

# Getting started with BatchReactor®

## Use Case 3: Simulation of mass transfer resistance

Software & Services In Process Simulation

*We guide You to efficiency*







ProSim

# Introduction

When simulating a vapor-liquid reactor with BatchReactor<sup>®</sup>, 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<sup>®</sup>.

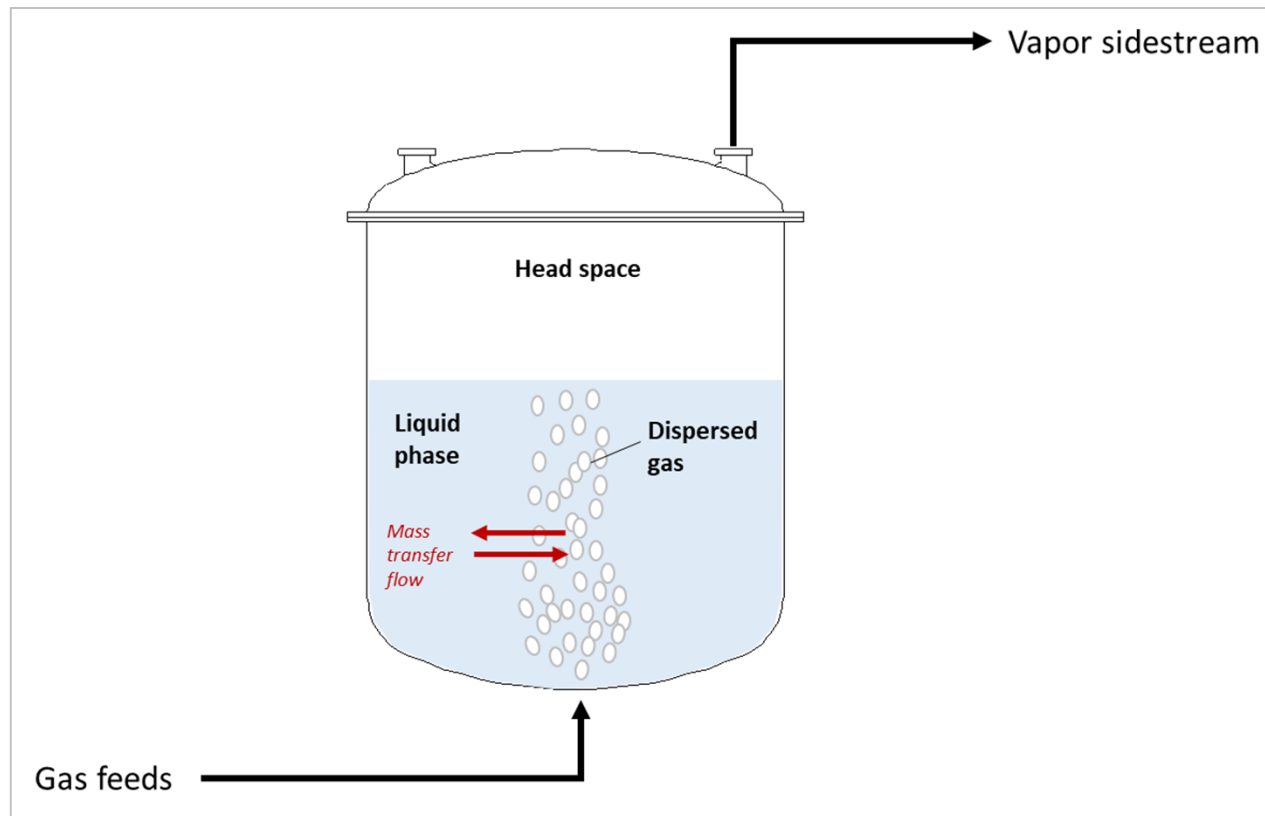
Here are the steps to follow:

-  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<sup>®</sup> - Use Case 1”

# Description of the model

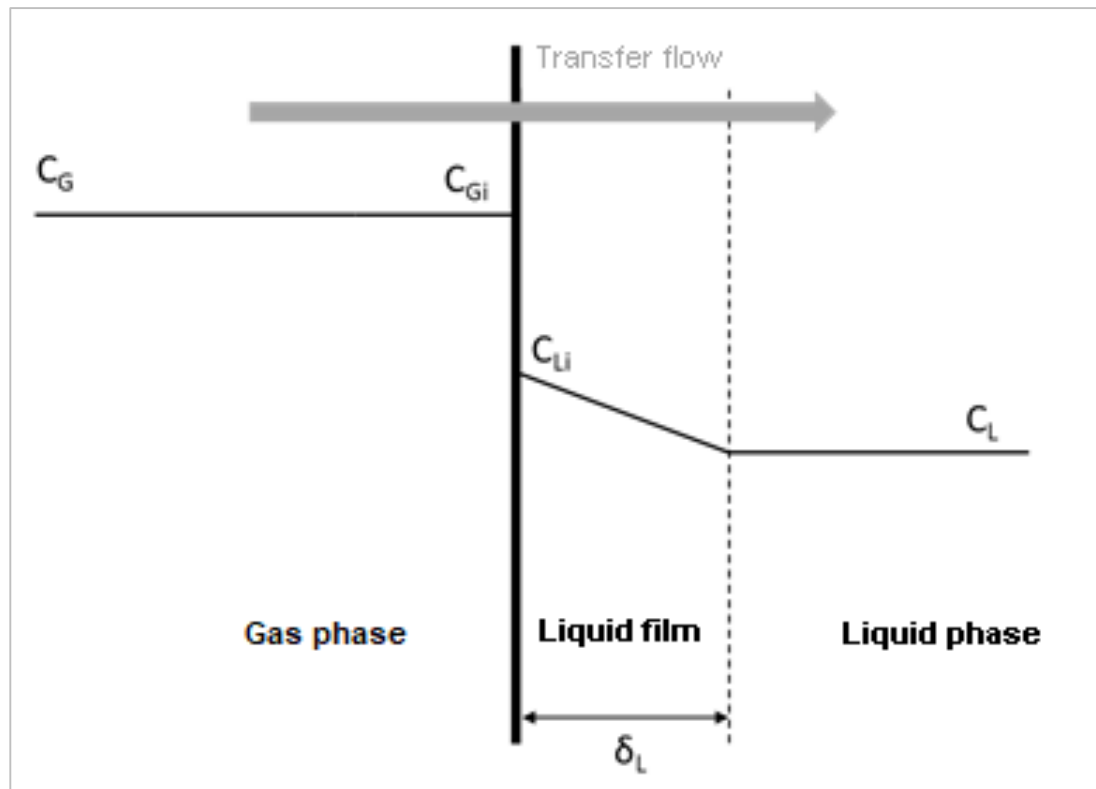
This tutorial is based on an example of a reactor that is fed with **pure oxygen** which creates a **dispersed gas phase** inside the liquid phase. The goal is to use the mass transfer model in order to analyse the influence of **mass transfer kinetic** on the composition of each phases.



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)
- $\delta_L$  : 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:

$\Phi$  Mass transfer flow (mol/(L.h))

$k_L a$  Volumetric mass transfer coefficient in the liquid phase (h<sup>-1</sup>)

**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



Calculators editor

EDITORS

CALCULATORS

EDITION

- +
- Add a new calculator
- Edit this calculator...**
- Edit the chemical reactions of this calculator...
- Clone this calculator
- X Delete the selection
- Default

FILE

- Open...
- Save As...

MODIFICATIONS

- Undo the last modification
- Redo the last modification

ORDER

- Move this calculator up
- Move this calculator down

This window helps you to manage a calculator list.

