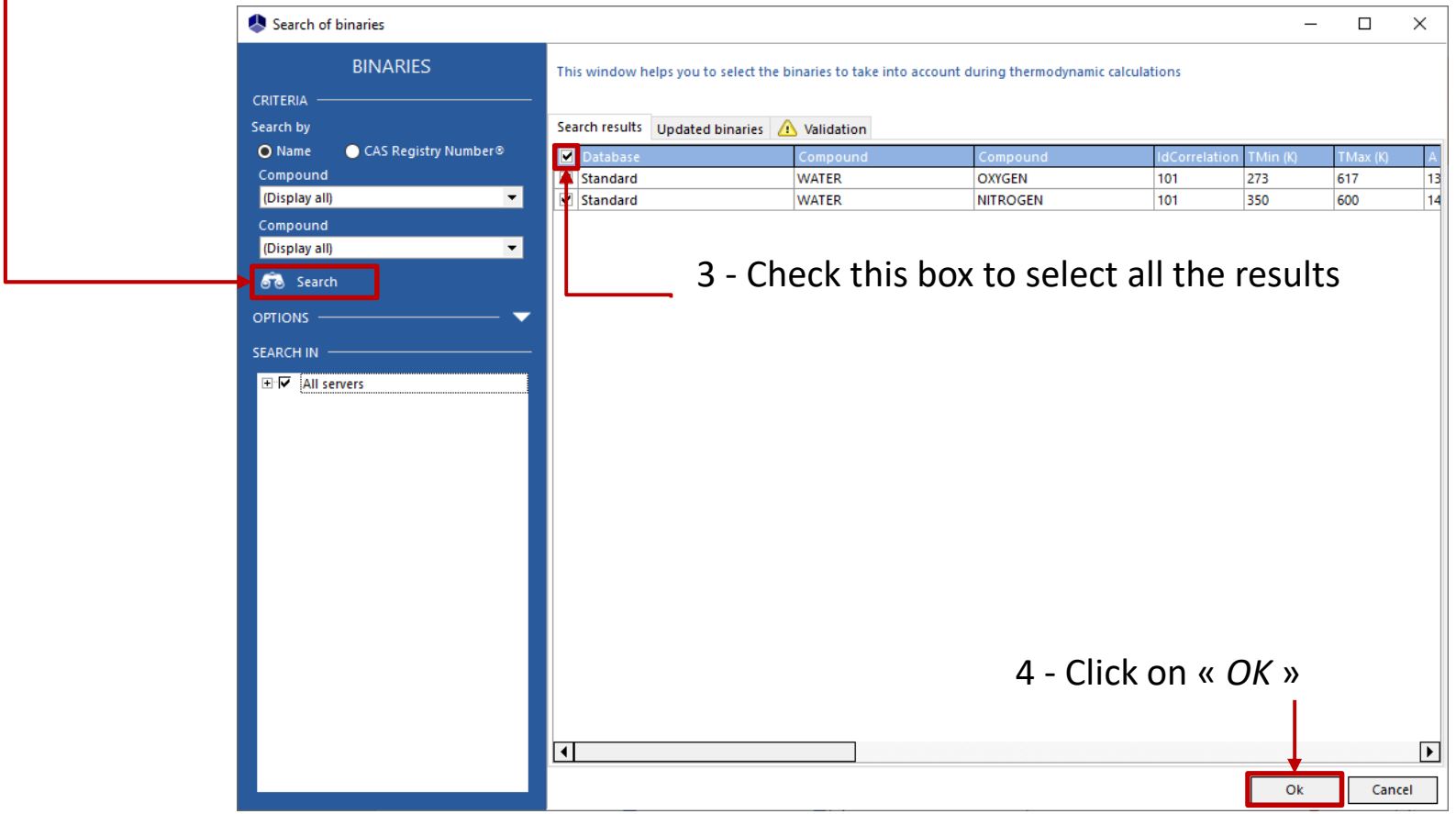


2 - Click here to access the parameters of the Henry's law

Step 1: Selection of the compounds

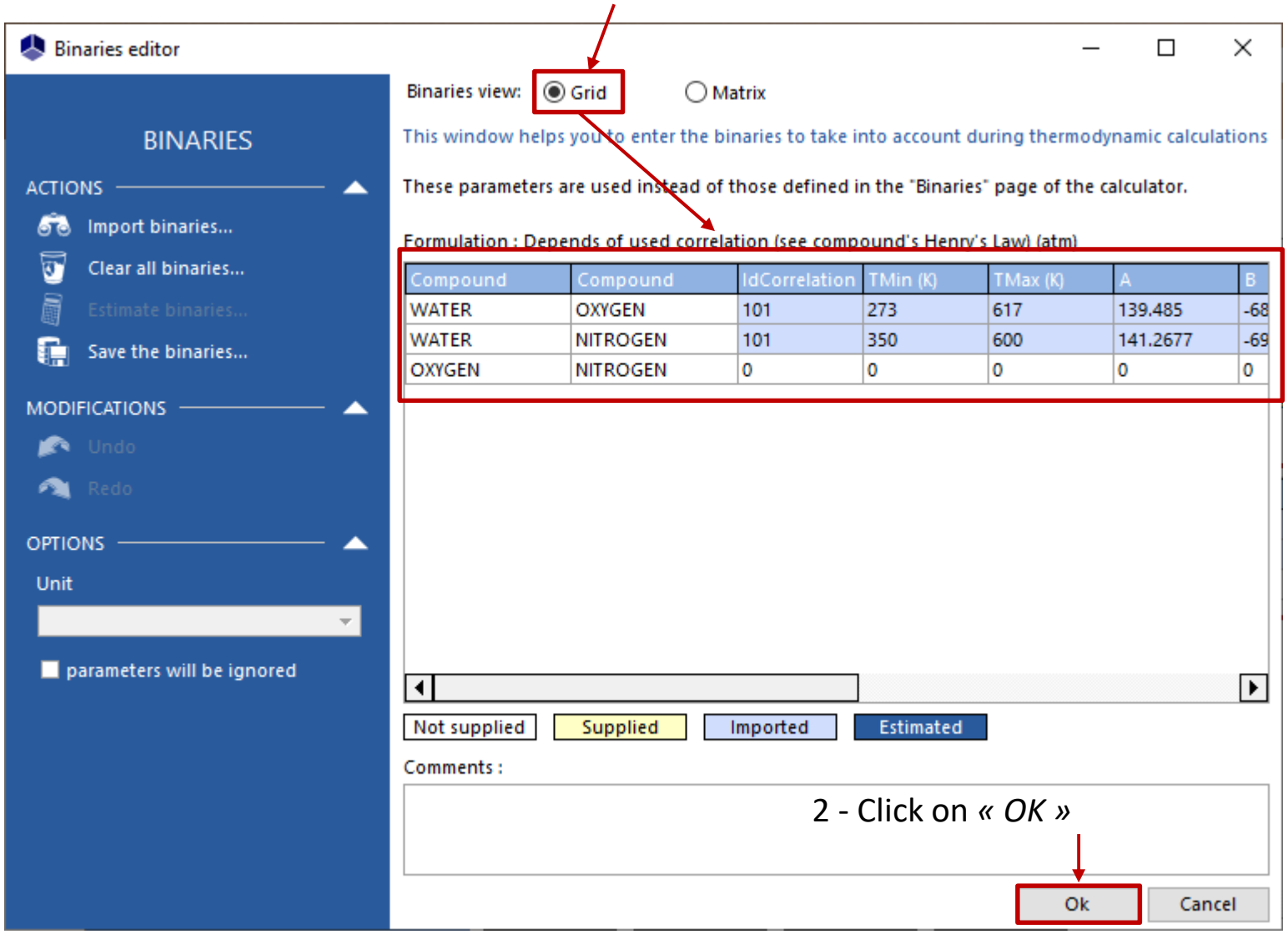
1 - Click on « *Import binaries* »

2 - Click on « *Search* »



