

# Getting started with BatchReactor®

Use Case 1: simulation of the chlorotoluene  
chlorination

Software & Services In Process Simulation

*We guide You to efficiency*



ProSim

# Introduction

This document presents the different steps to follow in order to simulate a batch reactor synthesis using BatchReactor software.

This presentation is based on a practical example: the chlorination of the chlorotoluene. This example is available on ProSim web site ([www.prosim.net](http://www.prosim.net)) or in the BatchReactor example directory.

The presentation includes 3 parts:

Part 1 - Example description

Part 2 - General description of the software interface

Part 3 - Description of the different steps to follow in order to run the simulation

# Part 1 - Example description

## Example description:

- Compounds and thermodynamic model
- Description of the reaction system
- Description of the equipment
- Operating mode

# Compounds and thermodynamic model

The following compounds are involved in the simulation:

Name	Formula	CAS Number(*)
o-Chlorotoluene	$C_7H_7Cl$	95-49-8
Chlorine	$Cl_2$	7782-50-5
Benzyl dichloride	$C_7H_6Cl_2$	98-87-3
Hydrogen chloride	HCl	7647-01-0
Benzotrichloride	$C_7H_5Cl_3$	98-07-7
Nitrogen	$N_2$	7727-37-9

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

# Compounds and thermodynamic model

The “NRTL” thermodynamic profile is selected, with the binary interaction parameters specified as follows (available parameters would be automatically loaded):

- Supplied for the following binaries:

Compounds		$C_{ij0}$	$C_{ji0}$	$A_{ij0}$	$C_{ijT}$	$C_{jiT}$	$a_{jiT}$
o-Chlorotoluene	Benzyl dichloride	-707.3	775.31	0.1939	0	0	0
o-Chlorotoluene	Benzotrichloride	-1246	1463.5	0.1584	0	0	0
Benzyl dichloride	Benzotrichloride	64.339	-79.04	0.4097	0	0	0

- Equal to 0 for the other binaries (coming down to considering ideal thermodynamic behaviour)

# Description of the reaction system

The reactor is initially composed of liquid chlorotoluene and is fed with vapor chlorine. Two chemical reactions are considered. For each reaction:

- The reaction takes place in the liquid phase
- The reaction heat is calculated from the standard enthalpies of formation
- The reaction is controlled by the kinetic
- The rate constant is calculated by the Arrhenius law:

$$k(T) = k^0 \exp\left(\frac{-E_a}{RT}\right)$$

With:

$k^0$	Pre-exponential factor → <u>Provided by the user</u>
$E_a$	Activation energy → <u>Provided by the user</u>
$R$	Ideal gas constant
$T$	Temperature

# Description of the reaction system

The main reaction is the following:



- Model expressed in molar concentrations
- Partial orders of 1 for the reactants and 0 for the products

Compound	Stoichiometry	Order
Chlorine	-1	1
o-Chlorotoluene	-1	1
Benzyl dichloride	1	0
Hydrogen chloride	1	0

- Kinetic parameters:

Pre-exponential factor ( $k^0$ )	$2.7203 \cdot 10^{17} \text{ s}^{-1}(\text{mol/l})^{-1}$
Activation energy ( $E_a$ )	130320 J/mol

# Description of the reaction system

A side reaction is considered:



- Model expressed in molar concentrations
- Partial orders of 1 for the reactants and 0 for the products

Compound	Stoichiometry	Order
Benzyl dichloride	-1	1
Chlorine	-1	1
Benzotrichloride	1	0
Hydrogen chloride	1	0

- Kinetic parameters:

Pre-exponential factor ( $k^0$ )	$580 \text{ s}^{-1}(\text{mol/l})^{-1}$
Activation energy ( $E_a$ )	42200 J/mol



# Description of the equipment

Two streams feed the reactor: the first is for the reactant and the second is for nitrogen sweeping.

The reactor characteristics are the following:

- **Vessel:** torispherical vessel with a volume of  $3\text{m}^3$  and a diameter of 1400 mm
- **Mixing device:** 3 retreating-blades impeller with a diameter of 700 mm, located at 450 mm from the bottom and rotating at 90 rpm
- **Wall heat exchanger:** external jacket, 50 mm thick and 1700 mm high
- **Wall materials:** stainless steel 316 with a thickness of 17 mm

# Description of the equipment

- **Utility fluid:**
  - Hot utility: 200 kg/h of steam at 6 bar
  - Cold utility: 4000 kg/h of water at 25°C
- **Thermal inertia:** the reactor is made of a material that has a weight of 800 kg and a specific heat of 500 J/kg/K
- **Heat losses:** negligible

# Description of the equipment

- The reactor is closed and equipped with a two-stages condenser. A vapor output stream is leaving the second stage
- The liquid condensates are collected in the storage tank
- The characteristics of the first condensation stage are the following:
  - Exchange area:  $15 \text{ m}^2$
  - Global heat exchange coefficient:  $300 \text{ kcal/h/m}^2/\text{ }^\circ\text{C}$
  - Utility:  $3000 \text{ kg/h}$  of water at  $20^\circ\text{C}$
- The characteristics of the second condensation stage are the following:
  - Exchange area:  $0.5 \text{ m}^2$
  - Global heat exchange coefficient:  $300 \text{ kcal/h/m}^2/\text{ }^\circ\text{C}$
  - Utility:  $100 \text{ kg/h}$  of a thermal fluid composed of ethylene glycol 40% available at  $15^\circ\text{C}$
- Pressure drop in both stages are neglected

# Operating mode

The reactor is initially composed of 2400 kg of chlorotoluene at 25°C and atmospheric pressure.

- **First step: heating**

The reactor is heated, maintaining a total reflux, until 58°C is reached. The reactor inerting is performed using a nitrogen stream with a flowrate of 1 kg/h at 25°C and atmospheric pressure. The reactor pressure is kept at atmospheric pressure.

# Operating mode

- **Second step: reaction**

The reactor is fed during 13 hours with 60 kg/h of chlorine at 3 bar and 25°C. The nitrogen sweeping is maintained. The reactor temperature is controlled at a value of 62°C by acting on the cooling water flowrate.

A PID controller is used, with the following parameters:

- Minimum / maximum values: 59°C / 65°C
- Type: feedback
- PID parameters: Gain = -5, Ti = 500 s, Td = 0
- Sample rate: 10 s
- Valve regulation: the valve equation is based on an “exponential” type and the Cv equals 30

# Part 2 - General description

## General description of the software interface:

- Home page
- Main window
- Toolbar
- Creating a new simulation file
- Selecting the unit system

# Home page

The screenshot shows the BatchReactor software interface. The top menu bar includes File, Edit, View, Configuration, Simulation, Elements, Shapes, Tools, and Help. Below the menu is a toolbar with various icons for file operations and simulation control. The main content area is divided into several sections:

- Getting started with...:** Contains links to "Getting started with BatchReactor® - Use Case 1: simulation of the chlorotoluene chloration" and "Getting started with Simulis Reactions® - Use Case 1: Features overview".
- Examples:** Lists various simulation examples such as "BATCHREA\_EX\_EN-Reer-Run-E1.pbpr" and "BATCHREA\_EX\_EN-Pressure-increase.pbpr".
- What's up?:** Contains "Release Note April 2020", "Covid-19", "Release Note July 2019", "Release note April 2019", and "New software for the simulation of heat exchangers".
- YouTube Videos:** A list of video titles including "Activated Carbon Lifetime - chemical process simulation with ProSim DAC software" and "WEBINAR: Energy audit why and how implementing pinch analysis?".
- Internet Site News Release Notes:** A search bar and a list of news items.
- Social Networks:** Icons for LinkedIn, Twitter, and YouTube.

Red callouts highlight the following areas:

- Last Projects:** Points to the "Files" section.
- Getting Started:** Points to the "Getting started with..." section.
- Examples:** Points to the "Examples" list.
- Internet Site News Release Notes:** Points to the "What's up?" section.
- YouTube Videos:** Points to the "YouTube Videos" section.
- Search in the Internet Site:** Points to the search bar in the "Internet Site News Release Notes" section.
- Social Networks:** Points to the LinkedIn, Twitter, and YouTube icons.

Social Networks

# Main window

Toolbar

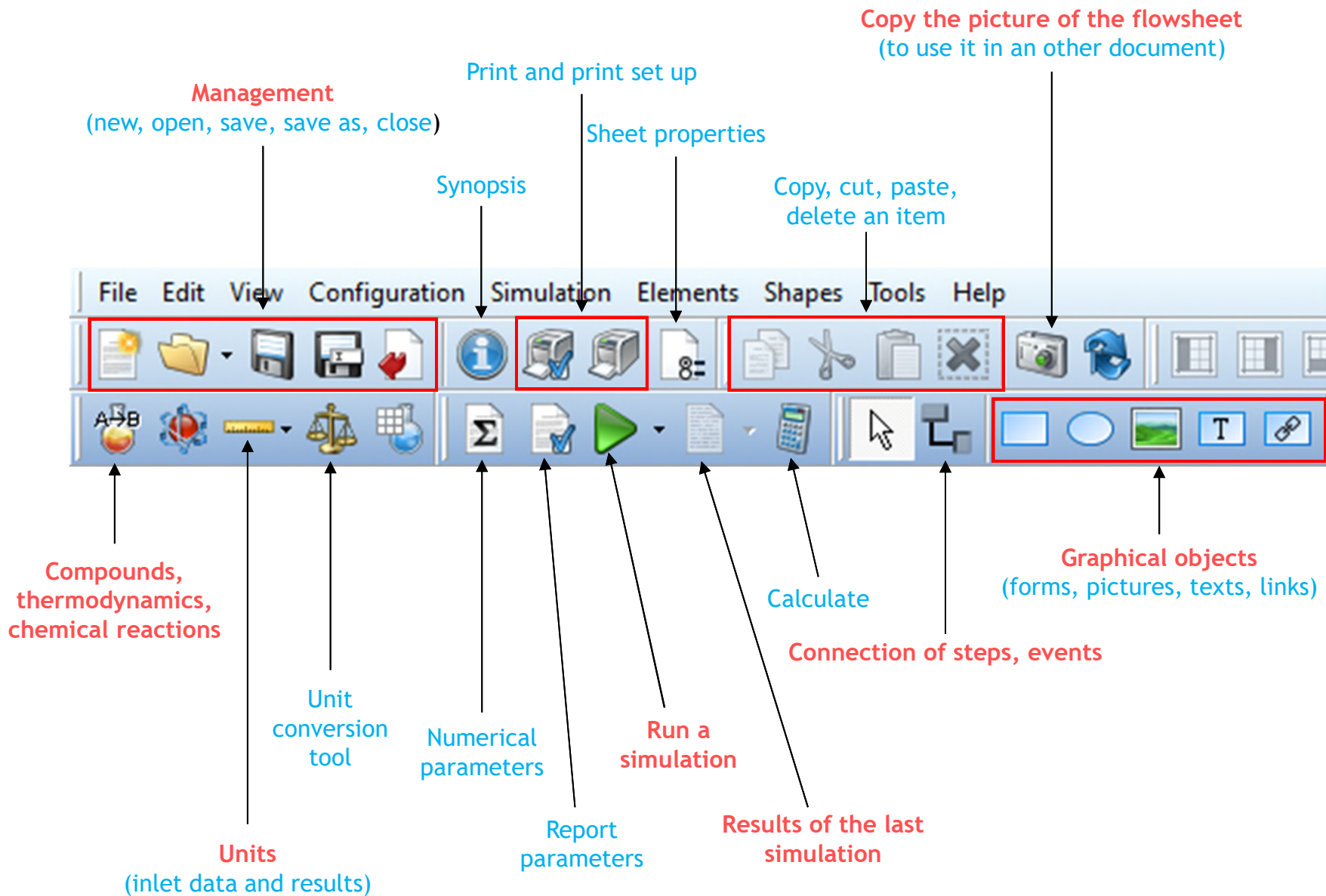
Selection of the step configuration tab

The screenshot displays the main window of the ProSim S.A. software, which is used for process simulation. The interface is divided into several key areas:

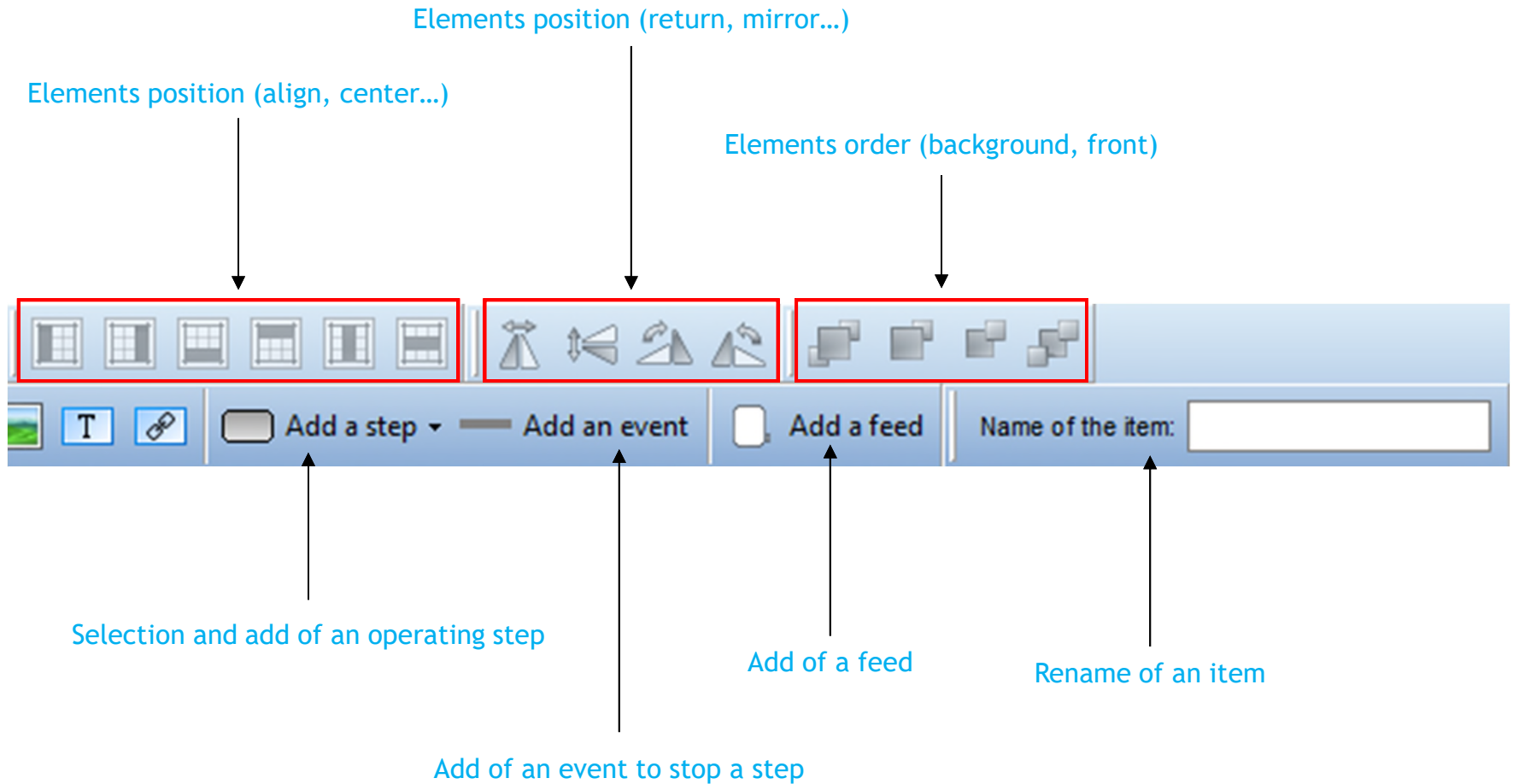
- Toolbar:** Located at the top, it contains various icons for file operations, simulation control, and element manipulation.
- Scenario Window:** On the left, a vertical flowchart shows the process steps. The 'Heating' step is currently selected and highlighted in purple, with a 'Reaction' step below it highlighted in green.
- Flowsheet Configuration Panel:** A central panel titled 'Flowsheet' provides detailed settings for the selected step. It includes:
  - Calculation mode:** Radio buttons for Monophasic (liquid), Diphasic (selected), and Monophasic (gas).
  - Diphasic reactor type:** Radio buttons for Open and Closed (selected).
  - Advanced options:** Checkboxes for 'With mass transfer model', 'With a liquid sidestream', 'With a condenser', 'With a decanter', and 'Vessel bottom geometry is known'.
  - Mixing device:** A dropdown menu set to 'Torispherical' with '3 retreating-blades impeller' selected.
  - Heat exchange options:** Checkboxes for 'Dissipated heat included', 'With an external heat exchanger', 'With an helical coil', and 'With a wall heat exchanger'.
  - External jacket:** A dropdown menu set to 'Joined'.
- Control panel:** A large diagram on the right shows a 3D schematic of a reactor vessel. It features a central 'Reactor' column with an agitator, and two side tanks labeled 'Reactant' and 'Inert' with pipes leading into the main vessel. This area is used to specify input parameters for the simulation.