#	Default	Name	Type	Reactive
1		[New calculator]	Native	No (0/0)

2 - Click on “*Edit this calculator*”

Comments:

Ok Cancel

# Step 1: Selection of the compounds

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

Thermodynamic calculator editor

This window helps you to define the context of your thermodynamic calculator

COMPOUNDS | MODEL | BINARIES | PARAMETERS

#	IUPAC Name	CAS Registry Number®
1	WATER	7732-18-5
2	OXYGEN	7782-44-7
3	NITROGEN	7727-37-9

Comments :

CAS Registry Numbers® are the intellectual property of the American Chemical Society; and are used by ProSim SA with the express permission of ACS. CAS Registry Numbers® have not been verified by ACS and may be inaccurate.

COMPOUNDS

FILE

- Open...
- Save as...
- Publish...

PACKAGE

- Show the package manager...
- Import a package...
- Build a package...
- Select a CAPE-OPEN package

SERVICES

- Calculate
- Export as a PSF file
- Diagrams
- Residue...
- Export as a PVT file
- Stream...
- Sigma profiles

MODIFICATIONS

- Undo
- Redo

CONFIGURATION

Name

[New calculator]

Comments

Calculator type

EDIT

- Import compounds...
- Edit this compound...
- Create a new compound
- Remove all the compounds
- Clone this compound
- Update the compounds
- Delete the selection

SERVICES

- Create a pseudo-compound...
- Temperature dependent properties...
- Editor array
- Compare with the original
- Compare the compounds

ORDER

- Move this compound up

Ok Cancel

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

Compound Editor

COMPOUNDS

PROPERTIES

VIEW

MODIFICATIONS

UNIT SYSTEMS

This window helps you visualize the compounds properties.

Complete

Properties	WATER	OXYGEN	NITROGEN
Identification			
Group contribution models			
Atomic			
Phase change			
Normal melting point	0 °C	-218.789 °C	-210.001 °C
Normal boiling point	100 °C	-182.962 °C	-195.806 °C
Enthalpy of fusion (melting point)	1434.4502868068...	106.11854684512...	172.08413001912...
Triple point temperature	0.01000000000000...	-218.789 °C	-210.001 °C
Triple point pressure	0.0060373056994...	0.0014803849000...	0.1235627929928...
Physical state at 25°C	Liquid	Supercritical	Supercritical
Physical state in aqueous solution at 25°C	<unknown>	<unknown>	<unknown>
Diffusion coefficient			
Enthalpy of vaporization (boiling point)			
Octanol-Water partition coefficient	<unknown>	<unknown>	<unknown>
soil sorption coefficient (Koc@20°C)			
Liquid vapor calculation type	<unknown>	Henry constant	Henry constant
Acentric factor	0.344861	0.0221798	0.0377215
Modified acentric factor	0.7023	0.021	0.04
Critical temperature	373.946 °C	-118.57 °C	-146.95 °C
Critical pressure	217.75474956822...	49.770540340488...	33.555391068344...
Critical volume	55.9472 cm <sup>3</sup> /mol	73.4 cm <sup>3</sup> /mol	89.21 cm <sup>3</sup> /mol
Critical compressibility factor	0.229	0.288	0.289
Critical density	0.0178739954814...	0.0136239782016...	0.0112095056608...
Heat of sublimation at the triple point	12141.491395793...		
Glass-transition temperature			
Combustion, security, toxicity			
Condensed phase			
Phase thermochemistry			

CAS Registry Numbers® are the intellectual property of the American Chemical Society; and are used by ProSim SA with the express permission of ACS. CAS Registry Numbers® have not been verified by ACS and may be inaccurate.

Ok Cancel

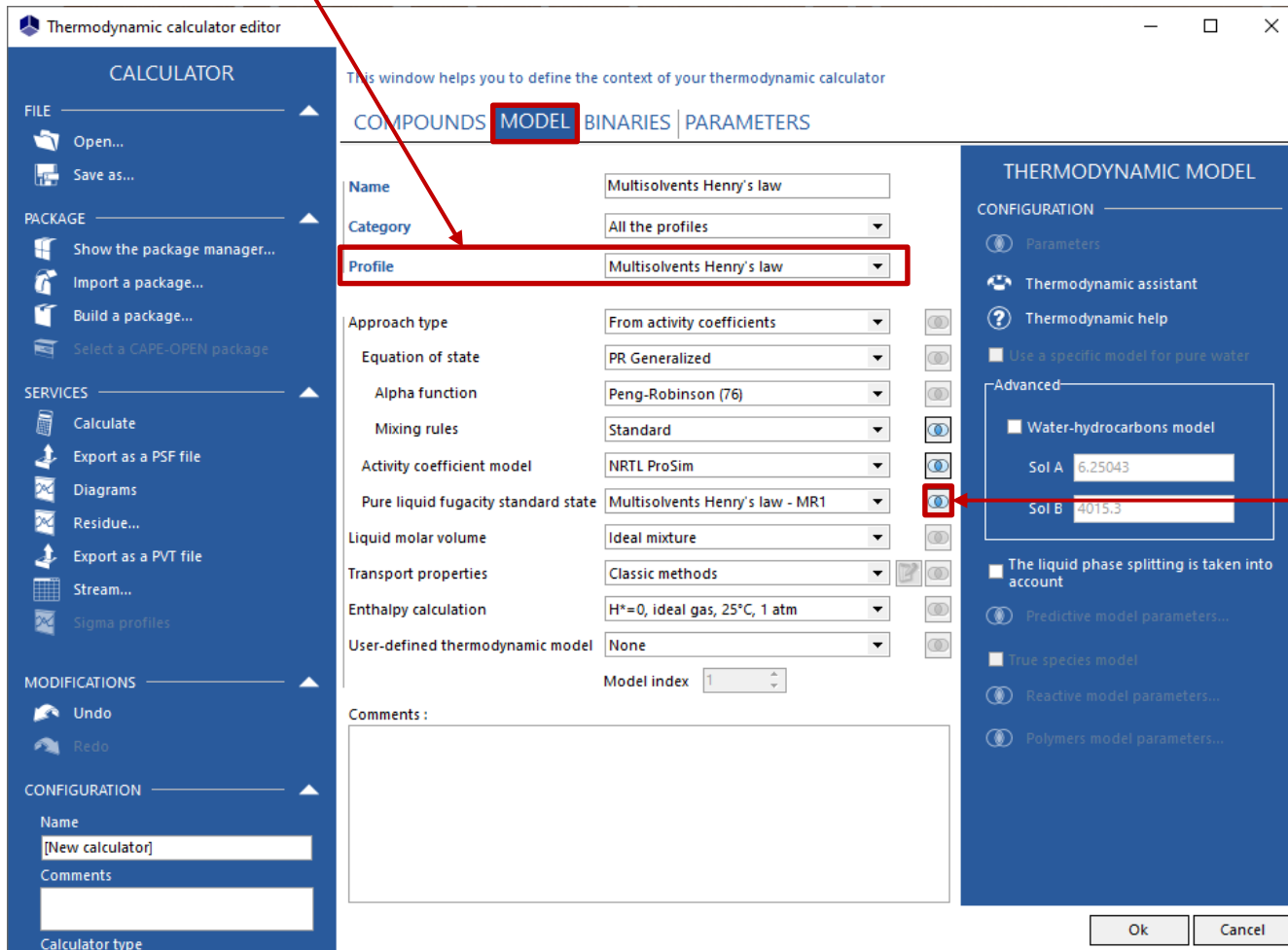
2 - For oxygen and nitrogen, select « *Henry constant* »