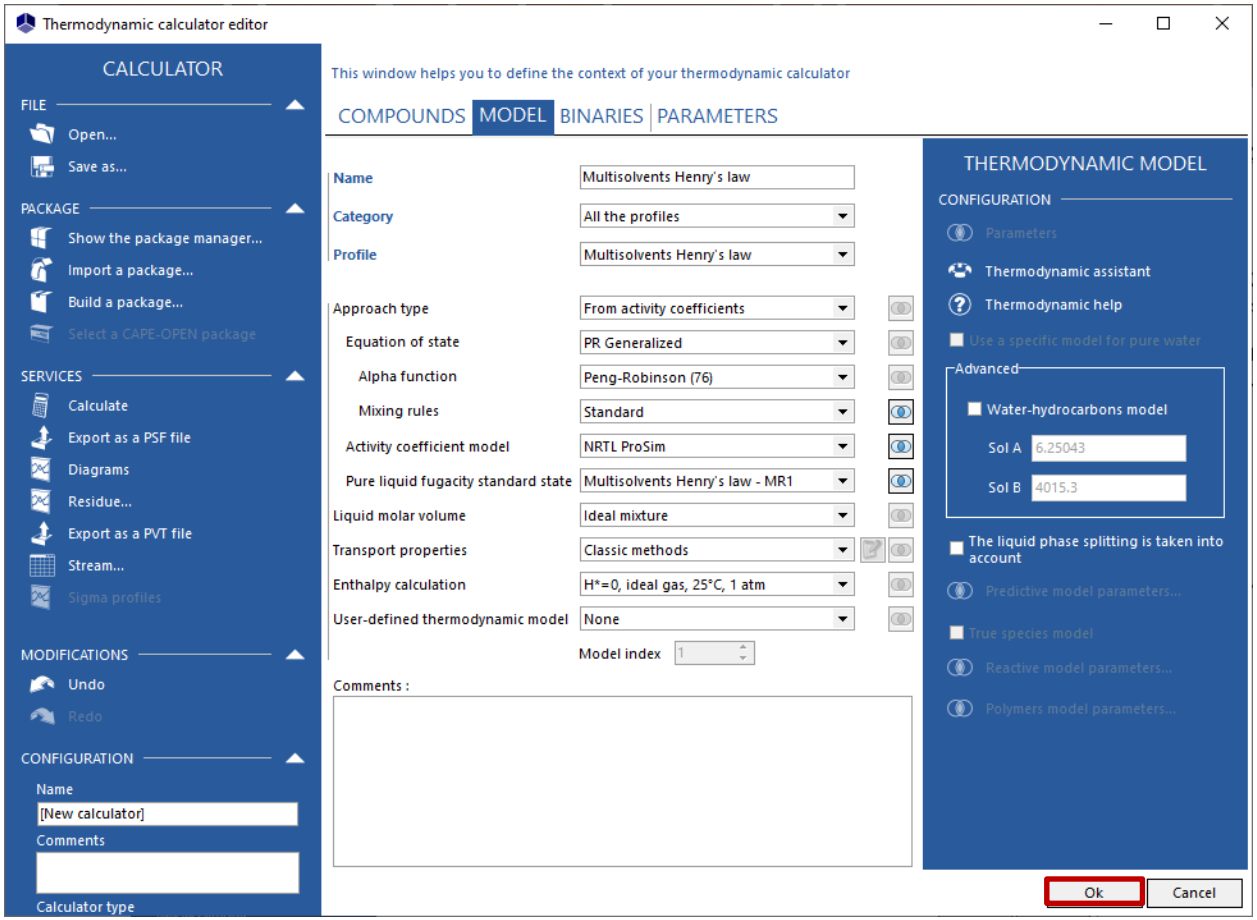
Step 1: Selection of the compounds

1 - The parameters of Henry's law are displayed here (binaries view: grid)



Step 1: Selection of the compounds

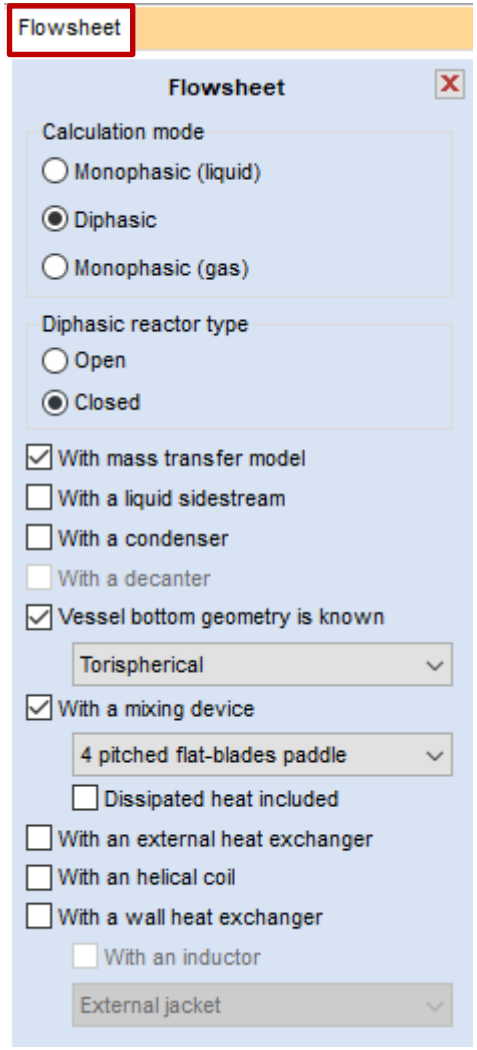
The configuration of the « *Thermodynamic calculator* » is now over. Click on « *OK* » to get back to the main interface.



For more information about compounds selection, please refer to *"Getting started with Simulis Thermodynamics - Use case 1"*

Step 2: configuration of the reactor topology and the mass transfer model

Back to the main interface, specify the reactor topology in the "*Flowsheet*" tab



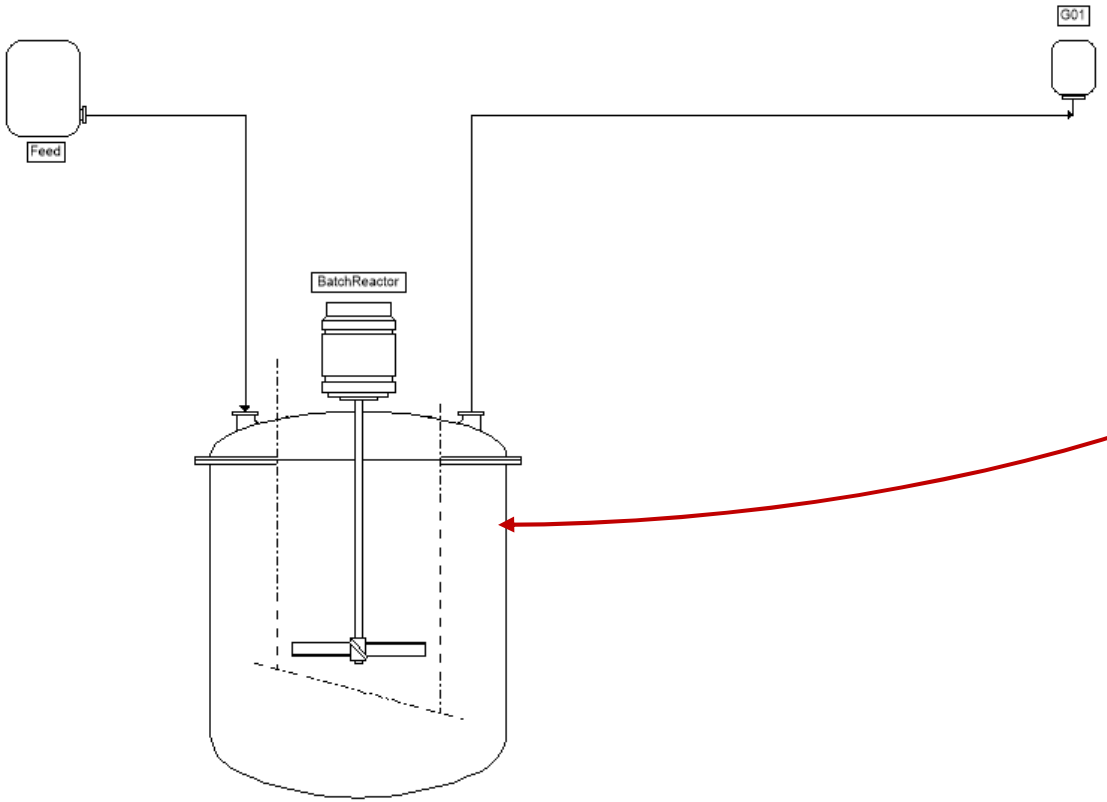
1 - Check the following options from the control panel:

- Calculation mode: diphasic
- Diphasic reactor type: closed
- With mass transfer model
- The vessel bottom geometry is "*Torispherical*"
- The mixing device is a "*4 pitched flat-blades paddle*"

Once the mass transfer model is configured, checking/unchecking the "*With mass transfer model*" option enables to switch between the mass transfer model and the equilibrium model (which is the default option)