# Toolbar



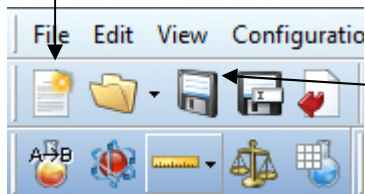
# Toolbar



# Creating a new simulation file



1- Click on « create a new document »



2- Save the file

3 - Fill the synopsis form (optional)

Synopsis

Title:

Subject:

Author:

Manager:

Company:

Category:

Keywords:

Comments:

OK Cancel

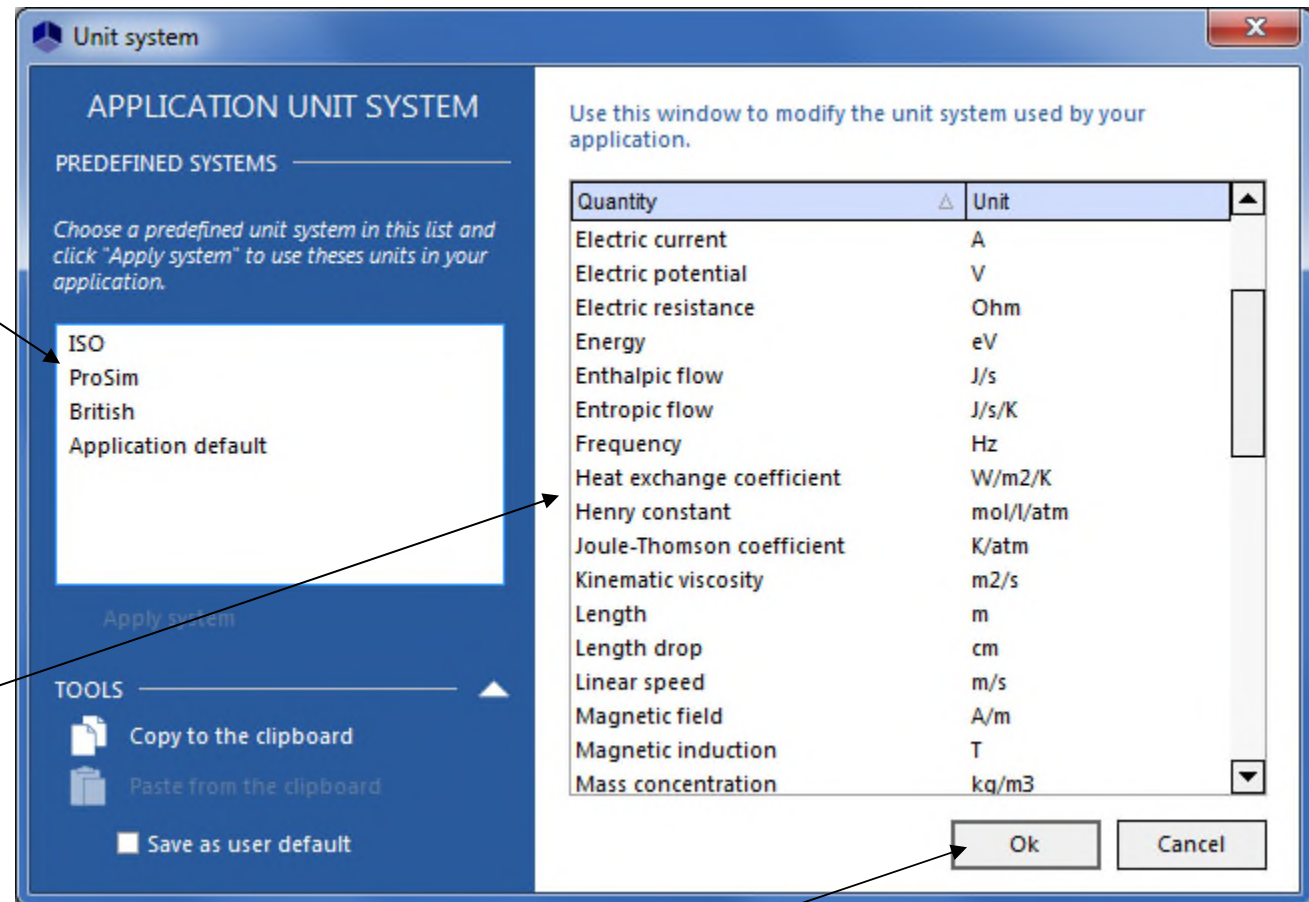
# Choosing the unit system



Click on this icon  in order to configure the unit system

1- Select a predefined unit system and click on “Apply system”

2- You can then customize the unit system



3- Click on “OK” to validate

# Part 3 - Simulation

## Description of the different steps to simulate the example

- Step 1: Select the compounds
- Step 2: Select the thermodynamic model
- Step 3: Describe the chemical reactions
- Step 4: Describe the equipment
- Step 5 : Describe the operating steps
- Step 6: Run the simulation
- Step 7: Analyze the simulation results

# Step 1: Select the compounds

1 - Click on the icon “Edit the thermodynamic and the compounds”



Calculators editor

CalcULATORS

EDITION

- ➕ Add a new calculator
- ✎ Edit this calculator...**
- ✎ Edit the chemical reactions of this calculator...
- 📄 Clone this calculator
- ✕ 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	Yes (2/2)

Comments:

Ok Cancel

2 - Click on “Edit this calculator”



For more information about selecting and editing the compounds, please consult “*Getting started with Simulis Thermodynamics, use case 1*”

# Step 1: Select the compounds

Thermodynamic calculator editor

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

COMPOUNDS | MODEL | PARAMETERS

#	IUPAC Name	CAS Registry Number <sup>®</sup>
---	------------	----------------------------------

Comments :

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

Calculator type

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

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

Ok Cancel

Click here to import the compounds from the database

# Step 1: Select the compounds

3 - Press “Enter” or click on “Search” to display the list of compounds that match your criteria

The screenshot shows the 'Search results' window. On the left, under 'COMPOUNDS', the search criteria are set to 'Name or synonym' with the text 'o-chlorotoluene'. The search options include 'Exact name' (checked), 'CAS Registry Number', 'Chemical formula', 'Specific ID', and 'Advanced'. The search is performed in the 'Standard 2021' database. The main panel shows the search results for 'NITROGEN', including its location, CAS Registry Number (7727-37-9), and Specific ID. A table of search results is displayed with columns for IUPAC name, Chemical formula, CAS Registry Number, Molecular weight, and Bubble temperature. The table contains one row for 'o-CHLOROTOLUENE' with a molecular weight of 126.583 and a bubble temperature of 432.300. On the right, a 'Selected compounds' list shows 'NITROGEN' as the selected item.

4 - The search results are shown here

2 - Multiple different research criteria can be used (in the example, research “o-chlorotoluene” by its name)

1 - Select the compounds server in which you want make the researches (by default, select the most recent one)



# Step 1: Select the compounds

1 - Double click on the compound to add it to your final selection

The screenshot displays the ProSim search results window. On the left, the 'COMPOUNDS' sidebar is visible, with the search criteria set to 'o-chlorotoluene'. The main search results table shows one entry for 'o-CHLOROTOLUENE' with a CAS Registry Number of 95-49-8. A red box highlights this entry in the table. An arrow points from the text '1 - Double click on the compound to add it to your final selection' to this entry. To the right of the table, the 'Selected compounds:' list contains the following items: o-CHLOROTOLUENE, CHLORINE, BENZYL DICHLORIDE, HYDROGEN CHLORIDE, BENZOTRICHLORIDE, and NITROGEN. An arrow points from the text '2 - Repeat the operation for the other compounds' to this list. At the bottom right of the window, a 'Close' button is highlighted with a red box, and an arrow points from the text '3 - Click on "Close" to end the compounds selection process' to it. The status bar at the bottom indicates '0 item(s) selected'.

#	IUPAC name (or co...)	Chemical for...	CAS Regi...	Molecular wei...	Bubble tem
7	o-CHLOROTOLUENE	C7H7Cl	95-49-8	126.583	432.300

Selected compounds:

- o-CHLOROTOLUENE
- CHLORINE
- BENZYL DICHLORIDE
- HYDROGEN CHLORIDE
- BENZOTRICHLORIDE
- NITROGEN

Close

2 - Repeat the operation for the other compounds

3 - Click on "Close" to end the compounds selection process

# Step 2: Select the thermodynamic model

1 - Click on the “Model” tab to access the thermodynamic model editor



The “Binaries” tab appears automatically when you select a model that requires binary interaction parameters

The screenshot shows the 'Thermodynamic calculator editor' window. The 'MODEL' tab is selected and highlighted with a red box. The 'Profile' dropdown menu is also highlighted with a red box and shows 'NRTL' selected. The 'Activity coefficient model' dropdown is also set to 'NRTL'. The 'THERMODYNAMIC MODEL' panel on the right is visible, showing various options like 'DOCUMENTATION', 'ADDITIONAL PARAMETERS', etc.

2 - Select the “NRTL” thermodynamic profile

# Step 2: Select the thermodynamic model

1 - Click on the “Binaries” tab, then enter the binary interaction parameters

Thermodynamic calculator editor

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

COMPOUNDS | MODEL | **BINARIES** | PARAMETERS

These parameters correspond to the general values and are used if the user has not provided specific parameters (buttons to the right of each option in the thermodynamic profile)

Binaries view:  Grid  Matrix

Formulation :  $g_{ij} - g_{jj} = C_{ij0} + C_{ijT}(T - 273.15)$ ,  $a_{ij} = a_{ij0} + a_{ijT}(T - 273.15)$

Compound	Compound	C <sub>ij0</sub>	C <sub>ji0</sub>	a <sub>ij0</sub>	C <sub>ijT</sub>	C <sub>jiT</sub>	a <sub>ijT</sub>
o-CHLOROTOLUEN	CHLORINE	0	0	0	0	0	0
o-CHLOROTOLUEN	BENZYL DICHLORIC	-707,3	775,314	0,1939	0	0	0
o-CHLOROTOLUEN	HYDROGEN CHLOR	0	0	0	0	0	0
o-CHLOROTOLUEN	BENZOTRICHLORIC	-1246	1463,5	0,1584	0	0	0
o-CHLOROTOLUEN	NITROGEN	0	0	0	0	0	0
CHLORINE	BENZYL DICHLORIC	0	0	0	0	0	0
CHLORINE	HYDROGEN CHLOR	0	0	0	0	0	0
CHLORINE	BENZOTRICHLORIC	0	0	0	0	0	0
CHLORINE	NITROGEN	0	0	0	0	0	0
BENZYL DICHLORIC	HYDROGEN CHLOR	0	0	0	0	0	0
BENZYL DICHLORIC	BENZOTRICHLORIC	64,339	-79,04	0,4097	0	0	0
BENZYL DICHLORIC	NITROGEN	0	0	0	0	0	0
HYDROGEN CHLOR	BENZOTRICHLORIC	0	0	0	0	0	0
HYDROGEN CHLOR	NITROGEN	0	0	0	0	0	0
BENZOTRICHLORIC	NITROGEN	0	0	0	0	0	0

Comments :

Unit: cal/mole

parameters will be ignored  
 parameters are automatically loaded

2 - Click on “OK”

Ok Cancel

# Step 3: Describe the chemical reactions

Back to the “Calculators editor” window, select “Edit the chemical reactions of this calculator”:

The screenshot shows the 'Calculators editor' window. The left sidebar contains a menu with the following items:

- EDITION
  - Add a new calculator
  - Edit this calculator...
  - Edit the chemical reactions of this calculator...**
  - Clone this calculator
  - 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

The main area of the window displays a table with the following data:

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

Below the table is a 'Comments:' field and 'Ok' and 'Cancel' buttons.

# Step 3: Describe the chemical reactions

1 - Select "Add a reaction"

The screenshot shows the 'Chemical reactions editor' window. On the left is a blue sidebar with the title 'CHEMICAL REACTIONS'. Under the 'REACTIONS' section, the 'Add a reaction' button is highlighted with a red box. Below it are options for editing, cloning, deleting, and adding literal expressions. The 'ORDER' section includes 'Move up the reaction' and 'Move down the reaction'. The 'MODIFICATIONS' section includes 'Undo' and 'Redo'. The 'PACKAGE' section includes 'Show the package manager...', 'Import a package...', and 'Build a package...'. The main area of the window contains a table with the following data:

#	Name	Type	Physical state	Model
1	[New reaction]	Kinetic	Liquid	Arrhenius

Below the table is a 'Comments:' text area and 'Ok' and 'Cancel' buttons at the bottom right.

2 - The reactions are displayed here

3 - Double click on the reaction to edit it

# Step 3: Describe the chemical reactions

1 - Select the “Kinetic” option

Chemical reaction editor

CHEMICAL REACTION

REACTION ▲

- Equilibrium
- Kinetic**
- Instantaneous

TOOLS ▲

- PDF Export (Print)

MODIFICATIONS ▲

- Undo
- Redo

HELP ▲

- Technical help...