3 - Click on « *OK* »



# Step 1: Selection of the compounds

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



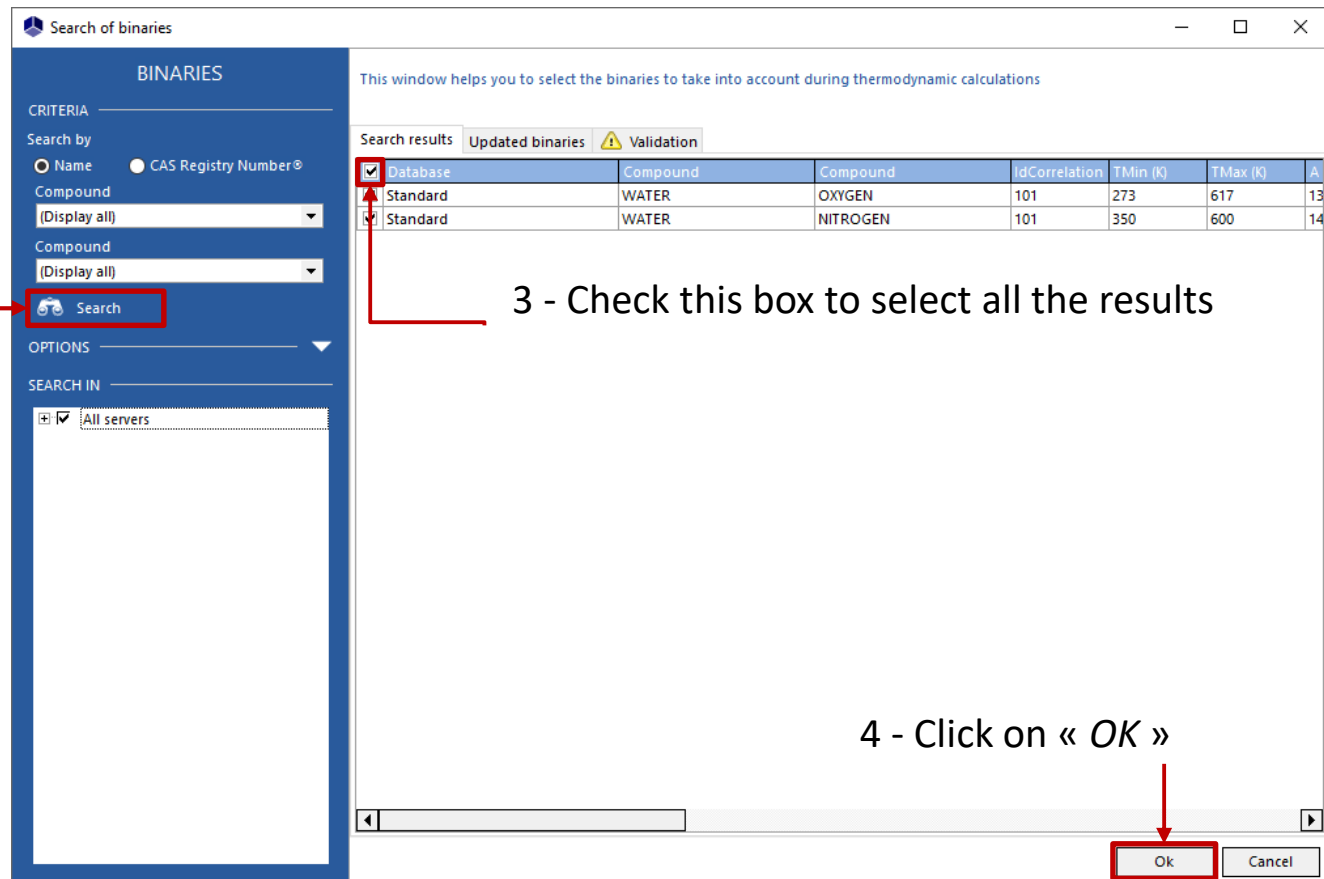
2 - Click here to access the parameters of the Henry's law

# Step 1: Selection of the compounds

1 - Click on « *Import binaries* »



2 - Click on « *Search* »



The dialog box "Search of binaries" is shown. It has a left sidebar with "BINARIES" and "CRITERIA" sections. The "Search by" section has radio buttons for "Name" and "CAS Registry Number", and two "Compound" dropdown menus. A "Search" button is highlighted with a red box. The main area has a "Search results" tab and a table with columns: "Database", "Compound", "Compound", "IdCorrelation", "TMin (K)", "TMax (K)", and "A". The table contains two rows of results. A red box highlights the "Database" column header and the first row. A red arrow points from the text "3 - Check this box to select all the results" to the checkbox in the "Database" column header. At the bottom right, the "Ok" button is highlighted with a red box, with a red arrow pointing from the text "4 - Click on « OK »".

3 - Check this box to select all the results

4 - Click on « OK »

Database	Compound	Compound	IdCorrelation	TMin (K)	TMax (K)	A
Standard	WATER	OXYGEN	101	273	617	13
Standard	WATER	NITROGEN	101	350	600	14

# Step 1: Selection of the compounds

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

Binaries editor

Binaries view:  Grid  Matrix

This window helps you to enter the binaries to take into account during thermodynamic calculations

These parameters are used instead of those defined in the "Binaries" page of the calculator.

Formulation : Depends of used correlation (see compound's Henry's Law) (atm)

Compound	Compound	IdCorrelation	TMin (K)	TMax (K)	A	B
WATER	OXYGEN	101	273	617	139.485	-68
WATER	NITROGEN	101	350	600	141.2677	-69
OXYGEN	NITROGEN	0	0	0	0	0

Not supplied Supplied Imported Estimated

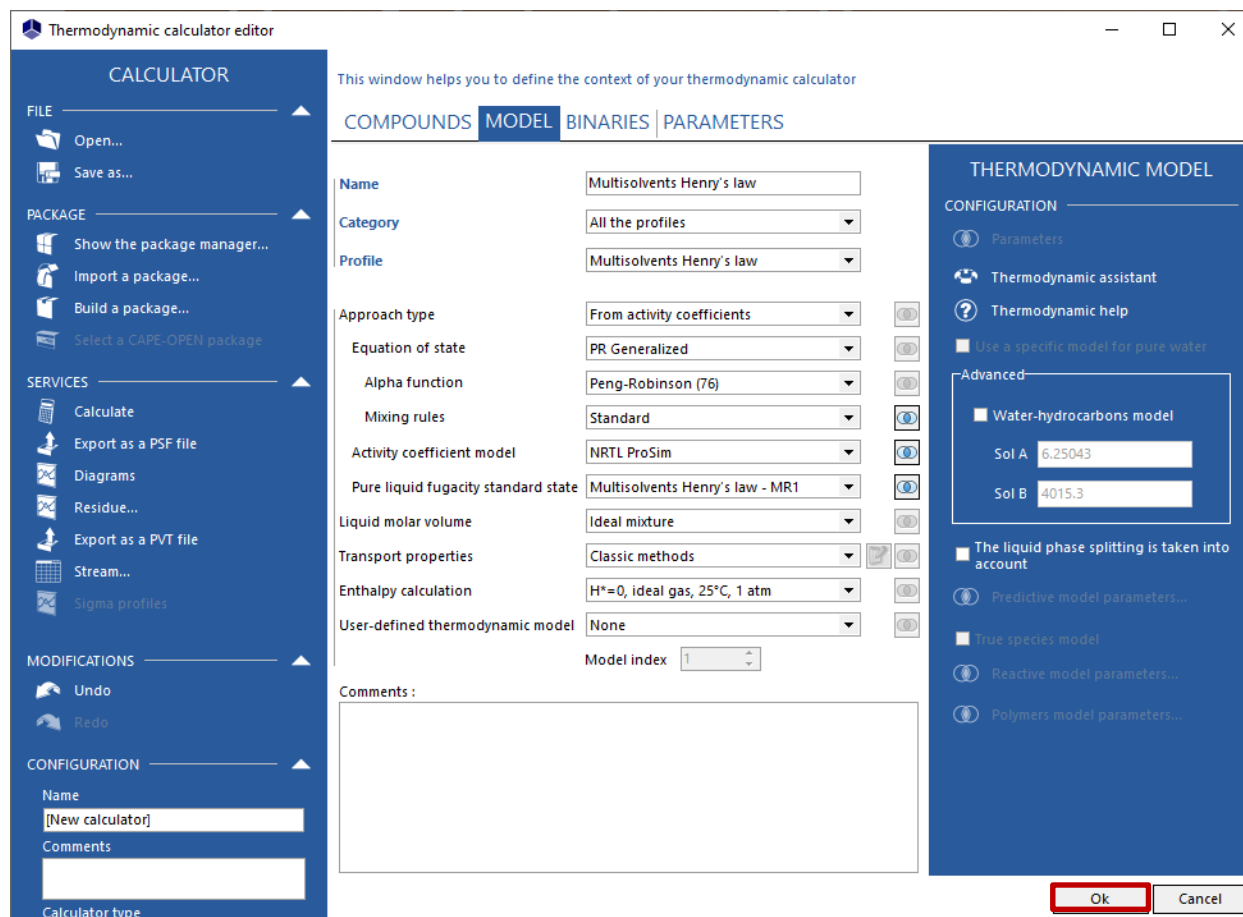
Comments :