Step 2: configuration of the reactor topology and the mass transfer model

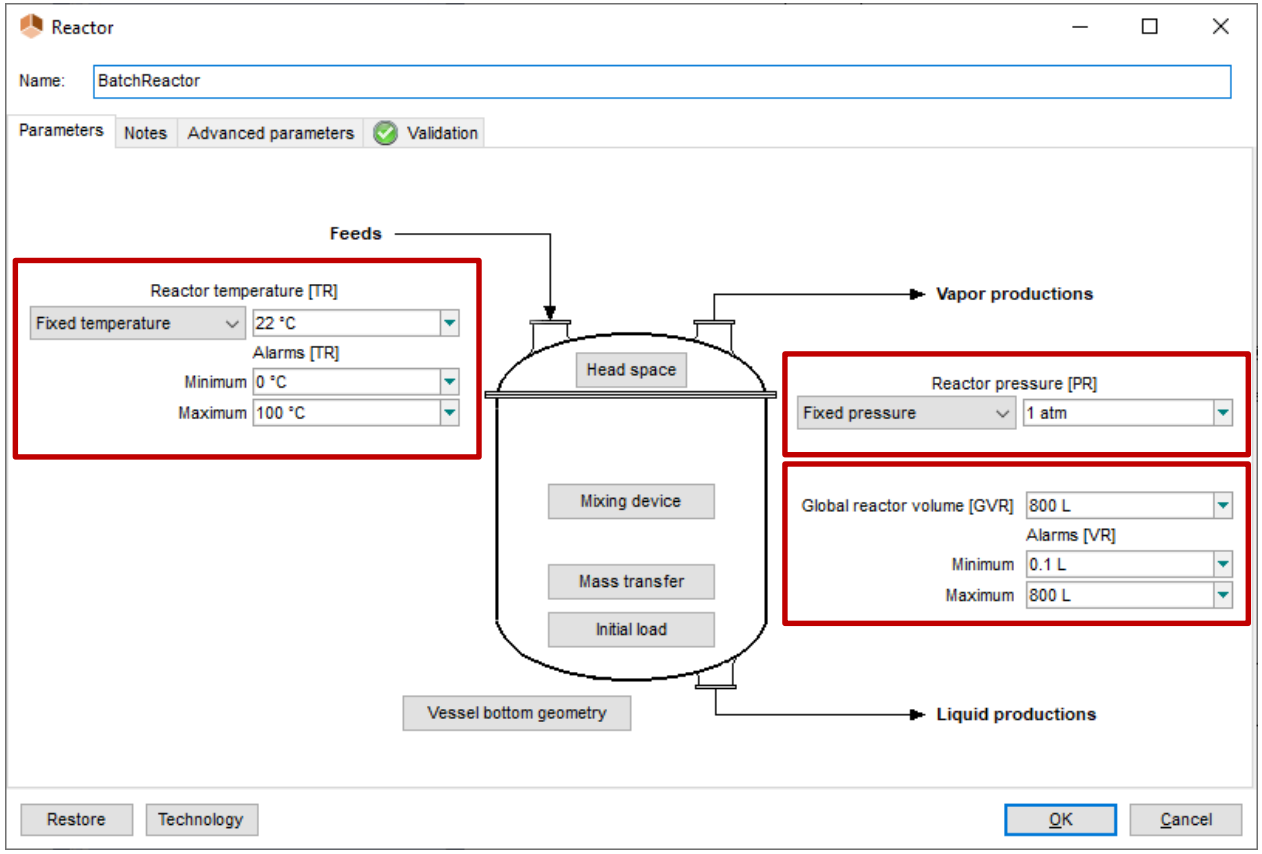
Back to the main interface, specify the reactor topology in the "*Flowsheet*" tab



2 - Double click on the reactor to provide the initial conditions and the global parameters

Step 2: configuration of the reactor topology and the mass transfer model

Specify the following parameters in the reactor configuration window:



1 - The initial conditions:

- T = 22°C
- P = 1 atm
- V = 800 L

2 - The alarms:

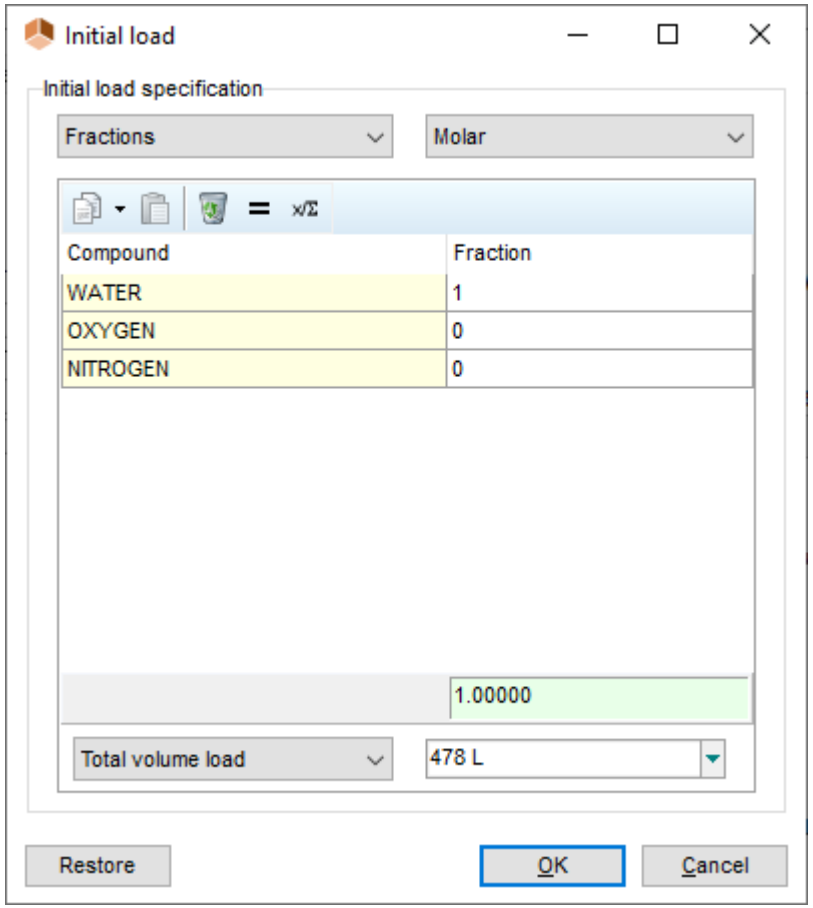
- Temperature
  Minimum: 0°C
  Maximum: 100°C
- Volume
  Minimum: 0,1 L
  Maximum: 800 L

Step 2: configuration of the reactor topology and the mass transfer model

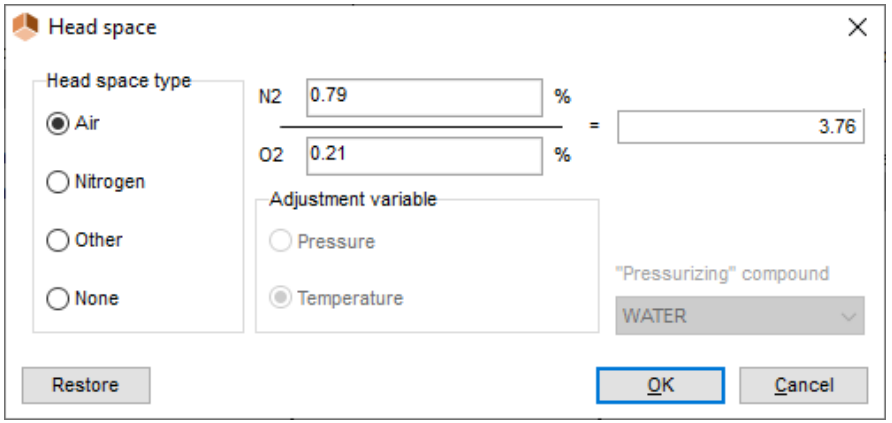
Specify the following parameters in the reactor configuration window:

3 - The initial load:

- 478 L of water — Initial load



- The head space is composed of air — Head space

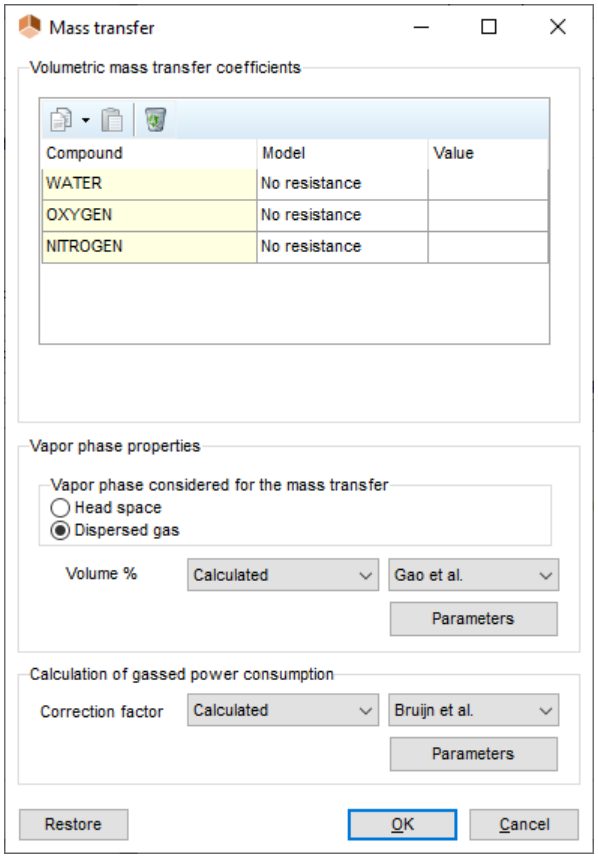


Step 2: configuration of the reactor topology and the mass transfer model

Specify the following parameters in the reactor configuration window:

4 - The mass transfer model:

Mass transfer



Configuration of the $k_L a$ (detailed in the step 4 of this document)

Vapor phase considered for the mass transfer

- Select "*Dispersed gas*"
- Select the "*Calculated*" option and the default correlation for the calculation of the dispersed gas volume %

Calculation of gassed power consumption

- Select the "*Calculated*" option and the default correlation

Press « *F1* » in order to access the help file including technical and practical details related to this model

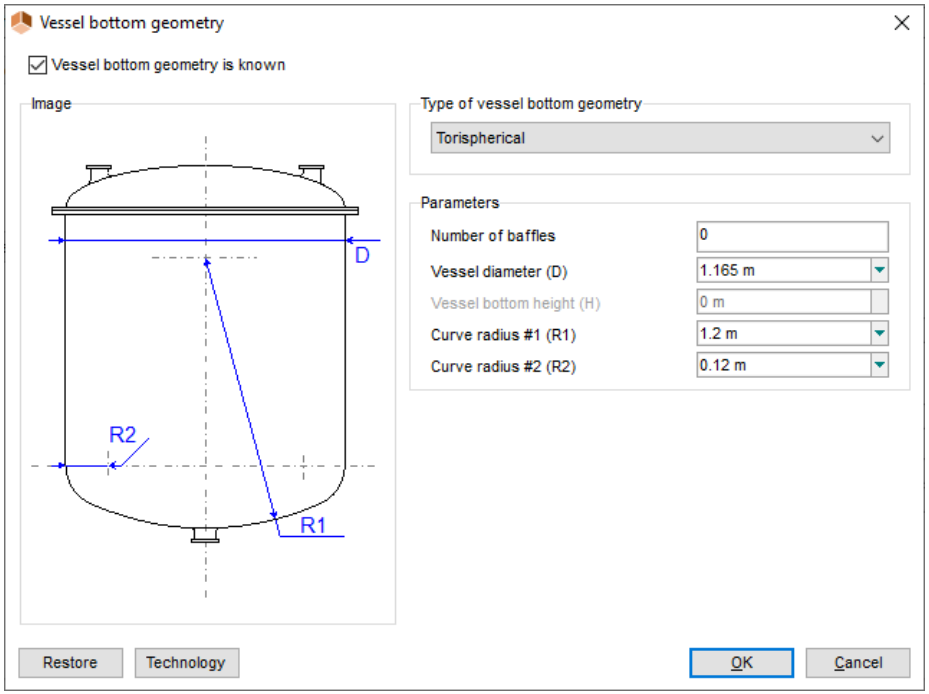
Step 2: configuration of the reactor topology and the mass transfer model

Specify the following parameters in the reactor configuration window:

5 - The geometric characteristics of the equipment:

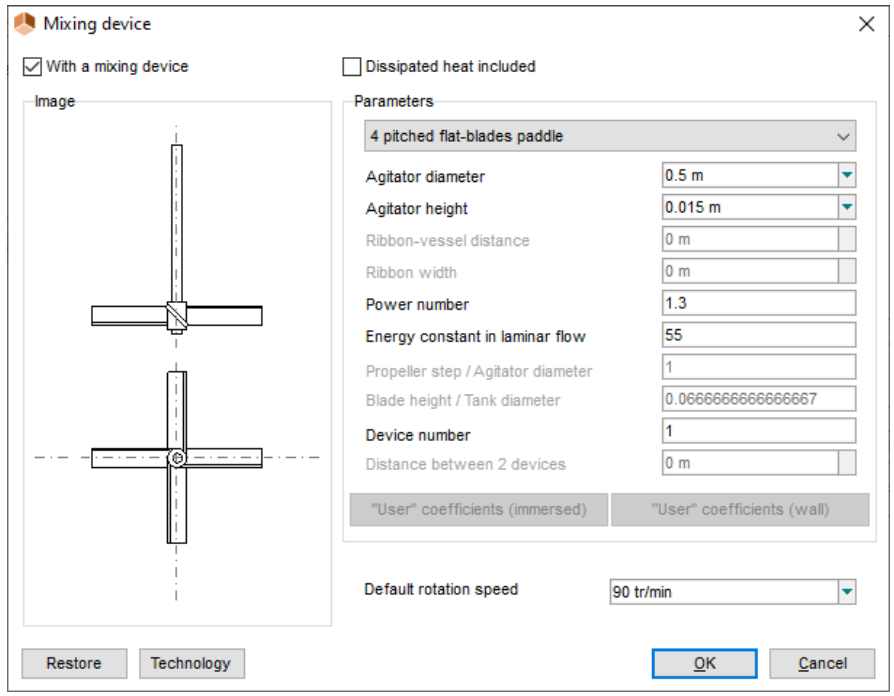
- Vessel bottom geometry

Vessel bottom geometry



- Mixing device

Mixing device



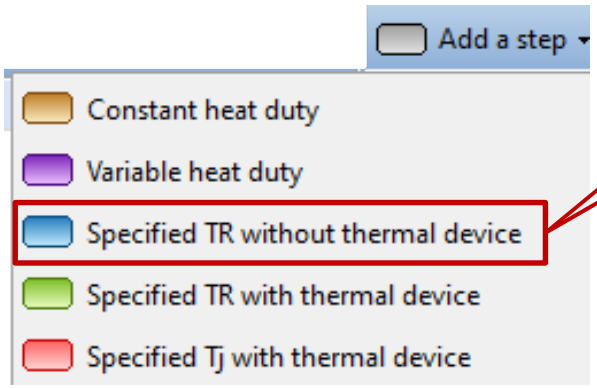
Step 3: description of the operating mode

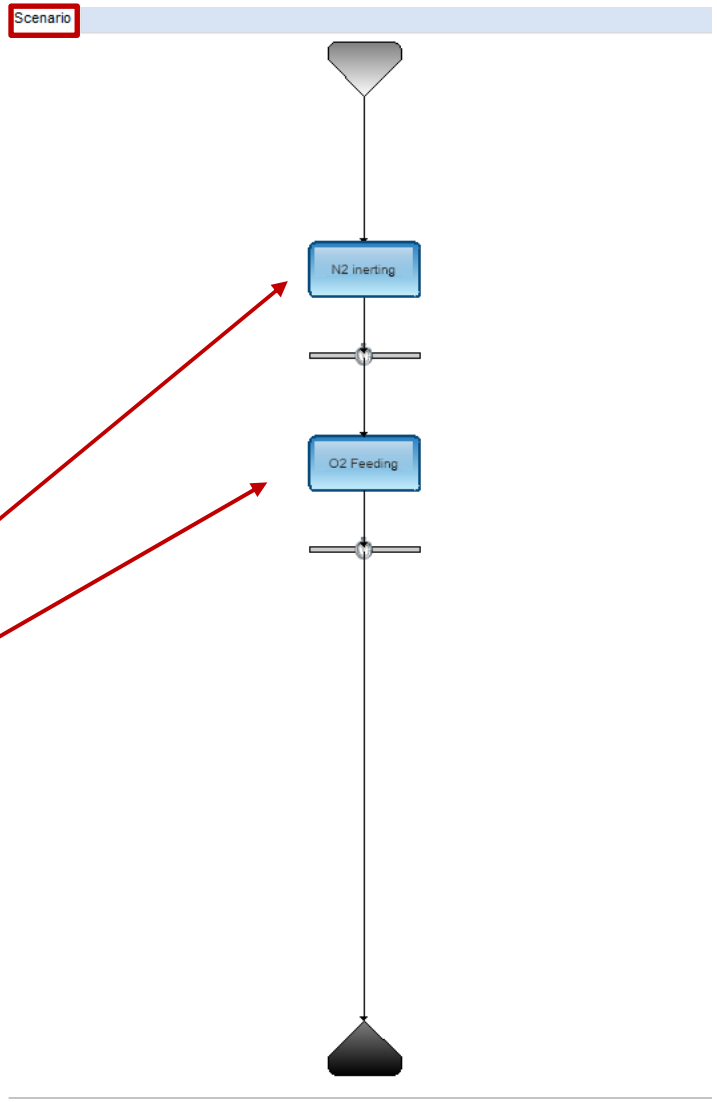
Back to the main interface, specify the operating mode in the "*Scenario*" tab

The operating mode is made of 2 isothermal operating steps:

- *One step with a nitrogen feed that enables to strip the oxygen initially present in the liquid phase.*
- *One step with an oxygen feed that enables to analyse the absorption of oxygen in the liquid phase.*