This window helps you to define the context of your chemical reaction

ID: {269A0068-E608-4508-A78F-5255247CDD41}

2 - Select the “General” tab

General Kinetic parameters Equation Notes

Name   Activated

User ID

Physical state

Reaction heat

Concentration model

Rate model

3 - Specify the general information

Properties		Stoichiometry and orders	
Name	CAS Registry Number® or...	Stoichiometry	Order
o-CHLOROTOLUENE	95-49-8	-1	1
CHLORINE	7782-50-5	-1	1
BENZYL DICHLORIDE	98-87-3	1	0
HYDROGEN CHLORIDE	7647-01-0	1	0
BENZOTRICHLORIDE	98-07-7	0	0
NITROGEN	7727-37-9	0	0

Ok Cancel

# Step 3: Describe the chemical reactions

Chemical reaction editor

REACTION ← →

This window helps you to define the context of your chemical reaction  
ID: {269A0068-E608-4508-A78F-5255247CDD41}

**General** Kinetic parameters Equation Notes

Name   Activated

User ID

Physical state

**Reaction heat**

Concentration model

Rate model

Properties		Stoichiometry and orders	
Name	CAS Registry Number® or...	Stoichiometry	Order
o-CHLOROTOLUENE	95-49-8	-1	1
CHLORINE	7782-50-5	-1	1
BENZYL DICHLORIDE	98-87-3	1	0
HYDROGEN CHLORIDE	7647-01-0	1	0
BENZOTRICHLORIDE	98-07-7	0	0
NITROGEN	7727-37-9	0	0

Ok Cancel

4 - Select the option to automatically calculate the reaction heat from the standard enthalpies of formation

# Step 3: Describe the chemical reactions

Chemical reaction editor

**CHEMICAL REACTION**

REACTION ———— ▲

- Equilibrium
- **Kinetic**
- Instantaneous

TOOLS ———— ▲

PDF Export (Print)

MODIFICATIONS ———— ▲

Undo

Redo

HELP ———— ▲

Technical help...

This window helps you to define the context of your chemical reaction

ID: {269A0068-E608-4508-A78F-5255247CDD41}

**General** Kinetic parameters Equation Notes

Name   Activated

User ID

Physical state

Reaction heat

Concentration model

Rate model

Properties		Stoichiometry and orders	
Name	CAS Registry Number® or...	Stoichiometry	Order
o-CHLOROTOLUENE	95-49-8	-1	1
CHLORINE	7782-50-5	-1	1
BENZYL DICHLORIDE	98-87-3	1	0
HYDROGEN CHLORIDE	7647-01-0	1	0
BENZOTRICHLORIDE	98-07-7	0	0
NITROGEN	7727-37-9	0	0

Ok Cancel

5 - Indicate the concentration model

6 - Select the Arrhenius model



# Step 3: Describe the chemical reactions

Chemical reaction editor

**CHEMICAL REACTION**

REACTION ▲

- Equilibrium
- Kinetic**
- Instantaneous

TOOLS ▲

- PDF Export (Print)

MODIFICATIONS ▲

- Undo
- Redo

HELP ▲

- Technical help...

This window helps you to define the context of your chemical reaction

ID: {269A0068-E608-4508-A78F-5255247CDD41}

**General** Kinetic parameters Equation Notes

Name   Activated

User ID

Physical state

Reaction heat

Concentration model

Rate model

Properties		Stoichiometry and orders	
Name	CAS Registry Number® or...	Stoichiometry	Order
o-CHLOROTOLUENE	95-49-8	-1	1
CHLORINE	7782-50-5	-1	1
BENZYL DICHLORIDE	98-87-3	1	0
HYDROGEN CHLORIDE	7647-01-0	1	0
BENZOTRICHLORIDE	98-07-7	0	0
NITROGEN	7727-37-9	0	0

2 - Enter the stoichiometry coefficients (“-” for reactants and “+” for products”) along with the partial orders

# Step 3: Describe the chemical reactions

Chemical reaction editor

CHEMICAL REACTION

REACTION ▾

- Equilibrium
- Kinetic**
- Instantaneous

TOOLS ▾

PDF Export (Print)

MODIFICATIONS ▾

Undo

Redo

HELP ▾

Technical help...

This window helps you to define the context of your chemical reaction

ID: {269A0068-E608-4508-A78F-5255247CDD41}

1 - Select the "Model" tab

General **Kinetic parameters** Equation Notes

Activation energy 130320 J/mol

Frequency factor 2,7203E17

Frequency factor unit

Quantity	Unit
Time	second
Concentration	mol/l
Molality	mol/kg
Pressure	atm

2 - Specify the kinetic parameters:

- $k^0 = 2.7203E17 \text{ s}^{-1}(\text{mol/l})^{-1}$
- $E_a = 130320 \text{ J/mol}$

Be careful with the units!

Ok Cancel

3 - Click on "OK"

# Step 3: Describe the chemical reactions

Follow the same procedure for the second reaction:

Chemical reactions editor

CHEMICAL REACTIONS

REACTIONS

- +** Add a reaction
- Edit this reaction...
- Clone this reaction
- Delete this reaction
- Literal expressions...

ORDER

- Move up the reaction
- Move down the reaction

MODIFICATIONS

- Undo
- Redo

PACKAGE

- Show the package manager...
- Import a package...
- Build a package...

This window helps you to manage your chemical reaction list

#	Name	Type	Physical state	Model
1	<input checked="" type="checkbox"/> o-Chlorotoluene + Cl2 =>	Kinetic	Liquid	Arrhenius
2	<input checked="" type="checkbox"/> [New reaction]	Kinetic	Liquid	Arrhenius

Comments:

Ok Cancel

1 - Click on "Add a reaction"

2 - Double click on the second reaction to edit it

# Step 3: Describe the chemical reactions

1 - Select the “Kinetic” option

Chemical reaction editor

CHEMICAL REACTION

REACTION ▲

- Equilibrium
- Kinetic**
- Instantaneous

TOOLS ▲

- PDF Export (Print)

MODIFICATIONS ▲

- Undo
- Redo

HELP ▲

- Technical help...

This window helps you to define the context of your chemical reaction

ID: {C4A9700F-FF7D-4181-8C6C-123037E5833D}

**General** Kinetic parameters Equation Notes

Name: Benzyl dichloride + Cl2 => Benzotrichloride + HCl  Activated

User ID:

Physical state: Liquid

Reaction heat: Calculated

Concentration model: Molar concentration

Rate model: Arrhenius

3 - Specify the general information

Properties		Stoichiometry and orders	
Name	CAS Registry Number® or...	Stoichiometry	Order
o-CHLOROTOLUENE	95-49-8	0	0
CHLORINE	7782-50-5	-1	1
BENZYL DICHLORIDE	98-87-3	-1	1
HYDROGEN CHLORIDE	7647-01-0	1	0
BENZOTRICHLORIDE	98-07-7	1	0
NITROGEN	7727-37-9	0	0

Ok Cancel

2 - Select the “General” tab

3 - Specify the general information

# Step 3: Describe the chemical reactions

Chemical reaction editor

REACTION ID: {C4A9700F-FF7D-4181-8C6C-123037E5833D}

General Kinetical parameters Equation Notes

Name: Benzyl dichloride + Cl2 => Benzotrichloride + HCl  Activated

User ID:

Physical state: Liquid

Reaction heat: Calculated 0 cal/mol

Concentration model: Molar concentration

Rate model: Arrhenius

Properties		Stoichiometry and orders	
Name	CAS Registry Number® or...	Stoichiometry	Order
o-CHLOROTOLUENE	95-49-8	0	0
CHLORINE	7782-50-5	-1	1
BENZYL DICHLORIDE	98-87-3	-1	1
HYDROGEN CHLORIDE	7647-01-0	1	0
BENZOTRICHLORIDE	98-07-7	1	0
NITROGEN	7727-37-9	0	0

Ok Cancel

4 - Select the option to automatically calculate the reaction heat from the standard enthalpies of formation

# Step 3: Describe the chemical reactions

Chemical reaction editor

CHEMICAL REACTION

REACTION ———— ▲

- Equilibrium
- Kinetic**
- Instantaneous

TOOLS ———— ▲

PDF Export (Print)

MODIFICATIONS ———— ▲

Undo

Redo

HELP ———— ▲

Technical help...

This window helps you to define the context of your chemical reaction

ID: {C4A9700F-FF7D-4181-8C6C-123037E5833D}

**General** Kinetic parameters Equation Notes

Name   Activated

User ID

Physical state

Reaction heat

Concentration model

Rate model

Properties		Stoichiometry and orders	
Name	CAS Registry Number® or...	Stoichiometry	Order
o-CHLOROTOLUENE	95-49-8	0	0
CHLORINE	7782-50-5	-1	1
BENZYL DICHLORIDE	98-87-3	-1	1
HYDROGEN CHLORIDE	7647-01-0	1	0
BENZOTRICHLORIDE	98-07-7	1	0
NITROGEN	7727-37-9	0	0

Ok Cancel

5 - Indicate the concentration model

6 - Select the Arrhenius model

# Step 3: Describe the chemical reactions

Chemical reaction editor

**CHEMICAL REACTION** This window helps you to define the context of your chemical reaction

REACTION ID: {C4A9700F-FF7D-4181-8C6C-123037E5833D}

Equilibrium  
 **Kinetic**  
 Instantaneous

**TOOLS**  
 PDF Export (Print)

**MODIFICATIONS**  
 Undo  
 Redo

**HELP**  
 Technical help...

**General** Kinetic parameters Equation Notes

Name: Benzyl dichloride + Cl<sub>2</sub> => Benzotrichloride + HCl  Activated

User ID:

Physical state: Liquid

Reaction heat: Calculated 0 cal/mol

Concentration model: Molar concentration

Rate model: Arrhenius

Properties		Stoichiometry and orders	
Name	CAS Registry Number® or...	Stoichiometry	Order
o-CHLOROTOLUENE	95-49-8	0	0
CHLORINE	7782-50-5	-1	1
BENZYL DICHLORIDE	98-87-3	-1	1
HYDROGEN CHLORIDE	7647-01-0	1	0
BENZOTRICHLORIDE	98-07-7	1	0
NITROGEN	7727-37-9	0	0

2 - Enter the stoichiometry coefficients (“-” for reactants and “+” for products”) along with the partial orders

# Step 3: Describe the chemical reactions

1 - Select the “Model” tab

2 - Specify the kinetic parameters:

- $k^0 = 2.7203E17 \text{ s}^{-1}(\text{mol/l})^{-1}$
- $E_a = 130320 \text{ J/mol}$

Be careful with the units!

3 - Click on “OK”



# Step 3: Describe the chemical reactions

Both reactions are now configured

Chemical reactions editor

This window helps you to manage your chemical reaction list

#	Name	Type	Physical state	Model
1	<input checked="" type="checkbox"/> o-Chlorotoluene + Cl2 =>	Kinetic	Liquid	Arrhenius
2	<input checked="" type="checkbox"/> Benzyl dichloride + Cl2 =>	Kinetic	Liquid	Arrhenius

CHEMICAL REACTIONS

REACTIONS

- Add a reaction
- Edit this reaction...
- Clone this reaction
- Delete this reaction
- Literal expressions...

ORDER

- Move up the reaction
- Move down the reaction

Click on “Literal expressions” to display the equation of reaction

Literal expression of the reactions

CHEMICAL REACTIONS

DISPLAY

- Chemical formula
- Compound name

TOOLS

- Copy

C7H7Cl + Cl2 → C7H6Cl2 + HCl

Cl2 + C7H6Cl2 → HCl + C7H5Cl3

Close

# Step 3: Describe the chemical reactions

Click on “OK” to validate the calculator and return to the main window:

Chemical reactions editor

CHEMICAL REACTIONS

REACTIONS

- Add a reaction
- Edit this reaction...
- Clone this reaction
- Delete this reaction
- Literal expressions...

ORDER

- Move up the reaction
- Move down the reaction

MODIFICATIONS

- Undo
- Redo

PACKAGE

- Show the package manager...
- Import a package...
- Build a package...

This window helps you to manage your chemical reaction list

#	Name	Type	Physical state	Model
1	<input checked="" type="checkbox"/> o-Chlorotoluene + Cl2 => I	Kinetic	Liquid	Arrhenius
2	<input checked="" type="checkbox"/> Benzyl dichloride + Cl2 =>	Kinetic	Liquid	Arrhenius

Comments:

Ok Cancel

Calculators editor

CALCULATORS

EDITION

- Add a new calculator
- Edit this calculator...
- Edit the chemical reactions of this calculator...
- Clone this calculator
- 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	<input checked="" type="checkbox"/>	[New calculator]	Native	Yes (2/2)

Comments:

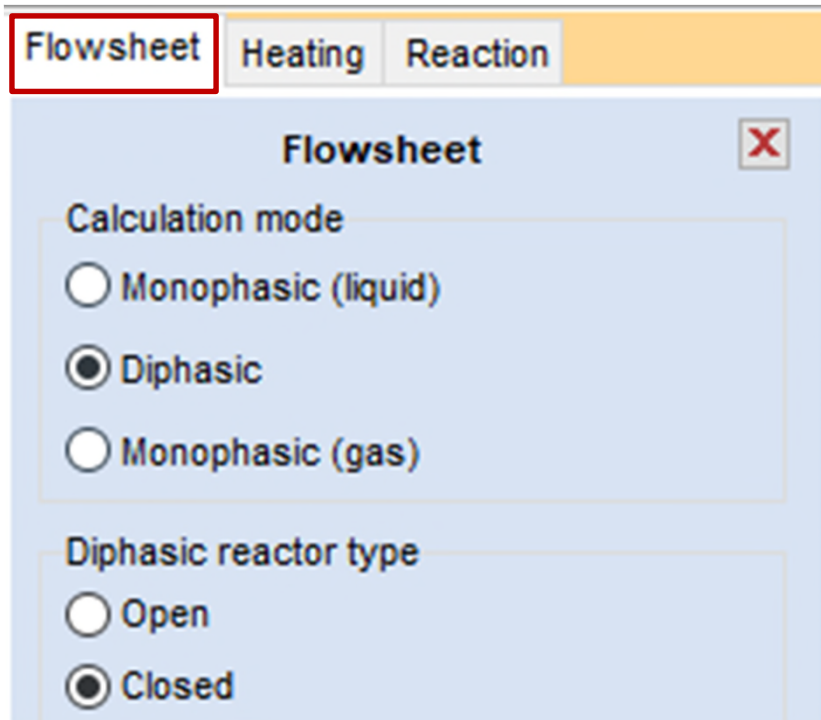
Ok Cancel



# Step 4: Describe the equipment

The “flowsheet” window allows to describe the following features:

- The general topology of the reactor
- The initial conditions inside the reactor
- The equipment characteristics



# Step 4: Describe the equipment

## Configure the control panel:

- 1 - Calculation mode: "Diphasic"
- 2 - Reactor type: "Closed"
- 3 - With a condenser
- 4 - Vessel bottom geometry: "torispherical"
- 5 - Mixing device: "3 retreating-blades impeller"
- 6 - With a wall heat exchanger:
  - External jacket
  - Joined