2 - Click on « OK »

Ok Cancel

# 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

**Flowsheet**

Calculation mode

Monophasic (liquid)

Diphasic

Monophasic (gas)

Diphasic reactor type

Open

Closed

With mass transfer model

With a liquid sidestream

With a condenser

With a decanter

Vessel bottom geometry is known

Torispherical

With a mixing device

4 pitched flat-blades paddle

Dissipated heat included

With an external heat exchanger






With an helical coil

With a wall heat exchanger

With an inductor

External jacket

## 1 - Check the following options from the control panel:

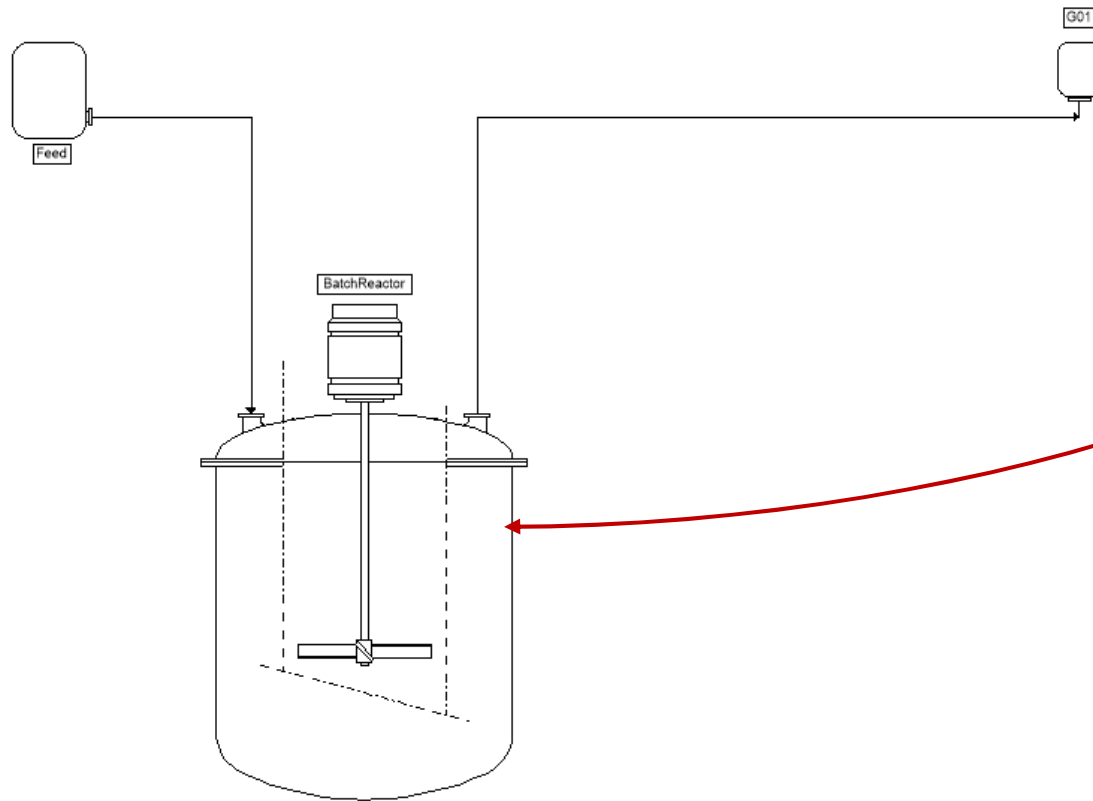
-  Calculation mode: diphasic
-  Diphasic reactor type: closed
-  With mass transfer model
-  The vessel bottom geometry is “*Torispherical*”
-  The mixing device is a “*4 pitched flat-blades paddle*”



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:

The screenshot shows the 'Reactor' configuration window for a 'BatchReactor'. The window is divided into several sections:

- Name:** BatchReactor
- Parameters:** Notes, Advanced parameters, Validation (checked)
- Reactor Model:** A 3D diagram of a stirred reactor with components labeled: Feeds, Head space, Mixing device, Mass transfer, Initial load, Vessel bottom geometry, Vapor productions, and Liquid productions.
- Reactor temperature [TR] (highlighted in red):**
  - Fixed temperature: 22 °C
  - Alarms [TR]:
    - Minimum: 0 °C
    - Maximum: 100 °C
- Reactor pressure [PR] (highlighted in red):**
  - Fixed pressure: 1 atm
- Global reactor volume [GVR] (highlighted in red):**
  - Global reactor volume [GVR]: 800 L
  - Alarms [VR]:
    - Minimum: 0.1 L
    - Maximum: 800 L
- Buttons:** Restore, Technology, OK, Cancel

## 1 - The initial conditions:

- $T = 22^{\circ}\text{C}$
- $P = 1 \text{ atm}$
- $V = 800 \text{ L}$

## 2 - The alarms:

- Temperature
  - Minimum:  $0^{\circ}\text{C}$
  - Maximum:  $100^{\circ}\text{C}$
- 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

Initial load specification

Fractions Molar

Compound	Fraction
WATER	1
OXYGEN	0
NITROGEN	0

Total volume load 478 L

The head space is composed of air

Head space

Head space type

Air

Nitrogen

Other

None

N2 0.79 %

O2 0.21 %

= 3.76

Adjustment variable

Pressure

Temperature

"Pressurizing" compound

WATER

Restore OK Cancel



# 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

Compound	Model	Value
WATER	No resistance	
OXYGEN	No resistance	
NITROGEN	No resistance	

Vapor phase considered for the mass transfer

Head space  
 Dispersed gas

Volume %

Calculation of gassed power consumption

Correction factor

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:

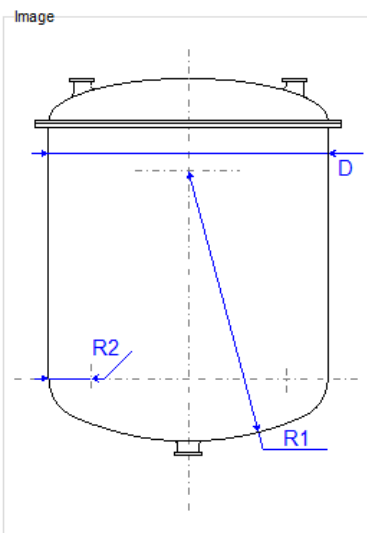
## 5 - The geometric characteristics of the equipment:

### Vessel bottom geometry

Vessel bottom geometry

Vessel bottom geometry is known

Image



Type of vessel bottom geometry  
Torispherical

Parameters

Number of baffles	0
Vessel diameter (D)	1.165 m
Vessel bottom height (H)	0 m
Curve radius #1 (R1)	1.2 m
Curve radius #2 (R2)	0.12 m

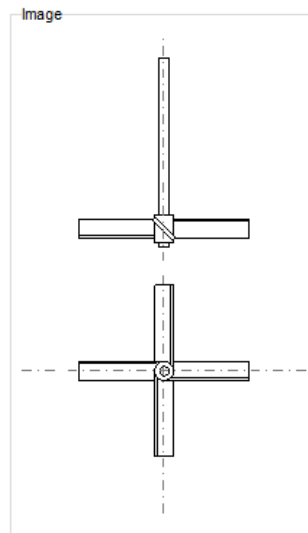
Restore Technology

### Mixing device

Mixing device

With a mixing device  Dissipated heat included

Image



Parameters

4 pitched flat-blades paddle

Agitator diameter	0.5 m
Agitator height	0.015 m
Ribbon-vessel distance	0 m
Ribbon width	0 m
Power number	1.3
Energy constant in laminar flow	55
Propeller step / Agitator diameter	1
Blade height / Tank diameter	0.0666666666666667
Device number	1
Distance between 2 devices	0 m

"User" coefficients (immersed) "User" coefficients (wall)

Default rotation speed 90 tr/min

Restore Technology

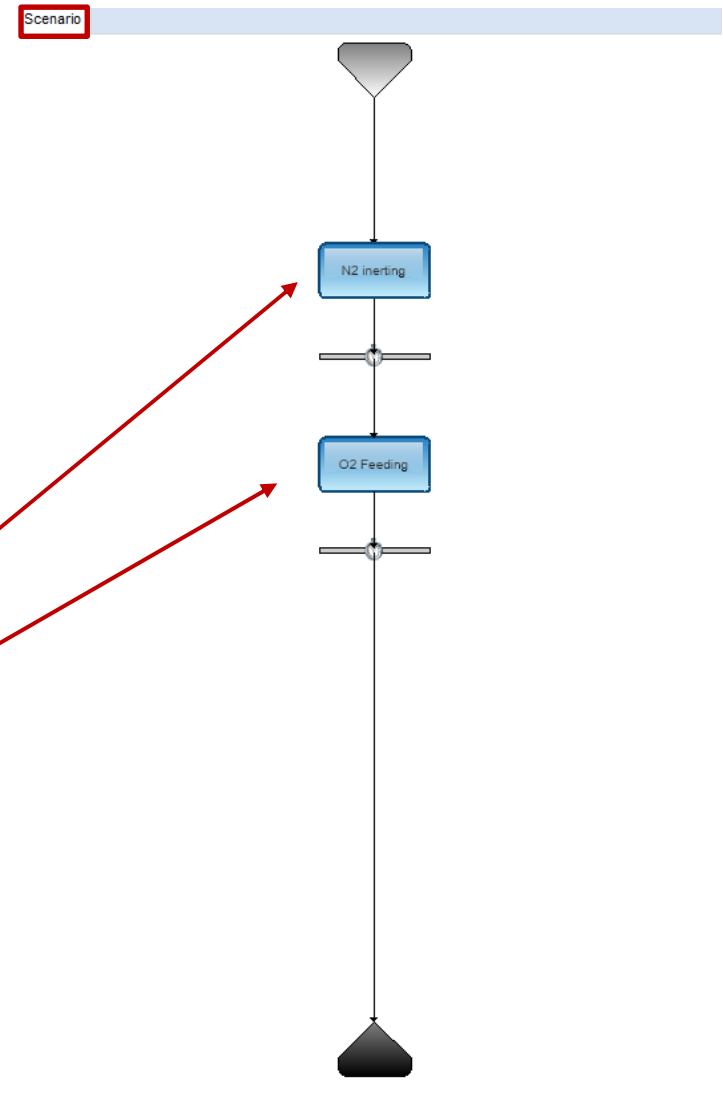
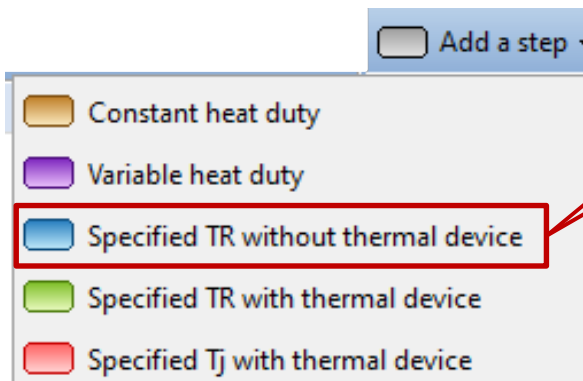
# Step 3: description of the operating mode

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 1<sup>st</sup> step

Step name: N<sub>2</sub> inerting

Feed:

Pure nitrogen

T = 22 °C

P = 1 atm

Flowrate = 354 l/h



Feed

Name: Feed

Parameters Notes Validation

Feed is open

Temperature specification  
Given temperature 22 °C

Pressure specification  
Given pressure 1 atm

Init flowrate specification flowrate variation

Fractions Molar

Compound	Fraction
WATER	0
OXYGEN	0
NITROGEN	1

Total volume flowrate 354 l/h

Thermodynamic calculator Default calculator

Restore OK Cancel

# 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 2<sup>nd</sup> step

Step name: O<sub>2</sub> Feeding

Feed:

Pure oxygen

T = 22 °C

P = 1 atm

Flowrate = 354 l/h



Feed

Name: Feed

Parameters Notes Validation

Feed is open

Temperature specification  
Given temperature 22 °C

Pressure specification  
Given pressure 1 atm

Init flowrate specification flowrate variation

Fractions Molar

Compound	Fraction
WATER	0
OXYGEN	1
NITROGEN	0

Total volume flowrate 354 l/h

Thermodynamic calculator Default calculator

Restore OK Cancel

# 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 each step, the end event corresponds to a time of 1h spent since the beginning of the step



Event
✕

Information

Name:

Parameters
Notes
✔ Validation

Event type

Time spent since beginning of simulation

Time spent since beginning of step

Temperature inside the reactor

Fraction inside the reactor

Concentration inside the reactor

Load of a component

Total load

Pressure inside the reactor

Parameter(s) of the event

Time of step






OK
Cancel

# 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)



**Report parameters** ✕

Composition printing Mass ▾

Flowrate printing Mass ▾

Time between each output 60 s ▾

Traced variables

Fractions

Concentrations

Volume and flowrates

Heat duty and temperature

Scale-up calculation

Type of the scale-up factor Volume ▾

Scale-up factor 2




Generation of the report (.docx)

Generation of the compounds and reactions files

Restore
OK
Cancel

# Step 4: Simulation of different configurations

The three following configurations can now be simulated:

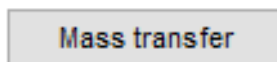
-  Configuration 1: with no transfer resistance
-  Configuration 2: with transfer resistance and the  $k_L a$  predicted by the software
-  Configuration 3: with transfer resistance and the  $k_L a$  regressed from experimental data



# Step 4: Simulation of different configurations

## Configuration 1: with no transfer resistance

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



Mass transfer

Volumetric mass transfer coefficients

Compound	Model	Value
WATER	No resistance	
OXYGEN	No resistance	
NITROGEN	No resistance	

Vapor phase properties

Vapor phase considered for the mass transfer

Head space

Dispersed gas

Volume %

Parameters

Calculation of gassed power consumption

Correction factor

Parameters

Restore

2 - Select the “*No resistance*” option for all compounds

3 - Save the file and run the simulation

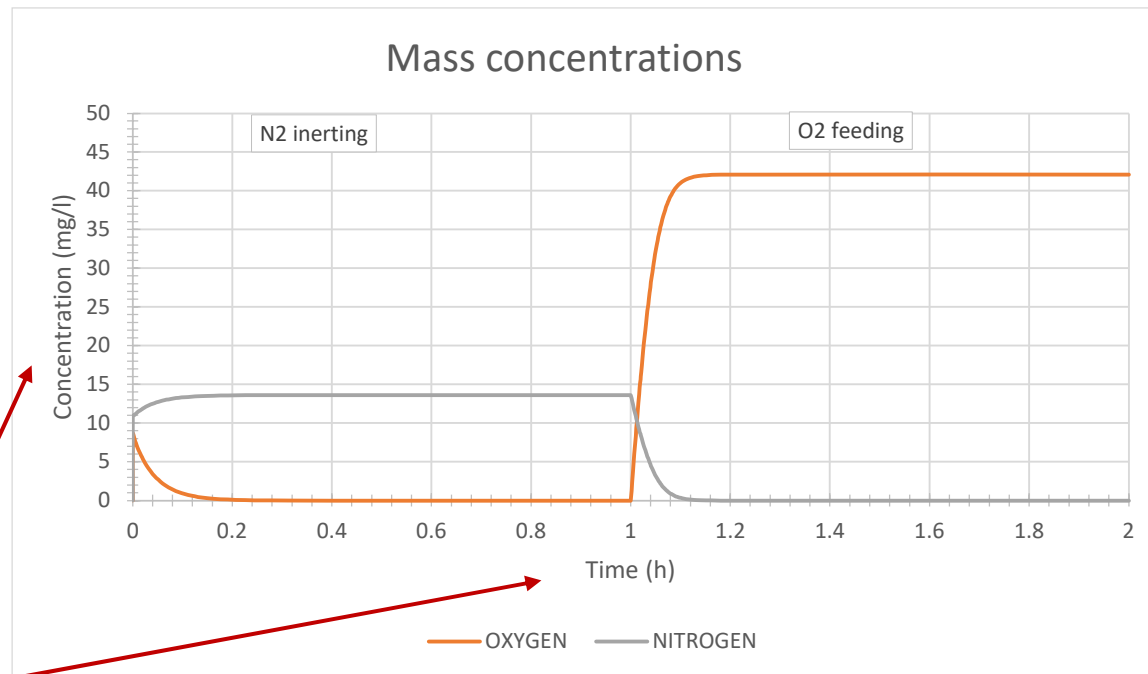


# Step 4: Simulation of different configurations

## Configuration 1: with no transfer resistance



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

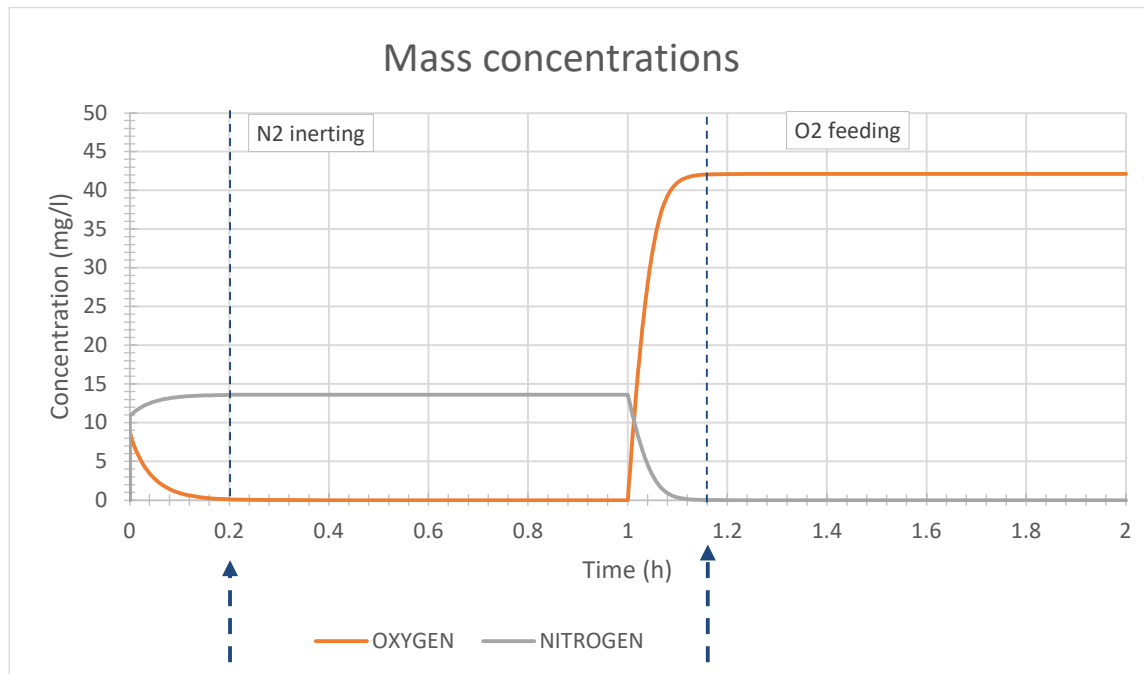


5 - You can adjust the graph scales in order to properly display the concentration profiles of nitrogen and oxygen

# 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  $P_{O_2} = 1$  atm and  $T = 22^\circ\text{C}$ )

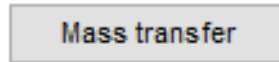
Required time to strip all the oxygen from the liquid phase

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



Mass transfer

Volumetric mass transfer coefficients

Compound	Model	Value
WATER	No resistance	
OXYGEN	Calculated	Middleton
NITROGEN	No resistance	

Correlations parameters

Vapor phase properties

Vapor phase considered for the mass transfer

Head space

Dispersed gas

Volume % Calculated Gao et al.

Parameters

Calculation of gassed power consumption

Correction factor Calculated Bruijn et al.