1 - Add two isothermal steps and connect them together



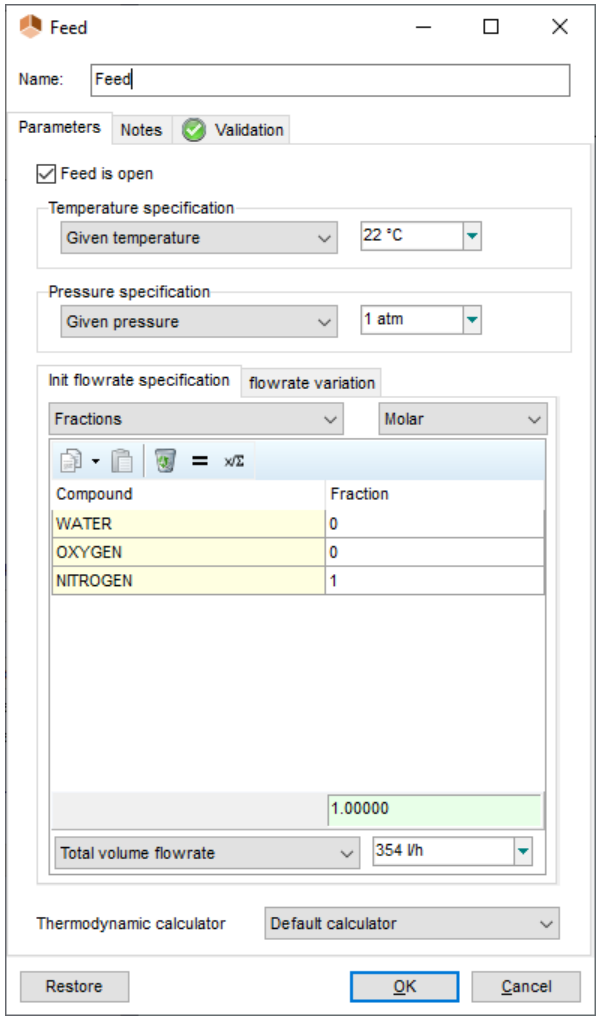


Step 3: description of the operating mode

Back to the main interface, specify the operating mode in the "*Scenario*" tab

2 - Specify the operating parameters of the 1st step

- Step name: N_2 inerting
- Feed:
  - Pure nitrogen
  - T = 22 °C
  - P = 1 atm
  - Flowrate = 354 l/h

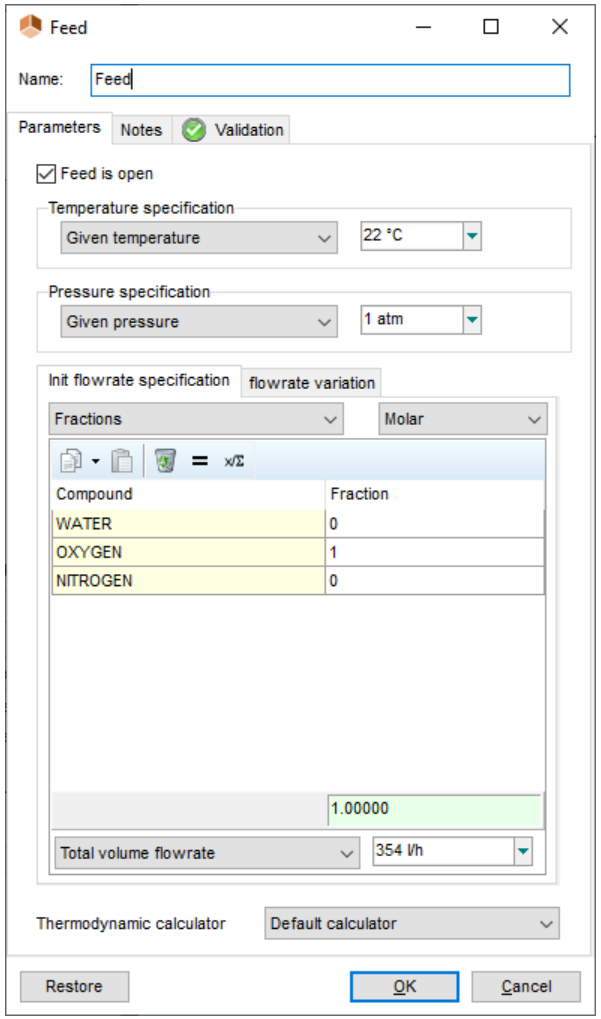


Step 3: description of the operating mode

Back to the main interface, specify the operating mode in the "*Scenario*" tab

3 - Specify the operating parameters of the 2nd step

- Step name: O_2 Feeding
- Feed:
  - Pure oxygen
  - T = 22 °C
  - P = 1 atm
  - Flowrate = 354 l/h

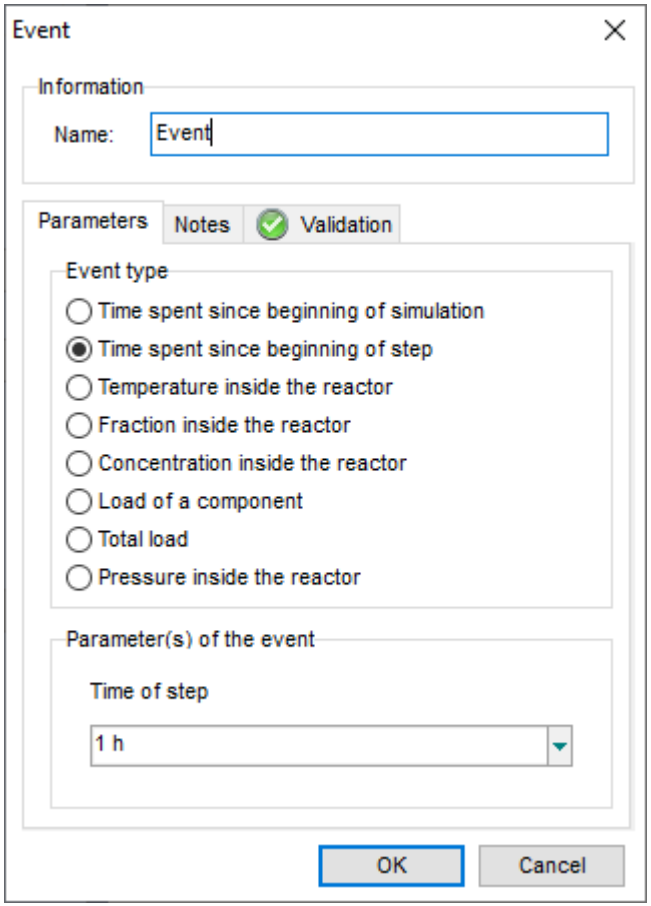


Step 3: description of the operating mode

Back to the main interface, specify the operating mode in the "*Scenario*" tab

4 - Specify the end events of the steps

- For <u>each</u> step, the end event corresponds to a time of 1h spent since the beginning of the step



Step 3: description of the operating mode

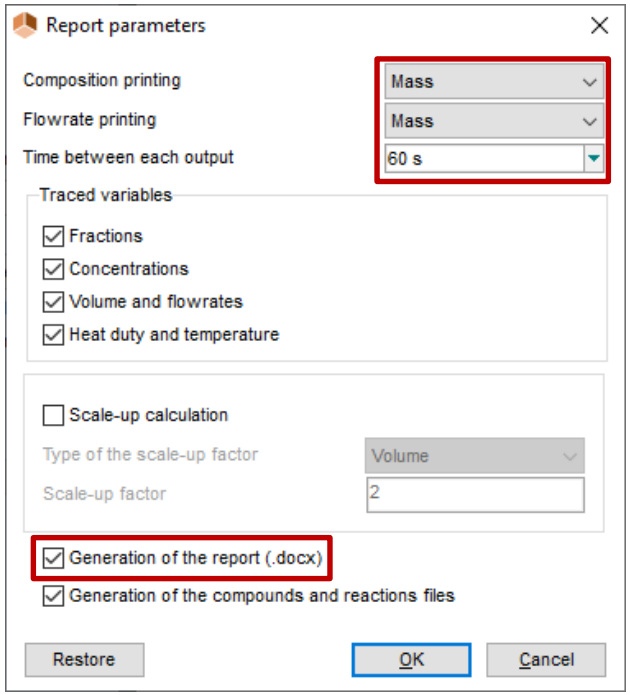
Back to the main interface, specify a unit system that is consistent with the experimental data

5 - Modify the "*Unit system for report*"

- Time: h
- Temperature: °C
- Pressure: atm
- Mass concentration: mg/L
- ... Feel free to customize the unit systems!