Flowsheet Heating Reaction

**Flowsheet** [X]

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

3 retreating-blades impeller

Dissipated heat included

With an external heat exchanger

With an helical coil

With a wall heat exchanger

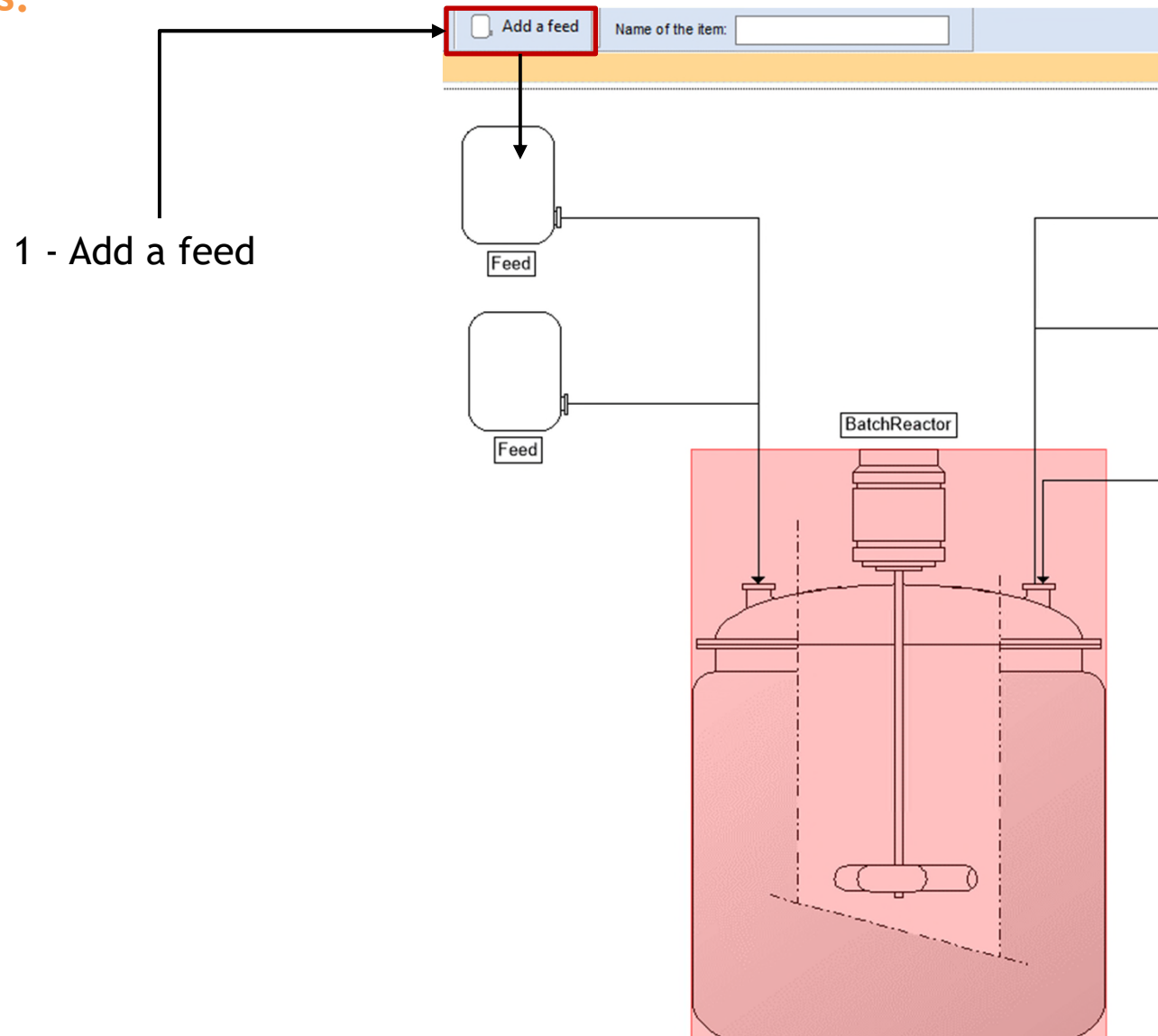
With an inductor

External jacket

Joined

# Step 4: Describe the equipment

## Configure the feeds:

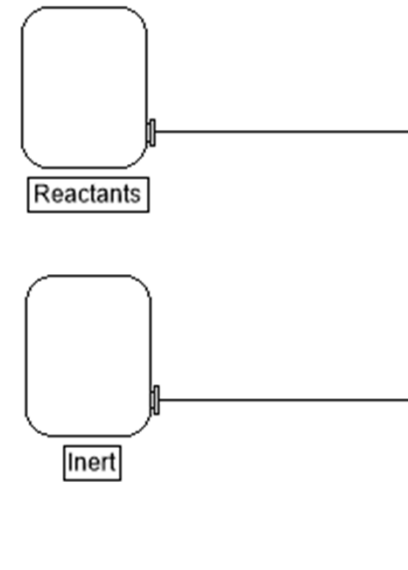
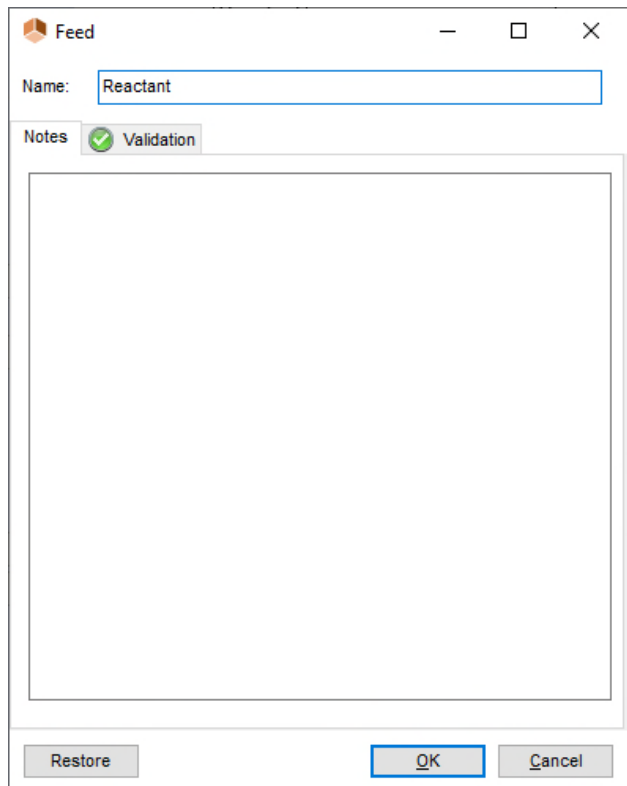


# Step 4: Describe the equipment

## Configure the feeds:

2 - Double click on the feeds to rename them:

- “Reactant”
- “Inert”



The feed characteristics will be specified in the operating steps

# Step 4: Describe the equipment

Double click on the reactor in order to open its configuration window:

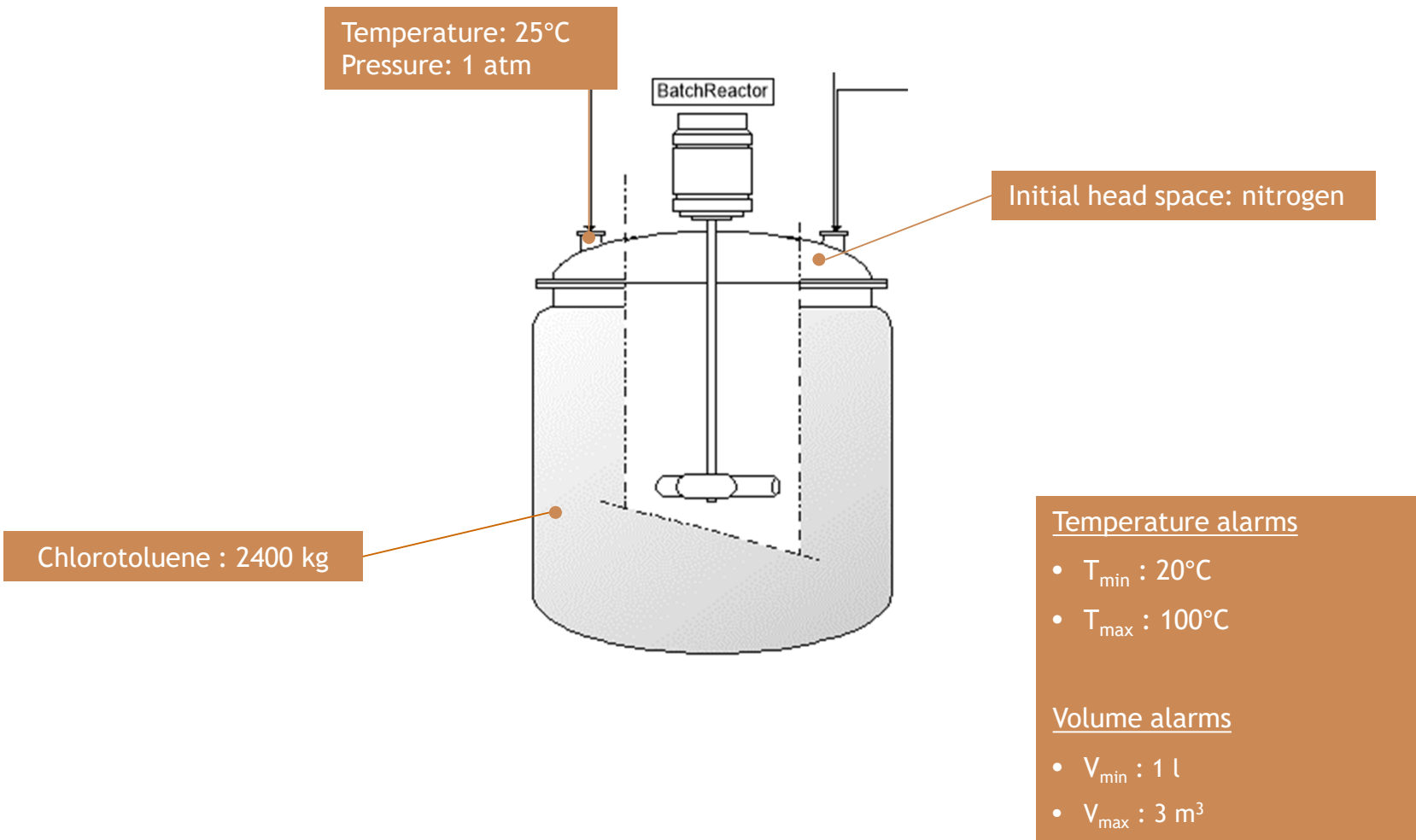
The image displays a software interface for configuring a reactor. On the left, a 'Flowsheet' panel shows various options for reactor configuration, including calculation mode (Ophasic, Monophasic (liquid), Monophasic (gas)), reactor type (Open, Closed), and various heat and mass transfer options. The main area shows a process flow diagram with a central 'BatchReactor' vessel, two 'Feed' tanks, a 'Condenser', a 'Bypass' line, and two 'Storage' tanks labeled 'S01' and 'TL01'. An arrow points from the reactor in the flowsheet to the configuration window on the right.

The 'Reactor' configuration window is titled 'BatchReactor' and contains the following parameters:

- Name:** BatchReactor
- Parameters:**
  - Reactor temperature [TR]: Fixed temperature 25 °C, Alarms [TR]: Minimum 20 °C, Maximum 100 °C
  - Reactor pressure [PR]: Fixed pressure 1 atm
  - Global reactor volume [GVR]: 3 m3, Alarms [VR]: Minimum 1, Maximum 3 m3
- Diagram:** A detailed schematic of the reactor vessel showing components like 'Feeds', 'Head space', 'Mixing device', 'Initial load', 'Vessel bottom geometry', 'Wall heat-exchanger', 'Wall materials', 'Vapor productions', 'Liquid productions', and 'By-pass'.
- Buttons:** Restore, Technology, Reference / Note, OK, Cancel

# Step 4: Describe the equipment

First, specify the initial conditions as well as the alarms:





# Step 4: Describe the equipment

- Initial conditions and alarms:

Reactor

Name:

Parameters **Notes** Advanced parameters **Validation**

Feeds

Vapor productions

Liquid productions

Reactor temperature [TR]

Fixed temperature

Alarms [TR]

Minimum

Maximum

Reactor pressure [PR]

Fixed pressure

Global reactor volume [GVR]

Alarms [VR]

Minimum

Maximum

Head space

Mixing device

Wall heat-exchanger

Wall materials

Initial load

Vessel bottom geometry

Liquid productions

Restore Technology Reference / Note

OK Cancel

# Step 4: Describe the equipment

- Initial load:

Initial load

Initial load specification

Partial loads Mass

Compound	
o-CHLOROTOLUENE	2400 kg
CHLORINE	0.000000 kg
BENZYL DICHLORIDE	0.000000 kg
HYDROGEN CHLORIDE	0.000000 kg
BENZOTRICHLORIDE	0.000000 kg
NITROGEN	0.000000 kg

Restore OK Cancel

# Step 4: Describe the equipment

- Head space:

Head space

Head space

Head space type

Air

Nitrogen

Other

None

N2  %

O2  %

Adjustment variable

Pressure

Temperature

"Pressurizing" compound

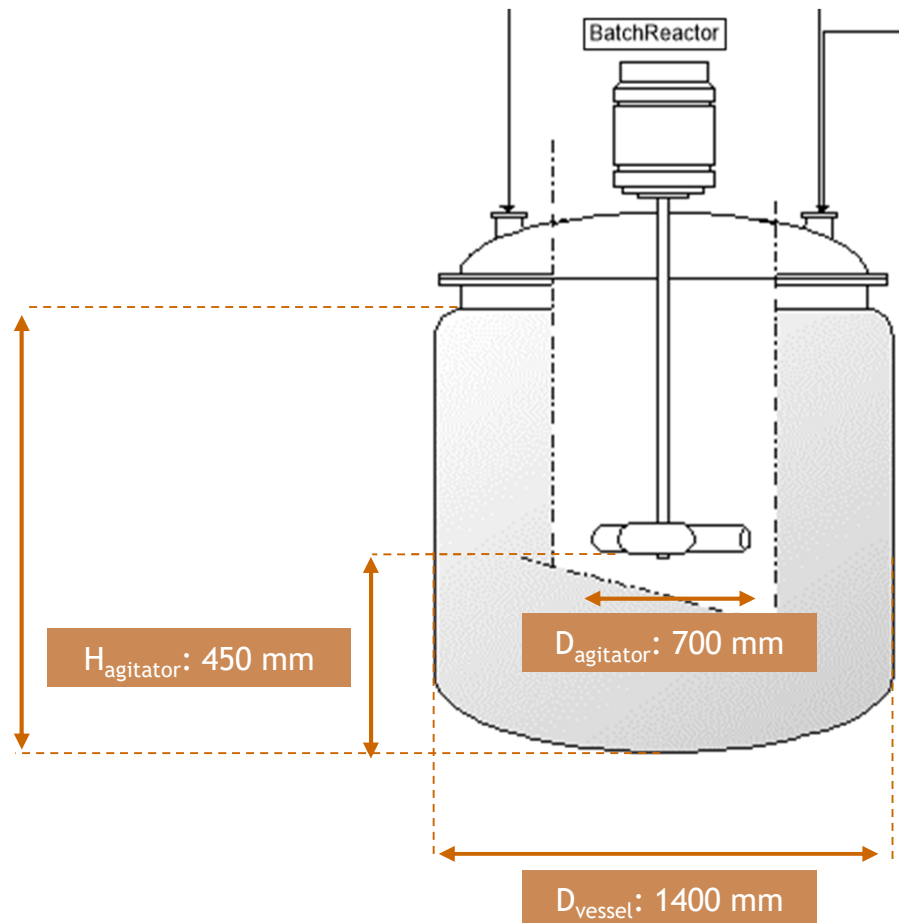
Restore

OK

Cancel

# Step 4: Describe the equipment

Configure the equipment geometry:



## Vessel:

- Number of baffles: 4
- Diameter: 1400 mm
- Curve radius #1: 1400 mm
- Curve radius #2: 140 mm

## Mixing device:

- Diameter: 700 mm
- Height: 450 mm

## External jacket:

- Height: 1700 mm
- Jacket-vessel distance: 50 mm

## Wall materials:

- Thickness: 17 mm
- Weight: 800 kg

# Step 4: Describe the equipment

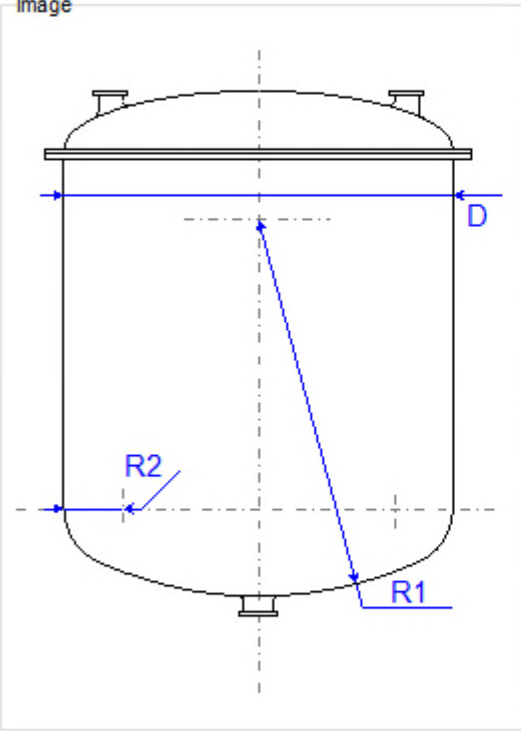
- Vessel bottom geometry:

Vessel bottom geometry

Vessel bottom geometry

Vessel bottom geometry is known

Image



Type of vessel bottom geometry

Torispherical

Parameters

Number of baffles	4
Vessel diameter (D)	1400 mm
Vessel bottom height (H)	0 m
Curve radius #1 (R1)	1400 mm
Curve radius #2 (R2)	140 mm

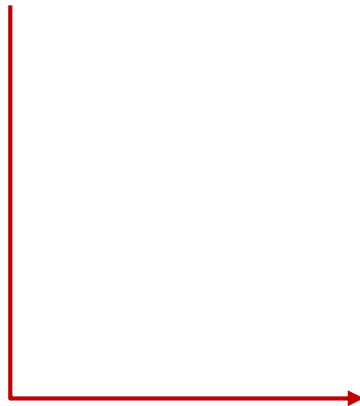
Reference / Note

Restore Technology OK Cancel

# Step 4: Describe the equipment

- Mixing device:

Mixing device



Mixing device
✕

With a mixing device

Image

Dissipated heat included

Parameters

3 retreating-blades impeller

Agitator diameter: 700 mm

Agitator height: 450 mm

Ribbon-vessel distance: 0 m

Ribbon width: 0 m

Power number: 0.9

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 (wall)

Reference / Note

Default rotation speed (\*): 60 rpm

(\* used for the scale-up or mass transfer calculation when no rotation speed has been defined for the step.