Parameters

Restore OK Cancel

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

3 - Save the file and run the simulation

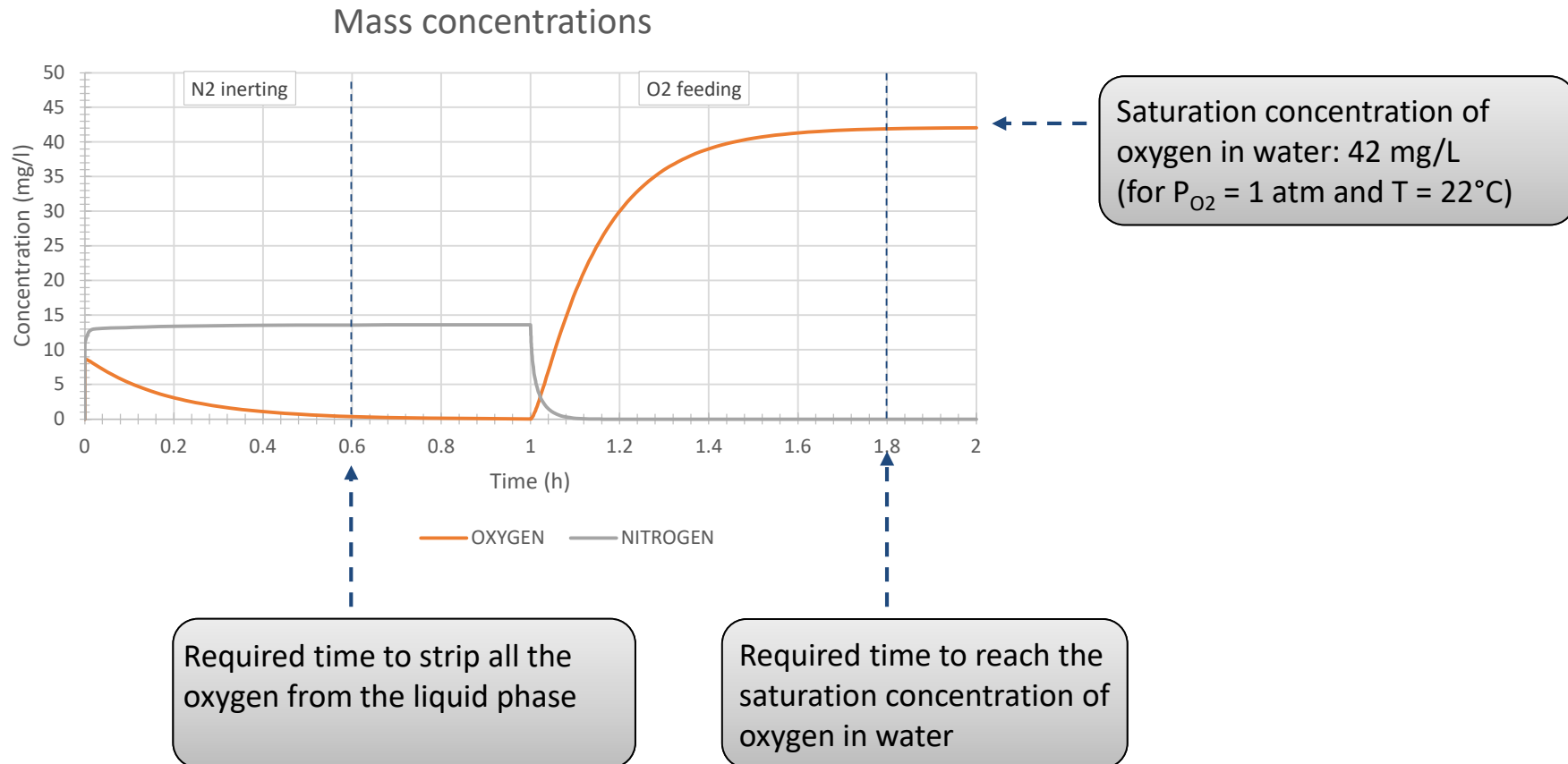


# Step 4: Simulation of different configurations

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

4 - For these operating conditions, the predicted value for the  $k_L a$  of oxygen equals  $6.8 \text{ h}^{-1}$ .

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



# 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]:

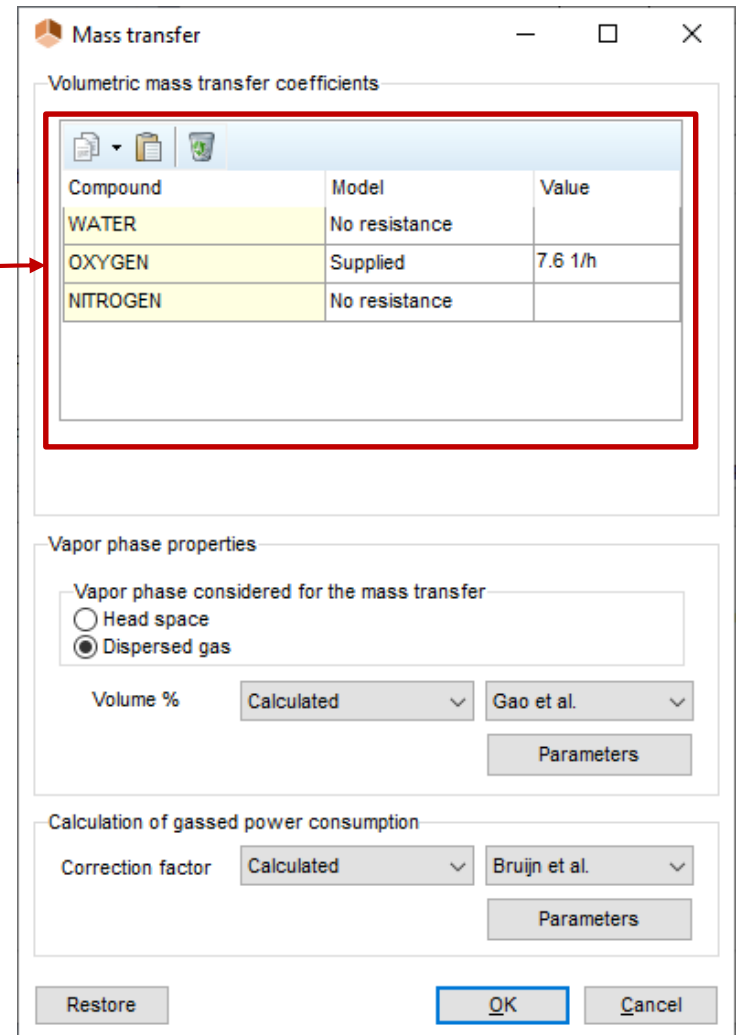
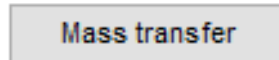
Time (h)	$C_L(O_2)$ (mg/L)
1.01	1.5
1.04	9.6
1.07	15.4
1.11	22.6
1.14	26.9
1.18	30.3
1.22	33.3
1.25	35.2
1.29	37
1.34	38.7
1.40	40.0
1.45	40.6
1.50	41.2

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

# 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

A screenshot of the "Mass transfer" dialog box. The dialog has a title bar with a close button. The main content is divided into three sections: "Volumetric mass transfer coefficients", "Vapor phase properties", and "Calculation of gassed power consumption". The "Volumetric mass transfer coefficients" section contains a table with three rows: WATER, OXYGEN, and NITROGEN. The OXYGEN row is highlighted in yellow and has "Supplied" in the Model column and "7.6 1/h" in the Value column. The "Vapor phase properties" section has radio buttons for "Head space" and "Dispersed gas", with "Dispersed gas" selected. Below are dropdown menus for "Volume %" (set to "Calculated") and "Gao et al." (set to "Gao et al."). The "Calculation of gassed power consumption" section has a dropdown for "Correction factor" (set to "Calculated") and "Brujin et al." (set to "Brujin et al."). At the bottom are buttons for "Restore", "OK", and "Cancel".