6 - Modify the "*Report parameters*"

- Composition and flowrate printing: mass
- Time between each output: 60s
- Generation of the report (.docx)



Step 4: Simulation of different configurations

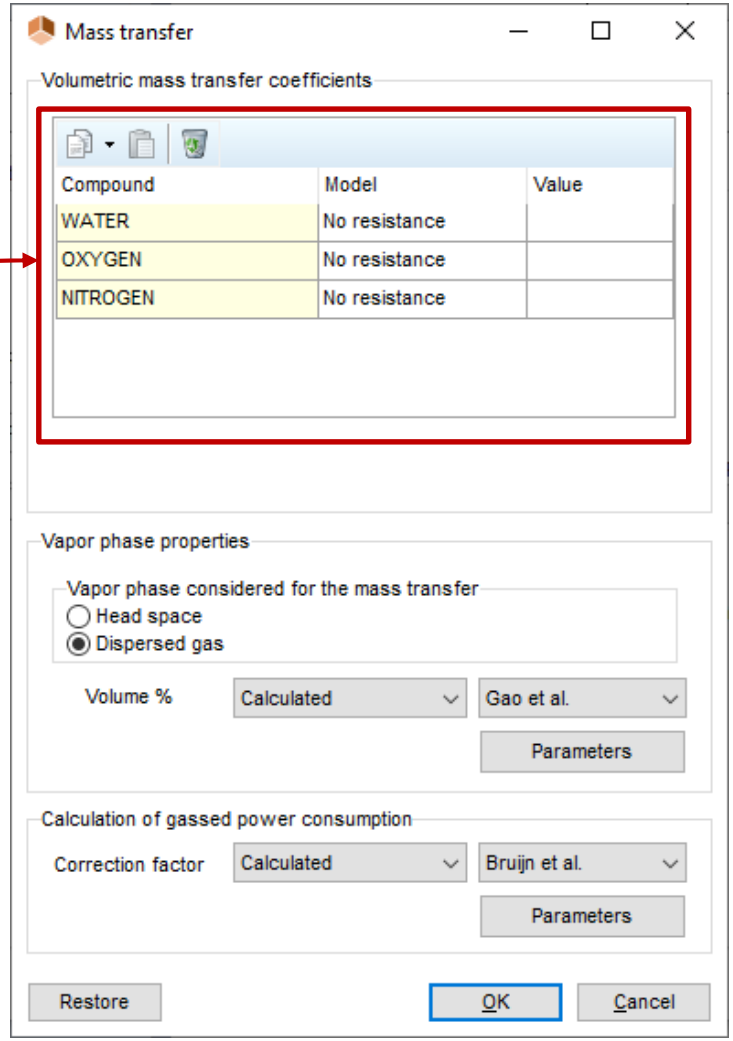
The three following configurations can now be simulated:

- Configuration 1: with no transfer resistance
- Configuration 2: with transfer resistance and the $k_L a$ predicted by the software
- Configuration 3: with transfer resistance and the $k_L a$ regressed from experimental data

Step 4: Simulation of different configurations

Configuration 1: with no transfer resistance

1 - Click on the "*Mass transfer*" button in the "*Flowsheet*" *tab*



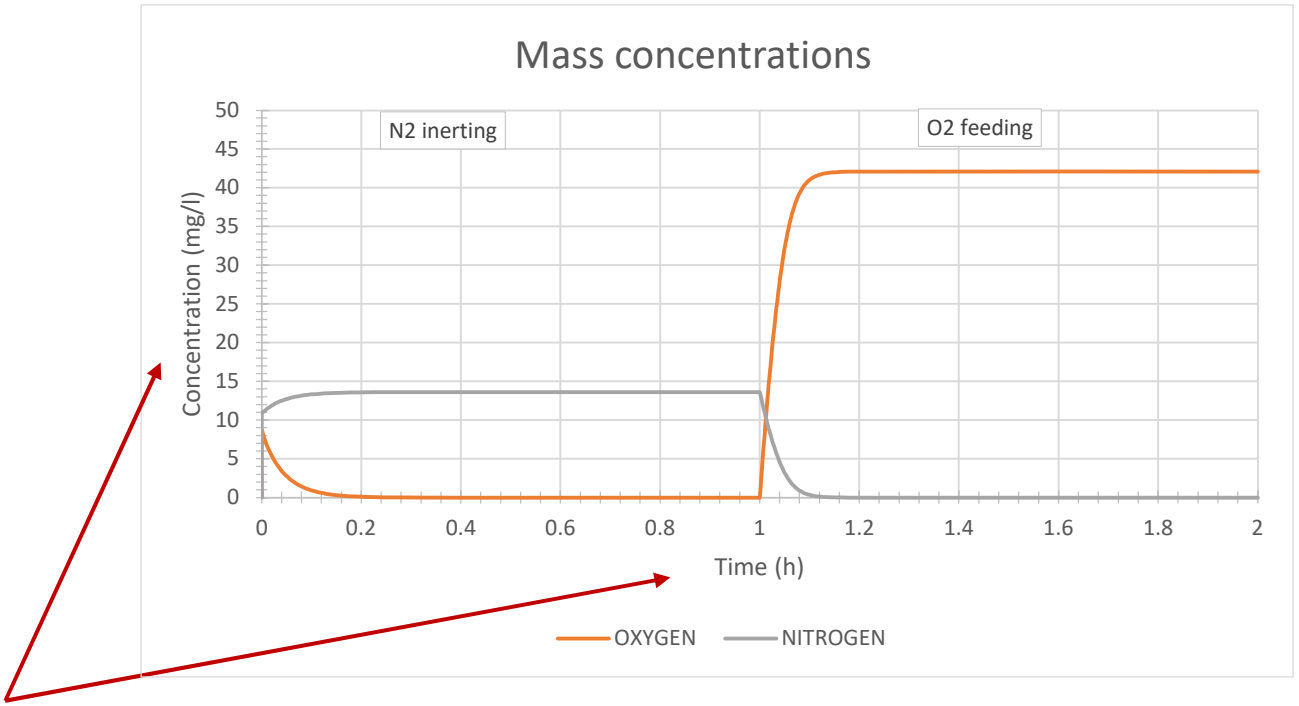
2 - Select the "*No resistance*" option for all compounds

3 - Save the file and run the simulation

Step 4: Simulation of different configurations

Configuration 1: with no transfer resistance

4 - Once the simulation is over, open the Word® report and access the profiles corresponding to the mass concentrations in the liquid phase

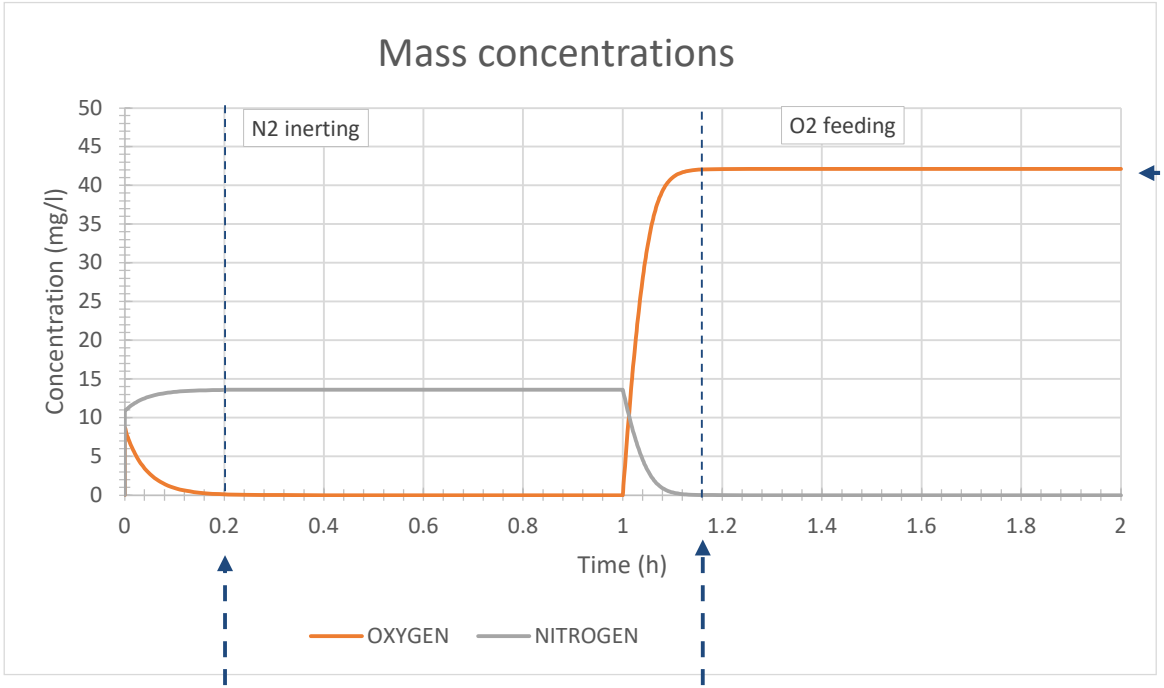


5 - You can adjust the graph scales in order to properly display the concentration profiles of nitrogen and oxygen

Step 4: Simulation of different configurations

Configuration 1: with no transfer resistance

6 - Finally, you can analyse the results:



Saturation concentration of oxygen in water: 42 mg/L (for P_{O2} = 1 atm and T = 22°C)