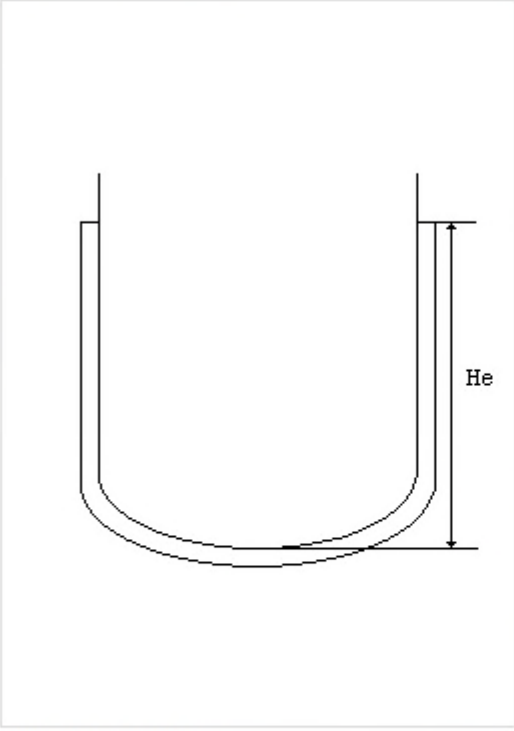
Restore
Technology
OK
Cancel

# Step 4: Describe the equipment

- Wall heat-exchanger:

Wall heat-exchanger

**External jacket geometry** ✕



**Layout**

Side only  
 Separated  
 Joined  
 Bottom

**Jacket characteristic**

None  
 Agitation nozzles  
 Dimple jacket  
 Spirally baffled

**Geometrical parameters**

Baffle step ( $E_c$ )	0 m
Jacket-vessel distance ( $E_e$ )	50 mm
Height of side (or total) jacket ( $H_e$ )	1700 mm
Side jacket-vessel bottom distance ( $H_j$ )	0 m
Jacket thickness ( $E_{de}$ )	0 m
Number of agitation nozzles	3
Throat diameter	0.015 m
Average roughness in the jacket	4.57E-5 m

**Utility flow direction**

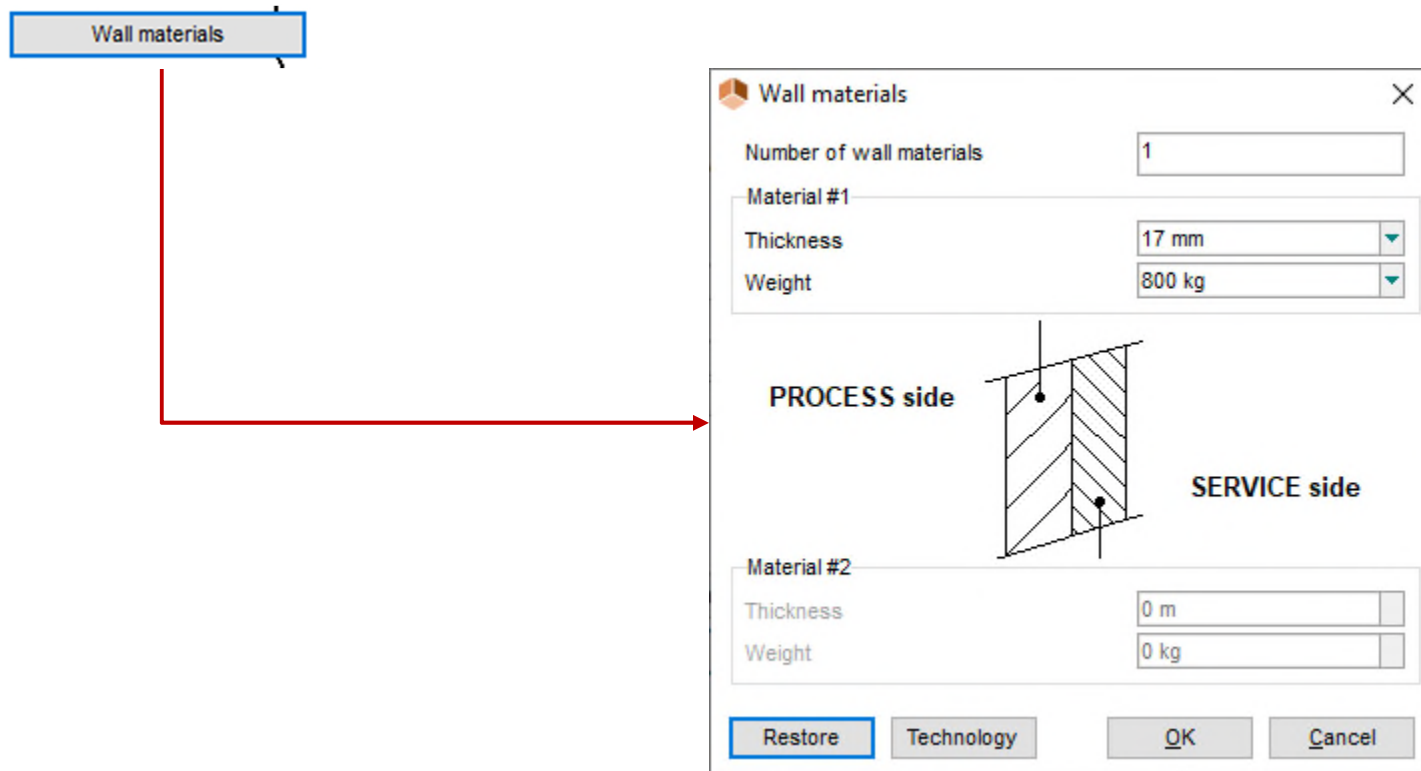
Up  
 Down

Restore Technology

OK Cancel

# Step 4: Describe the equipment

- Wall materials:

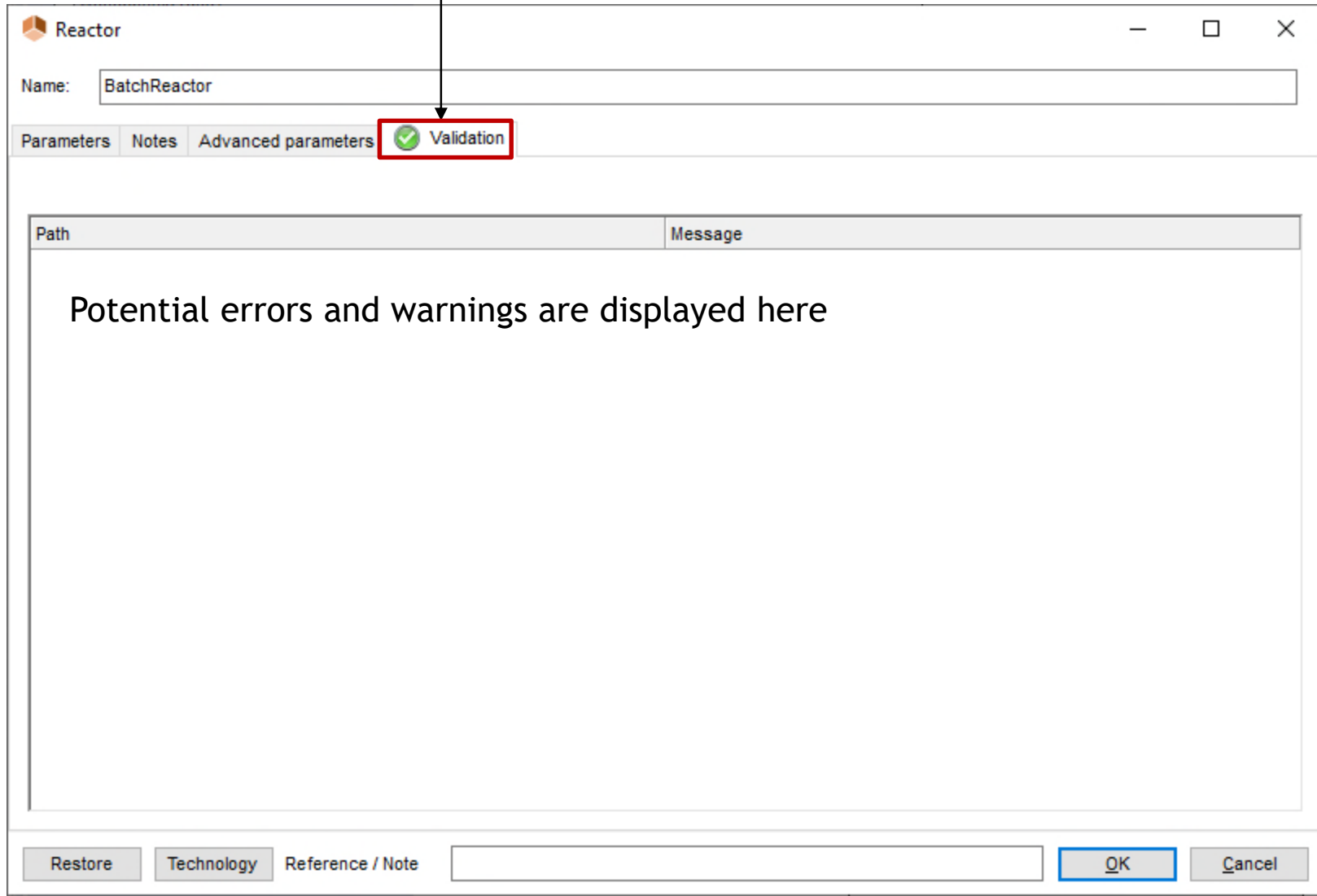


Note: it is possible to save/import equipment characteristics by clicking on the “Technology” button



# Step 4: Describe the equipment

Click on the “Validation” tab

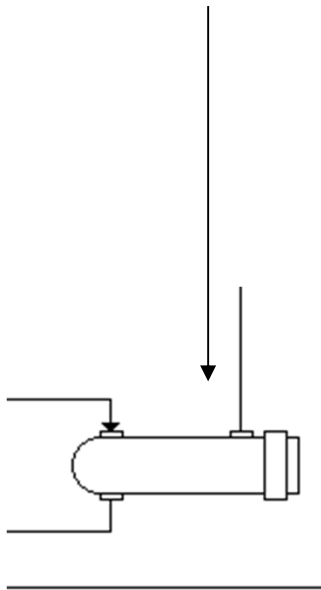


The screenshot shows the Reactor software window. The title bar reads "Reactor". Below the title bar is a text field labeled "Name:" containing the text "BatchReactor". Below the text field is a tabbed interface with four tabs: "Parameters", "Notes", "Advanced parameters", and "Validation". The "Validation" tab is selected and highlighted with a red box. An arrow points from the text "Click on the 'Validation' tab" to the "Validation" tab. Below the tabs is a table with two columns: "Path" and "Message". The table is currently empty. Below the table is a text area containing the text "Potential errors and warnings are displayed here". At the bottom of the window are several buttons: "Restore", "Technology", "Reference / Note", "OK", and "Cancel".