Compound	Model	Value
WATER	No resistance	
OXYGEN	Supplied	7.6 1/h
NITROGEN	No resistance	

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

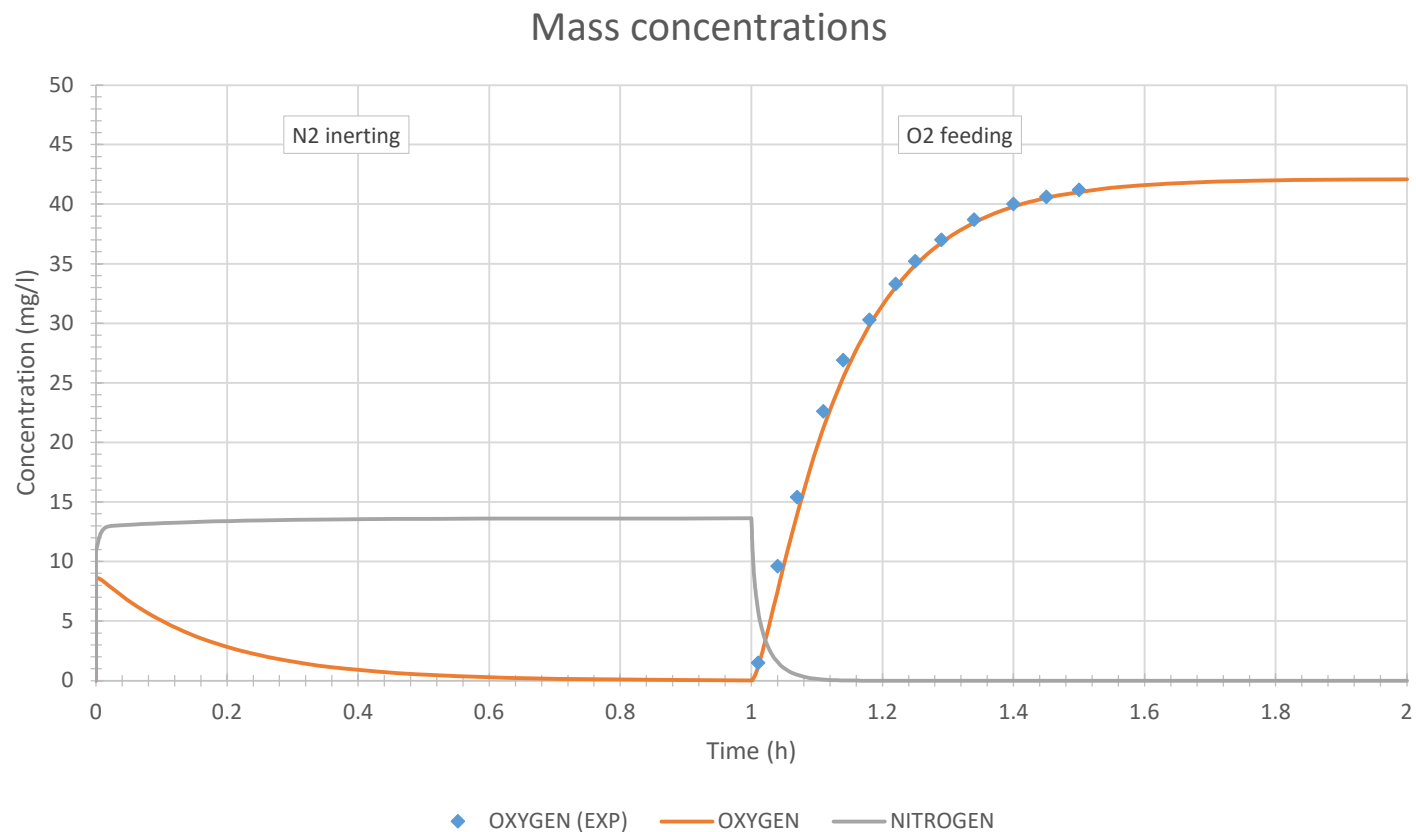
3 - Save the file and run the simulation



# 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)...

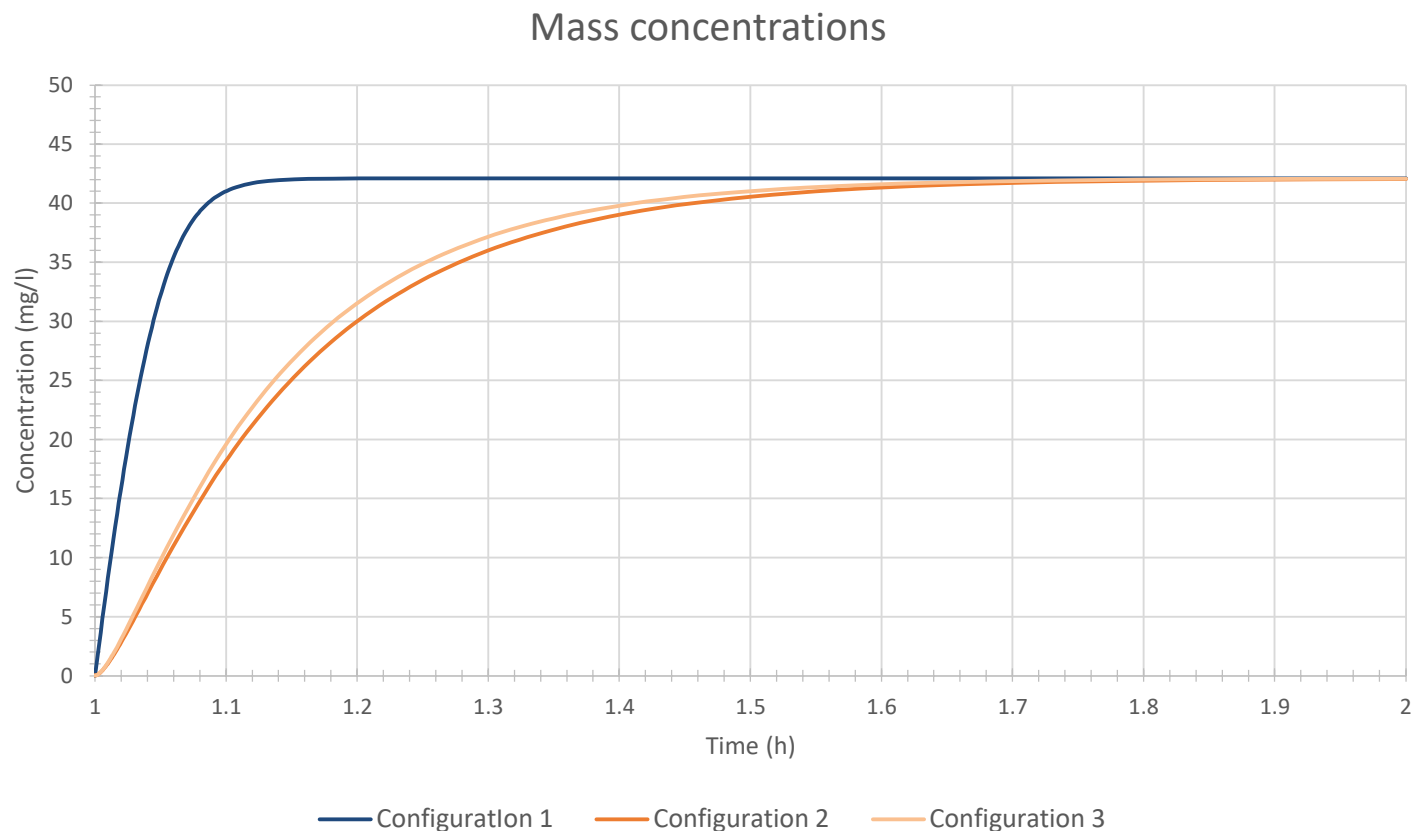




# Step 4: Simulation of different configurations




## 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 SA

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

☎: +33 (0) 5 62 88 24 30



# ProSim

Software & Services In Process Simulation

[www.prosim.net](http://www.prosim.net)  
[info@prosim.net](mailto:info@prosim.net)



### ProSim, Inc.

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

☎: +1 215 600 3759