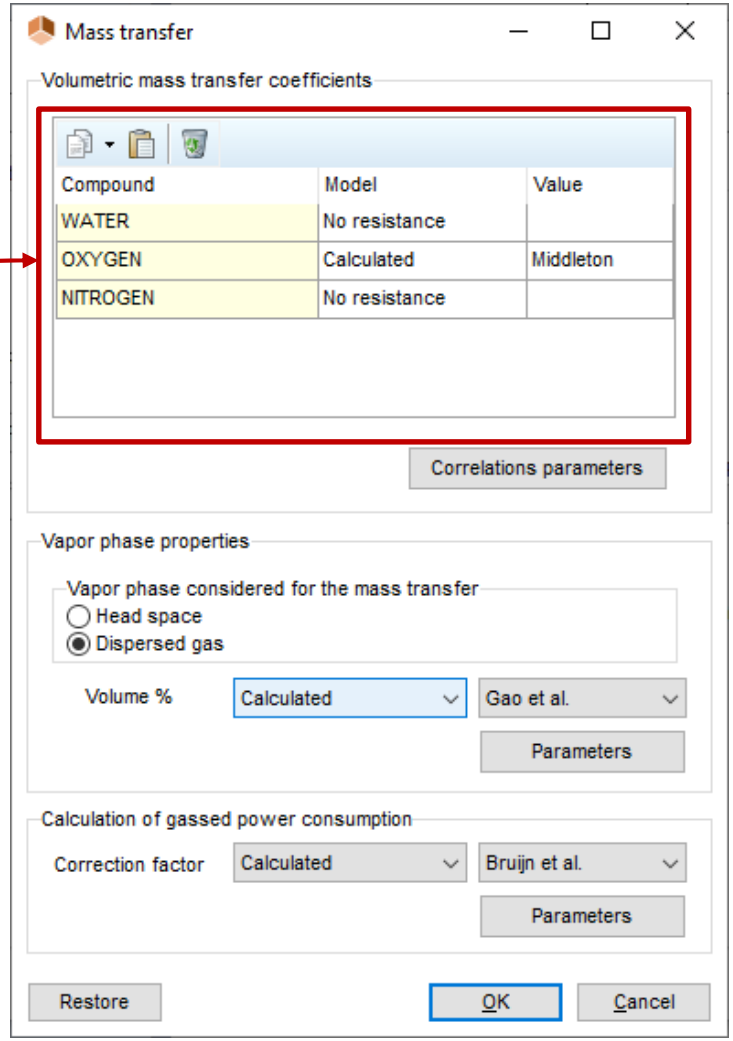
Required time to strip all the oxygen from the liquid phase

Required time to reach the saturation concentration of oxygen in water

Step 4: Simulation of different configurations

Configuration 2: with transfer resistance and the $k_L a$ predicted by the software

1 - Click on the "*Mass transfer*" button in the "*Flowsheet*" *tab*



2 - Select the "*Calculated*" option for the oxygen (and keep the *Middleton* correlation suggested by default)

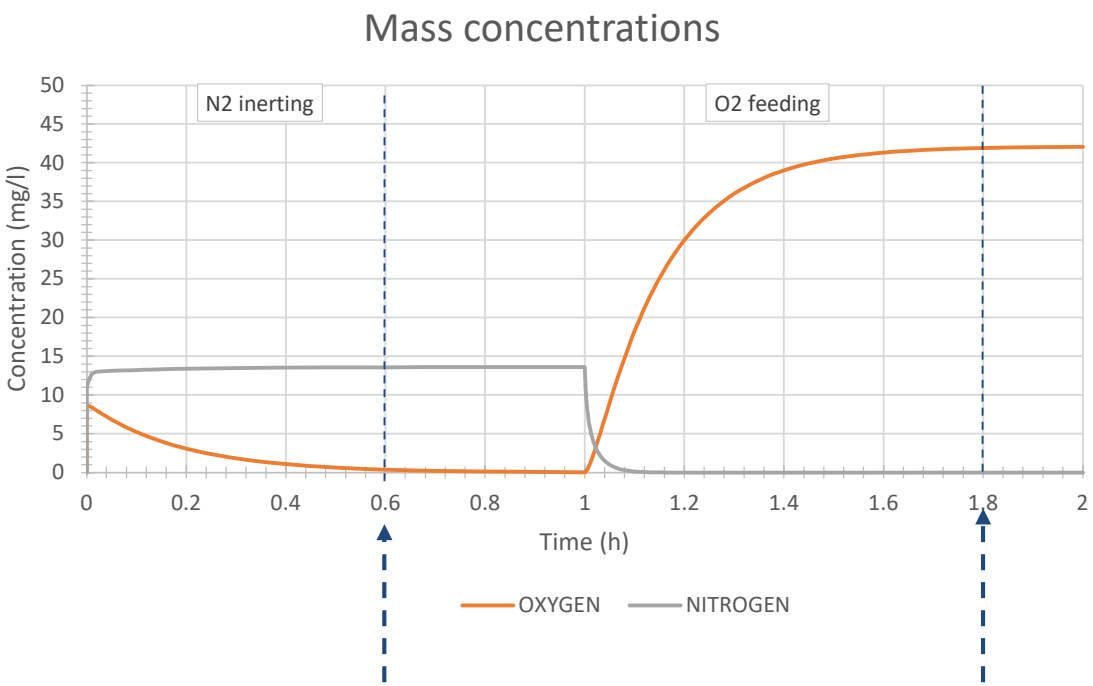
3 - Save the file and run the simulation

Step 4: Simulation of different configurations

Configuration 2: with transfer resistance and the k_La predicted by the software

4 - For these operating conditions, the predicted value for the k_La of oxygen equals **6.8 h^{-1}**.

5 - Analyse the impact of mass transfer resistance on the results...



Saturation concentration of oxygen in water: 42 mg/L (for P_{O2} = 1 atm and T = 22°C)

Required time to strip all the oxygen from the liquid phase

Required time to reach the saturation concentration of oxygen in water

Step 4: Simulation of different configurations

Configuration 3: with transfer resistance and the $k_L a$ regressed from experimental data

The concentration profile of oxygen absorbed in the liquid phase was measured by [SAR02]:

Time (h)	$C_L(O_2)$ (mg/L)
1.01	1.5
1.04	9.6
1.07	15.4
1.11	22.6
1.14	26.9
1.18	30.3
1.22	33.3
1.25	35.2
1.29	37
1.34	38.7
1.40	40.0
1.45	40.6
1.50	41.2

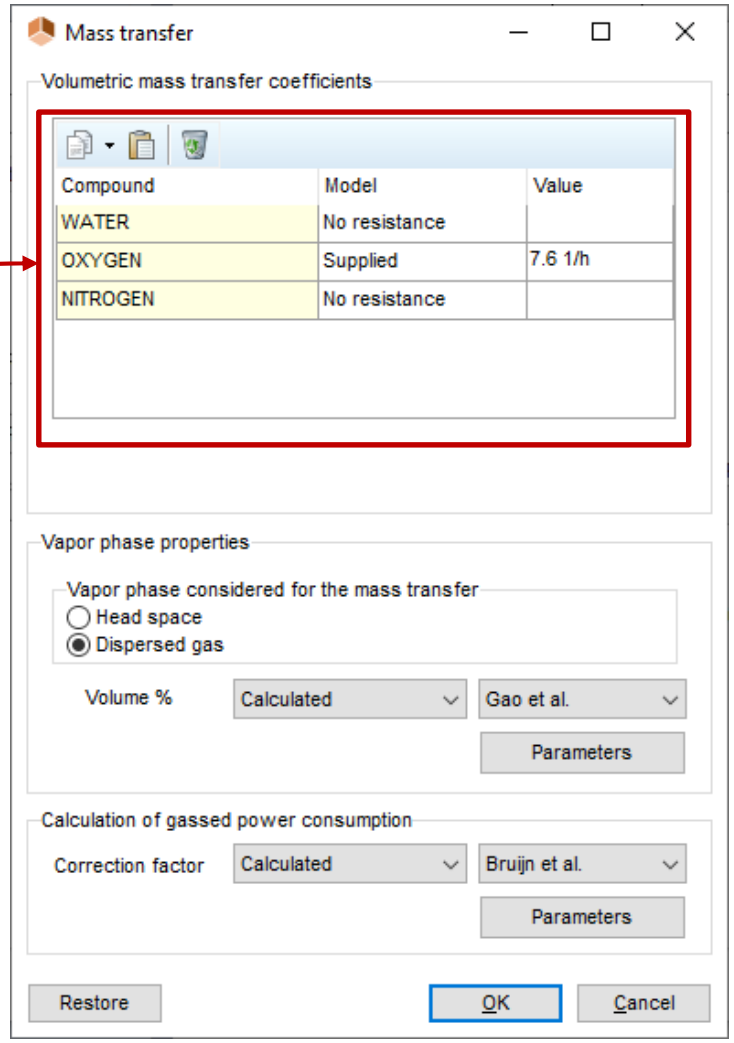
→ A case study was conducted in order to identify the $k_L a$ of oxygen. A value of **7.6 h^{-1}** was obtained (compared to **6.8 h^{-1}** predicted by the model)

[SAR02] : SARDEING R., « Hydrodynamique induite par un oxygénateur de surface : influence du design des agitateurs sur la qualité de dispersion », thèse INPT (2002)

Step 4: Simulation of different configurations

Configuration 3: with transfer resistance and the $k_L a$ regressed from experimental data