Path	Message
Potential errors and warnings are displayed here	

# Step 4: Describe the equipment

Double click on the condenser to access its configuration window



Enter the number of stages: 2  
Two condensers in series are then defined

Condenser

Name: Condenser

Parameters Notes Validation

Condenser geometry is known

Number of stages: 2

1st stage geometry 2nd stage geometry

Duplicate Technology

Reference / Note

Total number of tubes: 1

Tube layout: Square

Tube step (d1): 0 m

Tube thickness (d2): 0 m

Inside tube diameter (d3): 0 m

Number of passes (shell side): 1

Number of baffles: 1

Tube length: 0 m

Tube thermal conductivity: 100 W/m/K

Condenser orientation: Horizontal

Inside shell diameter (D): 0 m

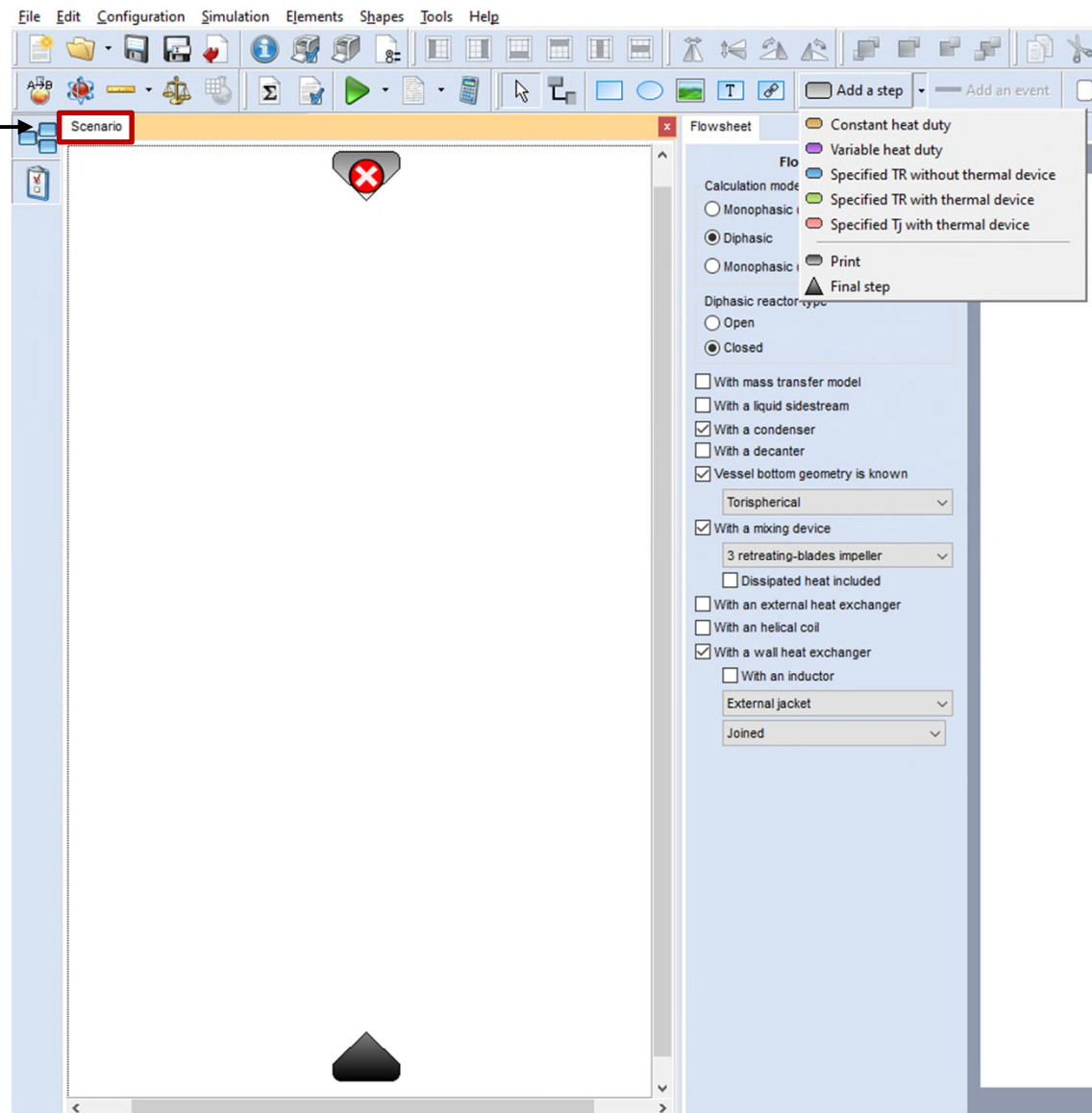
Baffle opening ratio (h/D): 0.25

Restore OK Cancel

A detailed cross-sectional diagram of a condenser. It shows a cylindrical shell with a hemispherical head on the left. The shell diameter is labeled 'D' and the baffle opening height is labeled 'h'. The diagram shows the internal tube bundle and the baffle structure.

# Step 5: Describe the operating steps

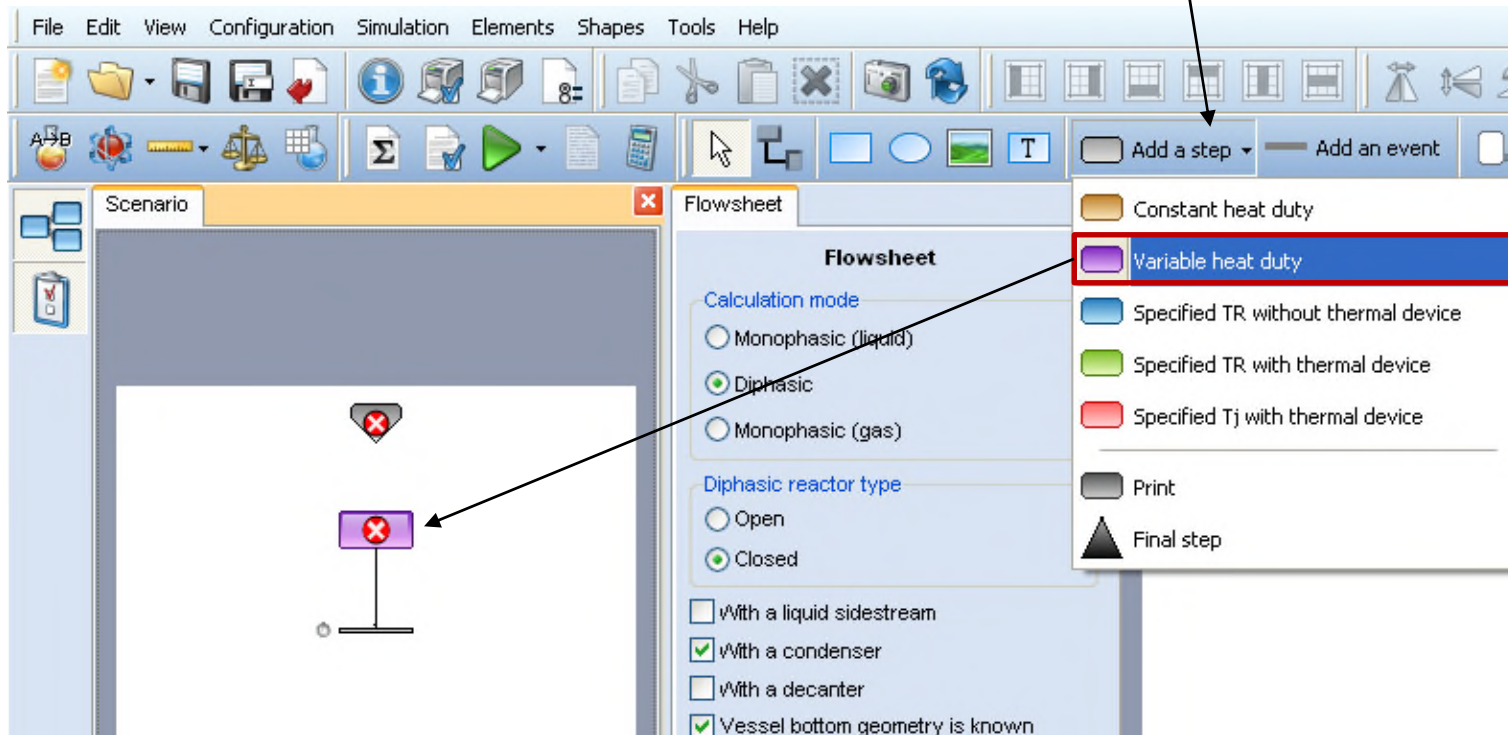
The operating mode is described in the “Scenario” tab and corresponds to a sequence of steps and events



# Step 5: Describe the operating steps

- Add the “heating” step:

1 - Click on “Add a step” and then on “Variable heat duty”



2 - Click on the “Scenario” tab.  
A new step and a new event are created

# Step 5: Describe the operating steps

- Connect the steps:

2 - Click on the first triangle (operation start) and then click on the first step.

1 - Click on “connection”

The screenshot shows the software interface for creating a flowsheet. The main workspace is divided into two panes: 'Scenario' and 'Flowsheet'. The 'Scenario' pane shows a diagram of a reactor with a purple 'Step' box. The 'Flowsheet' pane shows configuration options for a reactor, including 'Calculation mode' (Diphasic selected) and 'Diphasic reactor type' (Closed selected). A red box highlights a 'connection' icon in the toolbar, and an arrow points from the text '1 - Click on “connection”' to it. Another arrow points from the text '2 - Click on the first triangle (operation start) and then click on the first step.' to the 'Step' box in the Scenario window.

# Step 5: Describe the operating steps

- Configure the “heating” step:

The screenshot displays the software interface for configuring a step. The top toolbar includes icons for adding a step, event, and feed, along with a text input field for the item name. The flowsheet diagram shows a purple 'Step' block connected to a feed. The configuration window, titled 'Variable heat duty', is open, showing the following settings:

- Step name: Step
- 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: 
  - 3 retreating-blades impeller
- Dissipated heat included:
- With an external heat exchanger:
- With an helical coil:
- With a wall heat exchanger: 
  - External jacket
  - Joined
- With an inductor:

On the right, a 3D model of a 'BatchReactor' is shown with a red highlight, indicating its configuration. The reactor is connected to 'Reactants' and 'Inerte' feeds.

Double click on the operating step to access its configuration window

# Step 5: Describe the operating steps

- Configure the “heating” step:

The screenshot displays a software interface for configuring a process step. On the left, a flowsheet shows a funnel-shaped inlet connected to a purple rectangular box labeled 'Heating', which is then connected to a horizontal line with a valve symbol. The top toolbar contains various icons for navigation and configuration, including a play button, a document, a calculator, a mouse cursor, a square, a circle, a landscape, a text box, a link, and buttons for 'Add a step' and 'Add'. The 'Heating' step is highlighted in the toolbar. On the right, a configuration panel titled 'Variable heat duty' is open. The 'Step name' field is set to 'Heating' and is highlighted with a blue border. Below this, there are radio buttons for 'Calculation mode' (Monophasic (liquid), Diphasic, Monophasic (gas)) and 'Diphasic reactor type' (Open, Closed). A checkbox for 'With mass transfer model' is visible at the bottom.

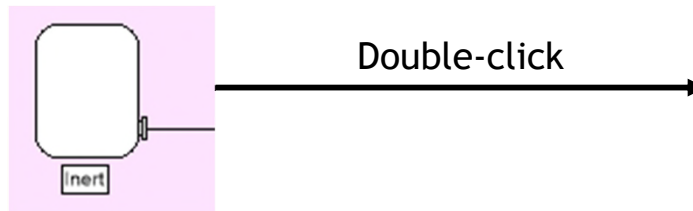
Rename the step “heating”

# Step 5: Describe the operating steps

- Configure the “heating” step:

Specify the properties of the “inert” feed:

- Check the “Feed is open” option
- Temperature: 25°C
- Pressure: 1 atm
- Nitrogen flowrate: 1 kg/h



Feed

Name:

Parameters  Notes  Validation

Feed is open

Temperature specification  
Given temperature:

Pressure specification  
Given pressure:

Init flowrate specification  flowrate variation

Partial flowrates

Compound	Flowrate
o-CHLOROTOLUENE	0.000000 kg/s
CHLORINE	0.000000 kg/s
BENZYL DICHLORIDE	0.000000 kg/s
HYDROGEN CHLORIDE	0.000000 kg/s
BENZOTRICHLORIDE	0.000000 kg/s
NITROGEN	1 kg/h

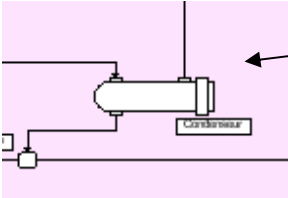
Calculator:

Restore



# Step 5: Describe the operating steps

- Configure the “heating” step:



1 - Double click on the condenser to open its configuration window

2 - Check the “condenser is open” box

3 - Condenser type: calculated

4 - In use stages: 2

# Step 5: Describe the operating steps

- Configure the “heating” step:

## Characteristics of the condenser 1<sup>st</sup> stage:

- Calculation type: at specified area and exchange coefficient
- Exchange coefficient: 300 kcal/h/m<sup>2</sup>/K
- Exchange area: 15 m<sup>2</sup>
- Utility fluid:
  - Water
  - Inlet temperature: 20°C
  - Mass flowrate: 3000 kg/h

Condenser

Name: Condenser

Parameters Notes Validation

State parameters

Condenser is open

Condenser type: Calculated condenser

In use stages: 2

1st used stage 2nd used stage

Calculation type: At specified area and exchange coefficient Duplicate

Exchange coefficient: 300 kcal/h/m<sup>2</sup>/K

Exchange area: 15 m<sup>2</sup>

Pressure drop: 0 Pa

Utility fluid

Fluid type: Water

Inlet temperature: 20 °C

Point #1

Reference temperature: 25 °C

Mass specific heat: 0 J/kg/K

Density: 0 kg/m<sup>3</sup>

Dynamic viscosity: 0 Pa.s

Thermal conductivity: 0 W/m/K

Point #2

Reference temperature: 25 °C

Mass specific heat: 0 J/kg/K

Density: 0 kg/m<sup>3</sup>

Dynamic viscosity: 0 Pa.s

Thermal conductivity: 0 W/m/K

Technology Reference / Note

Number of calculation steps: 10

Fouling factor (TUBES side): 0 W/m<sup>2</sup>/K

Fouling factor (SHELL side): 0 W/m<sup>2</sup>/K

Point number: 2

Mass flowrate: 3000 kg/h

Calculator: Default calculator

Restore OK Cancel

# Step 5: Describe the operating steps

- Configure the “heating” step:

## Characteristics of the condenser 2<sup>nd</sup> stage:

- Calculation type: at specified area and exchange coefficient
- Exchange coefficient: 300 kcal/h/m<sup>2</sup>/K
- Exchange area: 0.5 m<sup>2</sup>
- Utility fluid:
  - Click on “Technology” and import « Ethylene glycol 40% » from the database
  - Inlet temperature: -15°C
  - Mass flowrate: 100 kg/h

Condenser

Name: Condenser

Parameters Notes Validation

State parameters

Condenser is open

Condenser type: Calculated condenser

In use stages: 2

1st used stage: 2nd used stage

Calculation type: At specified area and exchange coefficient

Exchange coefficient: 300 kcal/h/m<sup>2</sup>/K

Exchange area: 0.5 m<sup>2</sup>

Pressure drop: 0 Pa

Utility fluid

Fluid type: Other

Inlet temperature: -15 °C

Point #1

Reference temperature: -20 °C

Mass specific heat: 3280 J/kg/K

Density: 1069 kg/m<sup>3</sup>

Dynamic viscosity: 0.0165 Pa.s

Thermal conductivity: 0.436 W/m/K

Point #2

Reference temperature: 100 °C

Mass specific heat: 3790 J/kg/K

Density: 1001 kg/m<sup>3</sup>

Dynamic viscosity: 0.00056 Pa.s

Thermal conductivity: 0.455 W/m/K

Technology: Ethylene glycol 40% (-20 100)

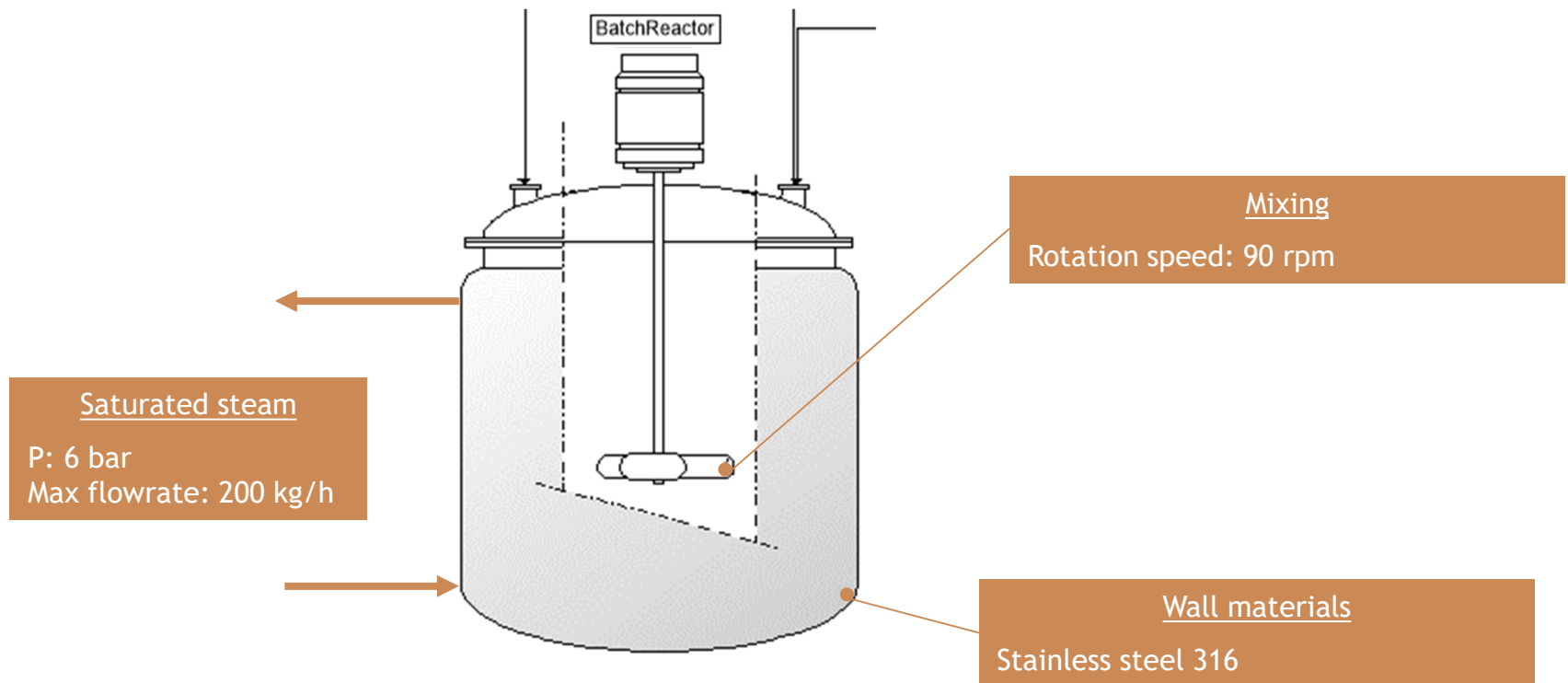
Calculator: Default calculator

Restore OK Cancel

# Step 5: Describe the operating steps

- Configure the “heating” step:

The characteristics of the heating device are the following:



# Step 5: Describe the operating steps

- Configure the “heating” step:

1 - Double click on the reactor icon to access its configuration window



2 - Enter the operating parameters:

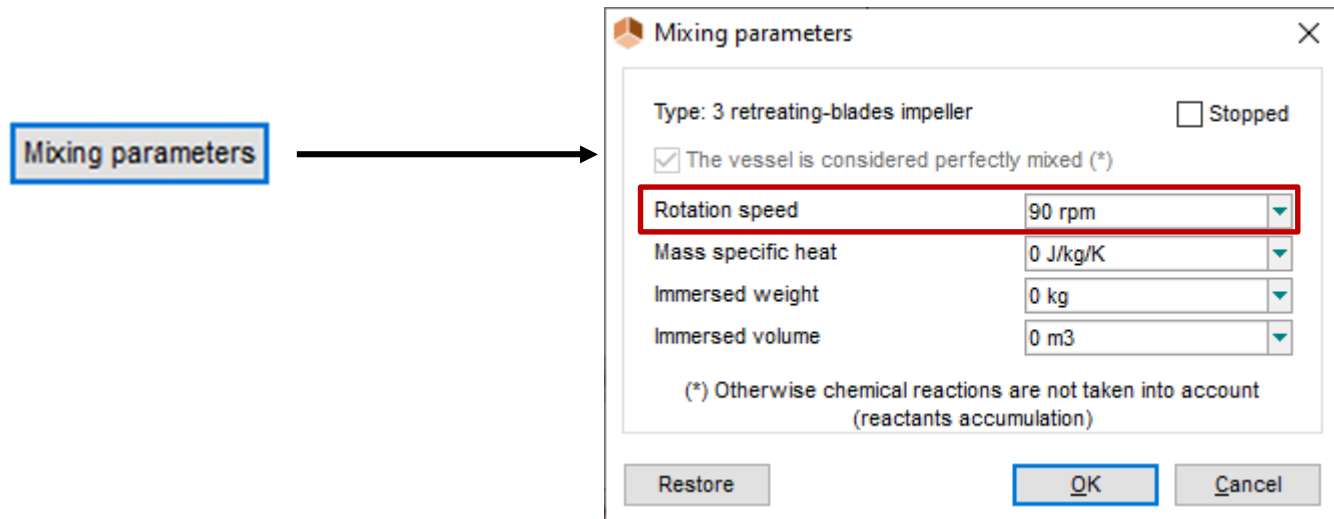
- Reflux ratio (1 for 100% reflux)
- Pressure specification

The screenshot shows the 'Reactor' configuration window for a 'BatchReactor'. The window has several tabs: 'Parameters', 'Notes', 'Advanced parameters', and 'Validation'. The 'Parameters' tab is active, showing a schematic of a reactor with various configuration options. The 'Reflux ratio' is set to 1, and the 'Pressure specification' is set to 1 atm. Other options include 'First feed' (Inert), 'Mixing parameters' (Constant molar fraction, o-CHLOROTOLUENE, Inert, Inert), 'Ti profile', 'Wall heat-exchanger', 'Wall materials', and 'Calculator' (Default calculator). The 'Reflux ratio' and 'Pressure specification' fields are highlighted with red boxes, and arrows point from the text on the left to these fields.

# Step 5: Describe the operating steps

- Configure the “heating” step:

Specify the mixing parameters:



# Step 5: Describe the operating steps

- Configure the “heating” step:

Specify the wall heat exchanger parameters:

Wall heat-exchanger

**Wall heat exchanger parameters**

The wall heat exchanger is in use

Maximum temperature difference process/utility: 0 K

Global exchange coefficient is supplied: 0 W/m<sup>2</sup>/K

Heat exchange coefficient is supplied (PROCESS side): 0 W/m<sup>2</sup>/K

Fouling factor: 0 W/m<sup>2</sup>/K

Heat exchange coefficient is supplied (SERVICE side): 0 W/m<sup>2</sup>/K

Fouling factor: 0 W/m<sup>2</sup>/K

**Utility fluid**

Fluid type: Saturated steam

Inlet temperature: 25 °C

Point number: 2

**Point #1**

Reference temperature: 25 °C

Mass specific heat: 0 J/kg/K

Density: 0 kg/m<sup>3</sup>

Dynamic viscosity: 0 Pa.s

Thermal conductivity: 0 W/m/K

Thermal expansion coefficient: 0 1/K

**Point #2**

Reference temperature: 25 °C

Mass specific heat: 0 J/kg/K

Density: 0 kg/m<sup>3</sup>

Dynamic viscosity: 0 Pa.s

Thermal conductivity: 0 W/m/K

Thermal expansion coefficient: 0 1/K

Mass flowrate: 200 kg/h

Pressure: 6 bar

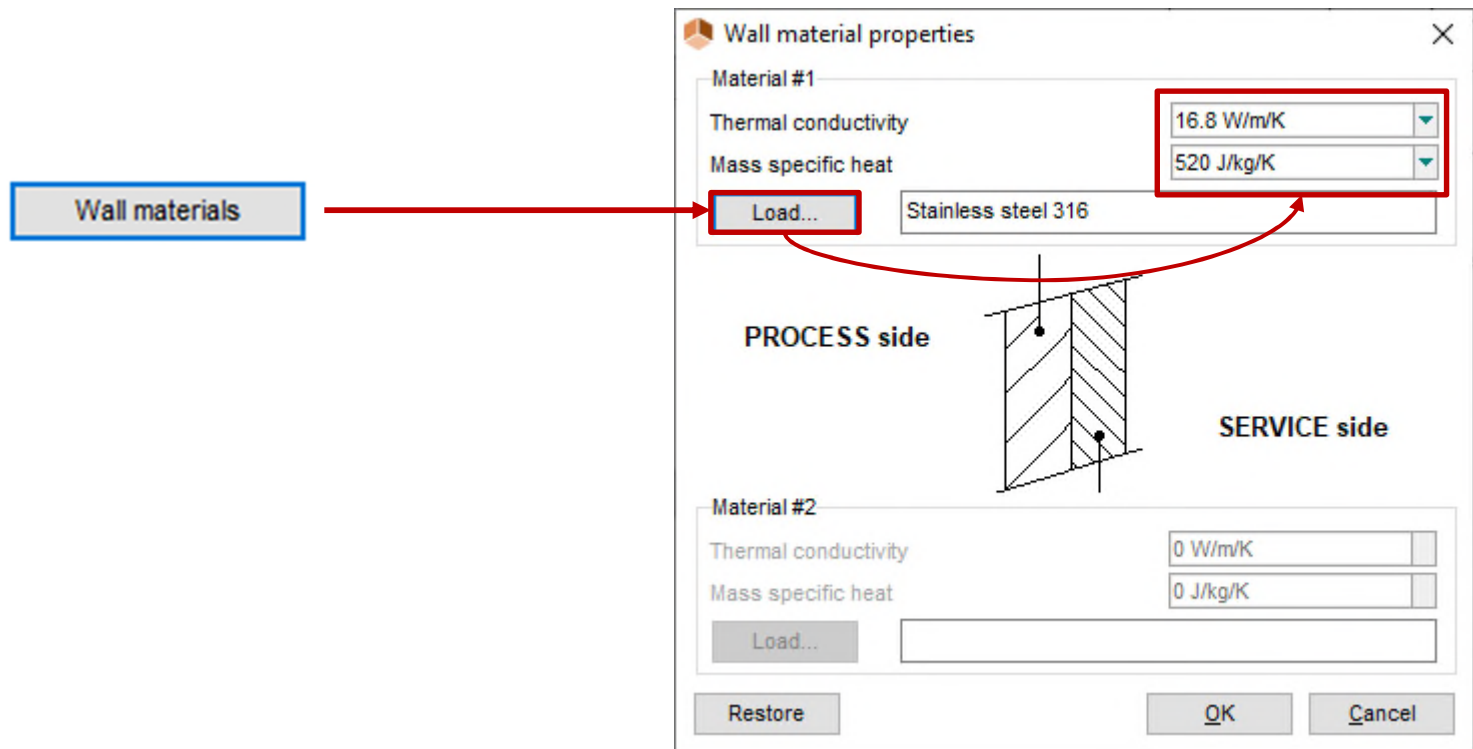
Technology: Reference / Note

Restore OK Cancel

# Step 5: Describe the operating steps

- Configure the “heating” step:

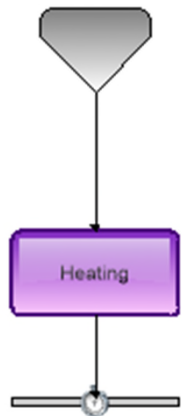
Wall materials: import the characteristics of the “Stainless steel 316” from the database:





# Step 5: Describe the operating steps

- Configure the “heating” step:



1 - Double click on the end event

2 - Specify the event name

3 - Select the event type: temperature of 58°C reached inside the reactor

Event

Information

Name: T(Reactor) = 58°C

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

Temperature

= 58 °C

OK Cancel

# Step 5: Describe the operating steps

- Configure the “reaction” step:

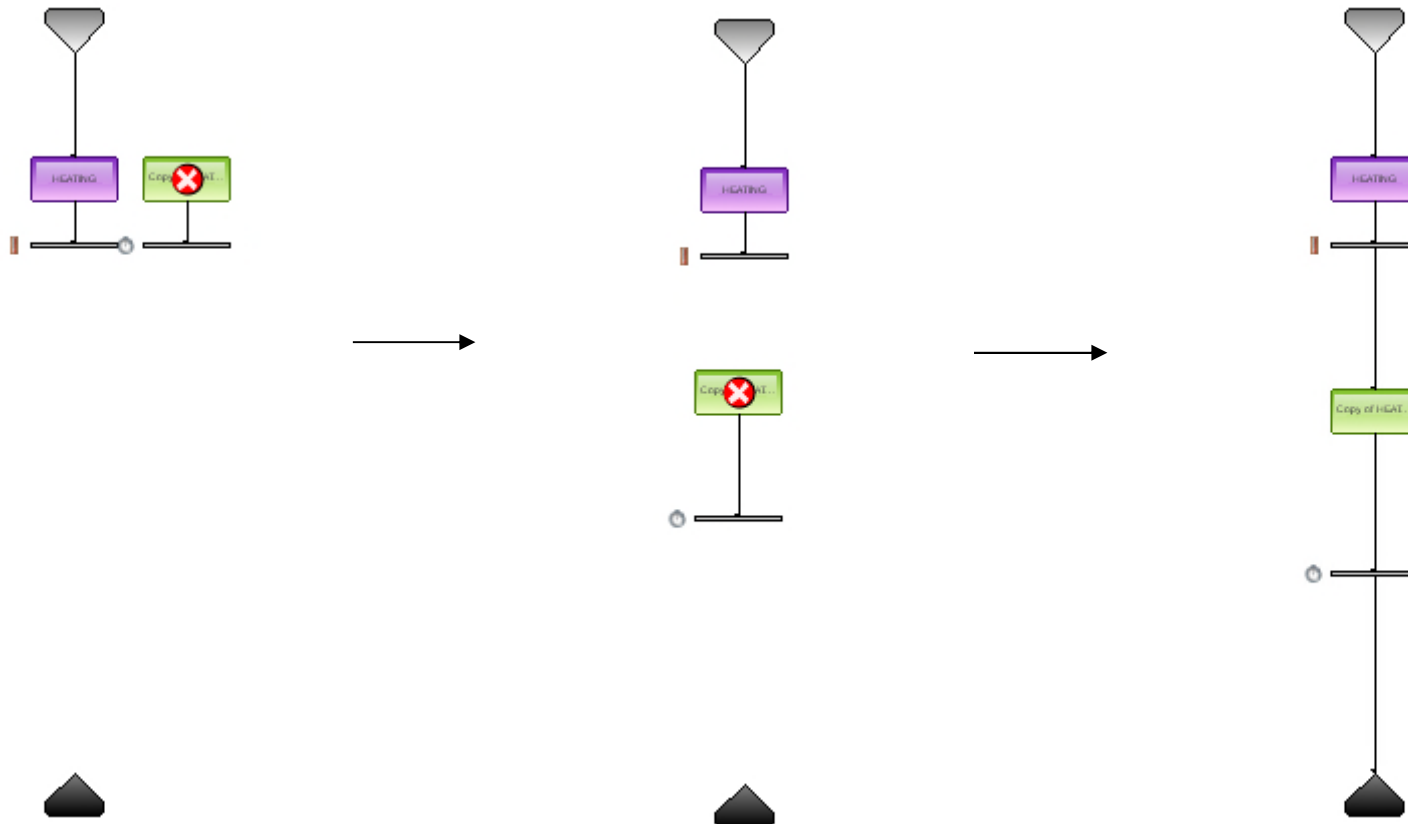
The image shows a software interface for configuring a process step. On the left, a schematic diagram features a purple rectangular block labeled 'Heating' connected to a funnel-shaped inlet at the top and a circular outlet at the bottom. A context menu is open over the 'Heating' block, listing options such as 'Start simulation from this step...', 'Duplicate', 'Duplicate to', 'Convert to', 'Order', 'Flip / Rotate', 'Alignment', and 'Delete selection'. The 'Duplicate to' option is selected, revealing a sub-menu with four choices: 'Constant heat duty', 'Specified Tj with thermal device', 'Specified TR without thermal device', and 'Specified TR with thermal device'. The 'Specified TR with thermal device' option is highlighted with a red border. To the right, a 'Flow' properties panel is partially visible, showing settings for 'Calculation mode' (Diphasic is selected), 'Diphasic reactor type' (Closed is selected), and 'With mass transfer'. A text box on the right contains the instruction: 'Right click on the first operating step and duplicate it to a new “specified TR with thermal device” step'. An arrow points from this text box to the 'Specified TR with thermal device' option in the sub-menu.