1 - Click on the "*Mass transfer*" button in the "*Flowsheet*" tab



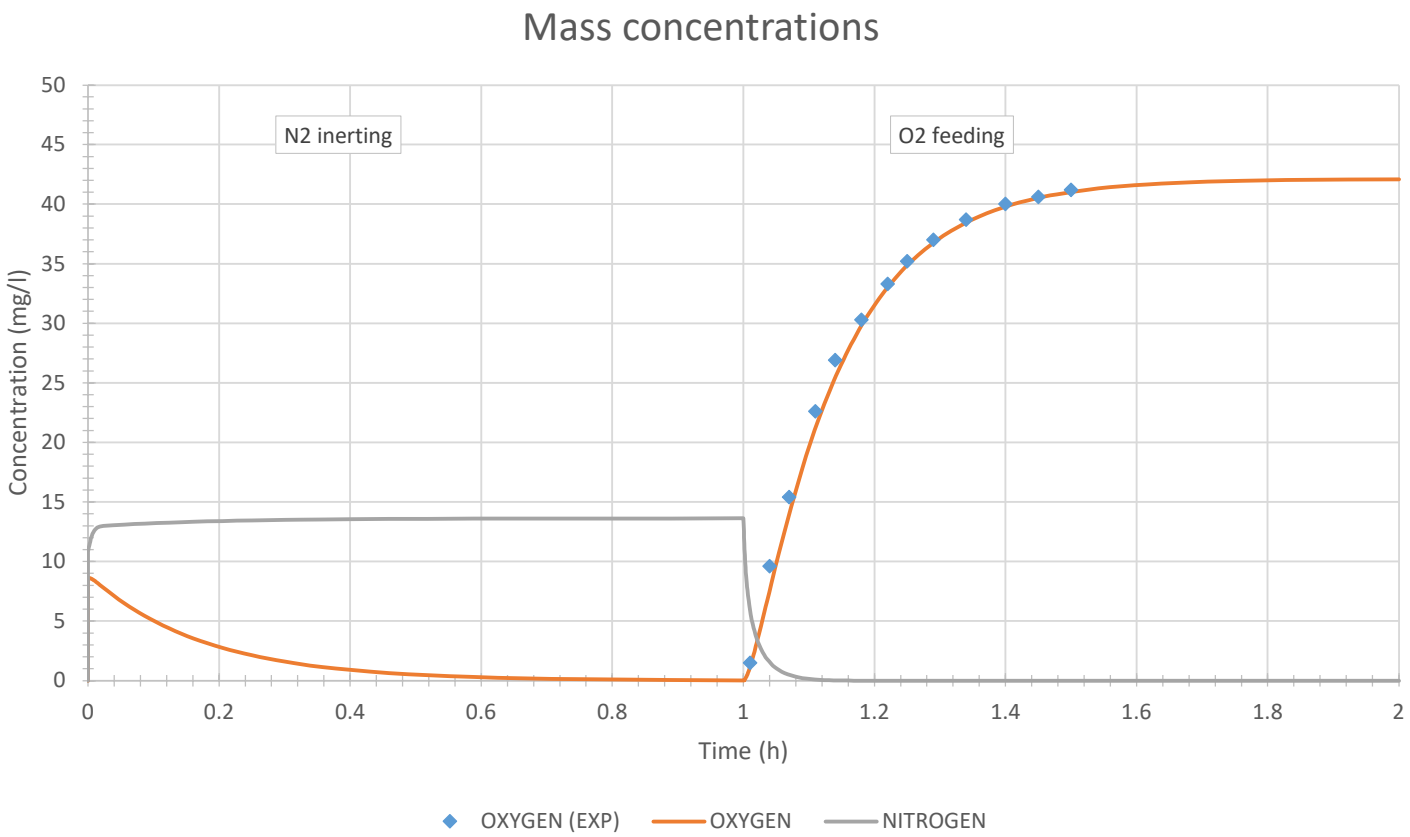
2 - Select the "*Supplied*" option for the oxygen and specify a $k_L a$ value of **7,6 h^{-1}**

3 - Save the file and run the simulation

Step 4: Simulation of different configurations

Configuration 3: with transfer resistance and the $k_L a$ regressed from experimental data

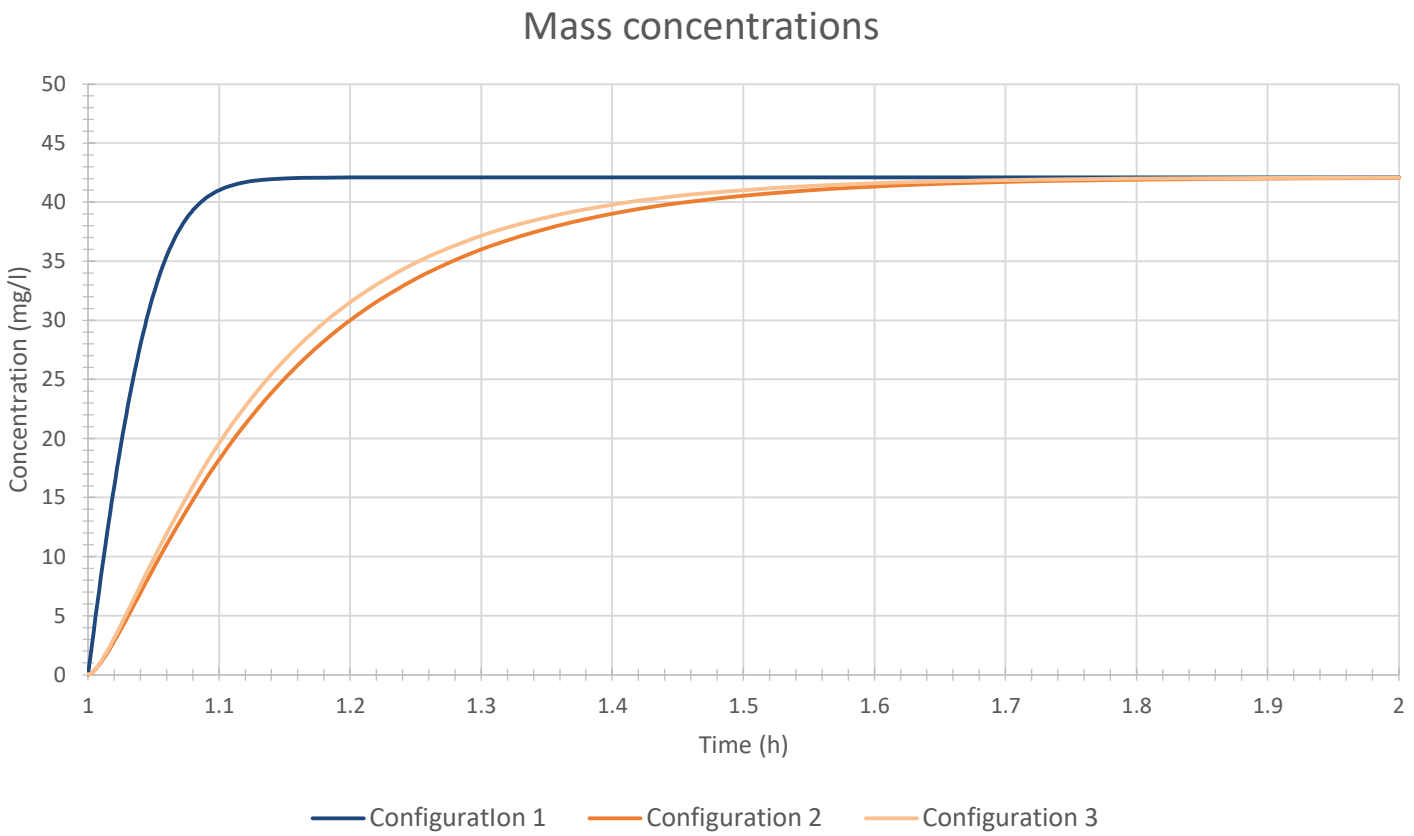
4 - Compare the theoretical results (orange curve) with the experimental data (blue dots)...



Step 4: Simulation of different configurations

To go further...

- Comparison of the profiles obtained during the oxygen absorption step, for the 3 configurations:



Step 4: Simulation of different configurations

To go further...

- Analyse the other profiles
  - Composition profiles of the gas and the liquid film
  - Mass transfer coefficients
  - Transfer flows
  - Heat duties
  - ...
- Add oxidation reactions with oxygen and analyse the influence of mass transfer resistance on the reactions conversion yields
- Analyse the influence of the technology, the geometric parameters and the operating conditions on the mass transfer kinetics.

ProSim

Software & Services In Process Simulation

ProSim SA
51, rue Ampère
Immeuble Stratège A
F-31670 Labège
France

☎: +33 (0) 5 62 88 24 30

www.prosim.net

info@prosim.net

ProSim, Inc.
325 Chestnut Street, Suite 800
Philadelphia, PA 19106
U.S.A.

☎: +1 215 600 3759