Duplicating a step prevents from providing a second time the input parameters that are similar in both steps

# Step 5: Describe the operating steps

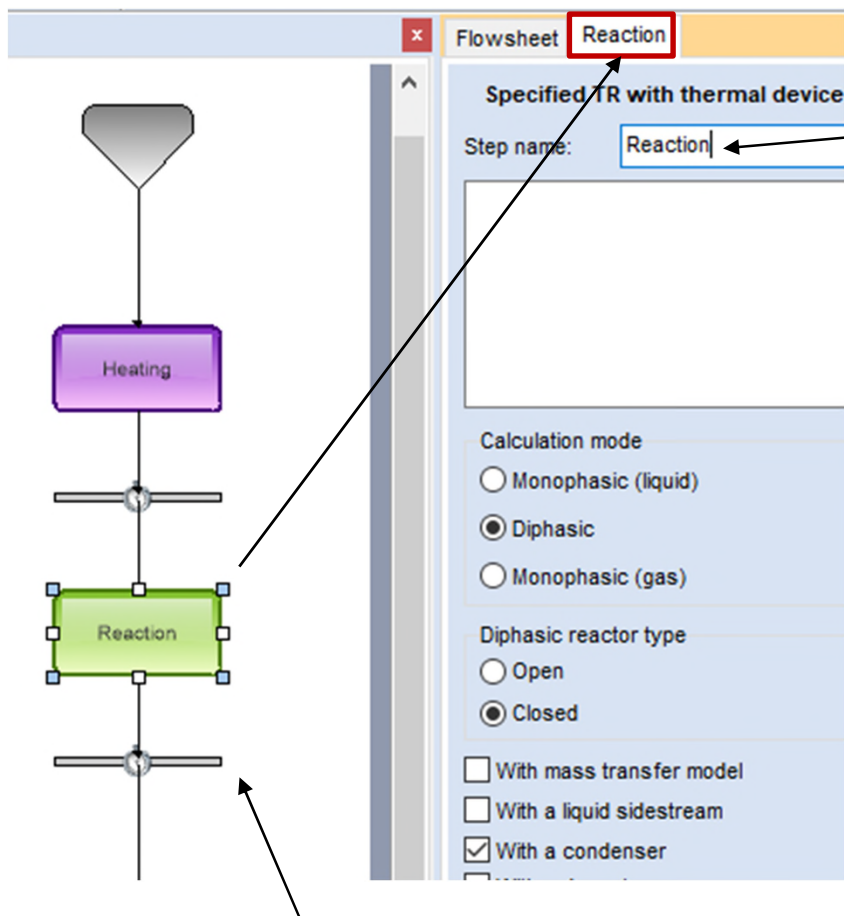
- Configure the “reaction” step:

Connect the new step to the ending event of the heating step and to the ending event of the simulation



# Step 5: Describe the operating steps

- Configure the “reaction” step:



2 - Rename the step “Reaction”

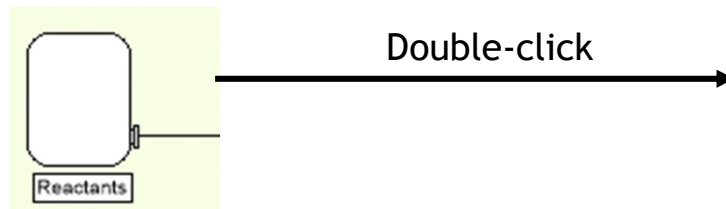
1 - Double click on the new step to access its configuration window

# Step 5: Describe the operating steps

- Configure the “reaction” step:

Specify the properties of the “Reactants” feed:

- Check the “Feed is open” option
- Temperature: 25°C
- Pressure: 3 bar
- Chlorine flowrate: 60 kg/h



Feed
— □ ×

Name:

Parameters

Notes

Validation

Feed is open

Temperature specification  
 Given temperature

Pressure specification  
 Given pressure

Init flowrate specification flowrate variation

Partial flowrates

Compound	Flowrate
o-CHLOROTOLUENE	0.000000 kg/s
CHLORINE	60 kg/h
BENZYL DICHLORIDE	0.000000 kg/s
HYDROGEN CHLORIDE	0.000000 kg/s
BENZOTRICHLORIDE	0.000000 kg/s
NITROGEN	0.000000 kg/s

Calculator

Restore
OK
Cancel

# Step 5: Describe the operating steps

- Configure the “reaction” step:

1 - Double click on the reactor icon to access its configuration window



2 - Check the “PID” option



The screenshot shows the 'Reactor' configuration window with the following details:

- Name:** BatchReactor
- Parameters:** Notes, Advanced parameters, Validation (with a red 'x' icon)
- First feed:** Inert
- Temperature specification:**
  - Minimum: 59°C
  - Set point value: 62°C
  - Maximum: 65°C
  - PID
- Command variable:** Service fluid flowrate
  - Minimum: 1 kg/h
  - Maximum: 10000 kg/h
- Pressure specification:**
  - 1 atm
  - Profile
  - Constant vapor flowrate
- Mixing parameters:**
  - Constant molar fraction
  - o-CHLOROTOLUENE
  - Inert
  - Inert
- Other components:** Wall heat-exchanger, Wall materials, Reflux ratio (1), G01, TL01, PID (on the right side of the reactor schematic).
- Calculator:** Default calculator
- Buttons:** Restore, OK, Cancel

# Step 5: Describe the operating steps

- Configure the “reaction” step:

## 3 - Specify the PID parameters:

### Temperature specification:

- Set point value: 62°C
- Minimum value: 59°C
- Maximum value: 65°C

### Command variable:

- Command variable:  
Service fluid flowrate
- Minimum value: 1 kg/h
- Maximum value: 10 t/h

Reactor

Name: BatchReactor

Parameters Notes Advanced parameters Validation

First feed: Inert

Temperature specification:

- Minimum: 59°C
- Set point value: 62°C
- Maximum: 65°C

Command variable: Service fluid flowrate

- Minimum: 1 kg/h
- Maximum: 10000 kg/h

Reflux ratio: 1

Pressure specification:

- 1 atm
- Profile
- Constant vapor flowrate

Mixing parameters:

- Constant molar fraction
- o-CHLOROTOLUENE
- Inert
- Inert

Wall heat-exchanger

Wall materials

Calculator: Default calculator

Restore OK Cancel

# Step 5: Describe the operating steps

- Configure the “reaction” step:

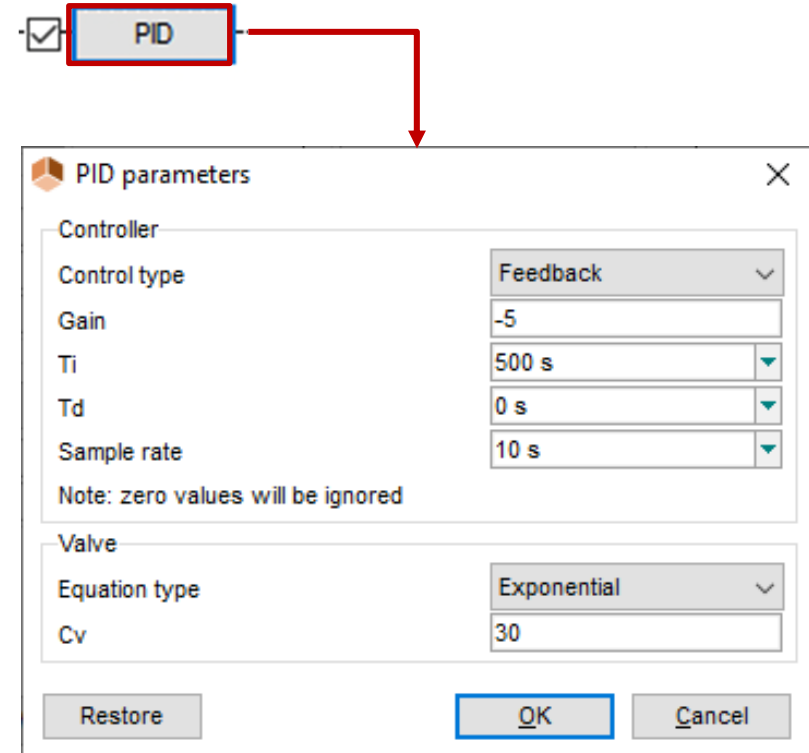
4 - Click on “PID” in order to specify the following parameters:

## Controller:

- Control type: Feedback
- Gain: -5
- $T_i$ : 500 s
- $T_d$ : 0 s
- Sample rate: 10 s

## Valve:

- Equation type: exponential
- Cv : 30





# Step 5: Describe the operating steps

- Configure the “reaction” step:

Specify the characteristics of the cooling system:

- Water
- Temperature: 25°C
- Mass flowrate: 4000 kg/h

Wall heat exchanger parameters

The wall heat exchanger is in use

Maximum temperature difference process/utility: 0 K

Global exchange coefficient is supplied: 0 W/m<sup>2</sup>/K

Heat exchange coefficient is supplied (PROCESS side): 0 W/m<sup>2</sup>/K

Fouling factor: 0 W/m<sup>2</sup>/K

Heat exchange coefficient is supplied (SERVICE side): 0 W/m<sup>2</sup>/K

Fouling factor: 0 W/m<sup>2</sup>/K

Utility fluid

Fluid type: Water

Inlet temperature: 25 °C

Point number: 2

Mass flowrate: 4000 kg/h

Pressure: 6 bar

Point #1

Reference temperature: 25 °C

Mass specific heat: 0 J/kg/K

Density: 0 kg/m<sup>3</sup>

Dynamic viscosity: 0 Pa.s

Thermal conductivity: 0 W/m/K

Thermal expansion coefficient: 0 1/K

Point #2

Reference temperature: 25 °C

Mass specific heat: 0 J/kg/K

Density: 0 kg/m<sup>3</sup>

Dynamic viscosity: 0 Pa.s

Thermal conductivity: 0 W/m/K

Thermal expansion coefficient: 0 1/K

Technology Reference / Note

Restore OK Cancel

Wall heat-exchanger

# Step 5: Describe the operating steps

- Configure the “reaction” step:

It is not necessary to configure the following elements that are identical to the first operating step:

- Mixing parameters
- Wall materials
- Reflux
- Pressure specification
- Condenser characteristics

# Step 5: Describe the operating steps

- Configure the “reaction” step:

The diagram shows a vertical process flow starting with a grey funnel at the top, followed by a purple 'Heating' block, a valve, a green 'Reaction' block, another valve, and finally a black inverted funnel at the bottom. To the right, an 'Event' dialog box is open, showing configuration options for an event named 't = 13 h'. The dialog has tabs for 'Parameters', 'Notes', and 'Validation' (which is checked). Under 'Event type', several radio buttons are listed, with 'Time spent since beginning of step' selected. Below this, a dropdown menu shows 'Time of step' set to '13 h'. At the bottom of the dialog are 'OK' and 'Cancel' buttons. Five numbered arrows point from text instructions to specific elements in the diagram and dialog box.

- 1 - Double click on the event
- 2 - Enter the event name
- 3 - Select “time spent since beginning of step”
- 4 - Enter the time of step
- 5 - Click on “OK”

# Step 6: Run the simulation

1 - Click on the “Report parameters”



2- Set up the general report parameters

**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: 3

Generation of the report (.docx)

Generation of the compounds and reactions files

Restore      OK      Cancel

3 - Change the “time between each output” to 60 s in order to get smoother curves

Possibility to perform scale-up calculations

4 - Save the file



5 - Run the simulation

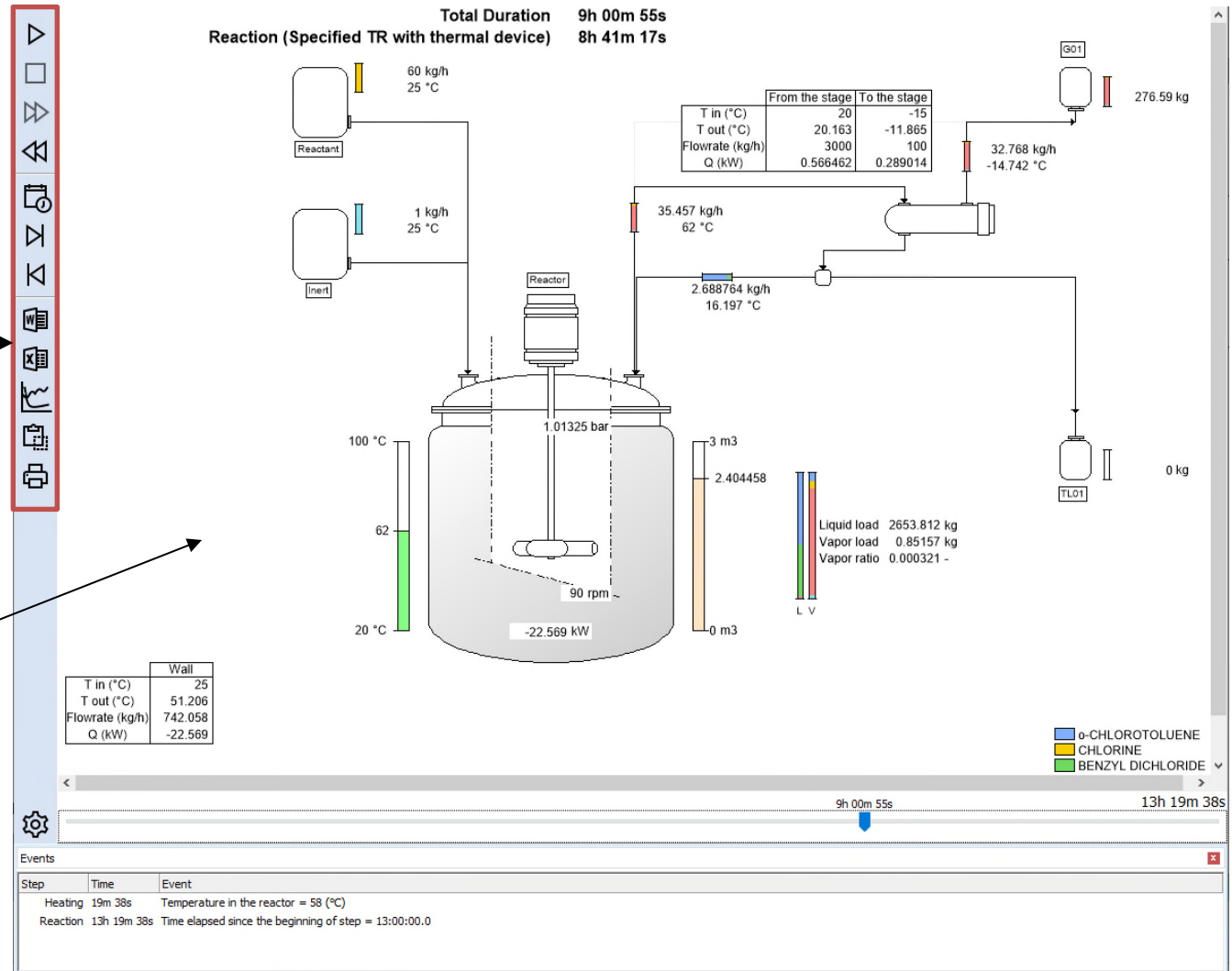


# Step 6: Run the simulation

The following window displays in real time the process operating variables:

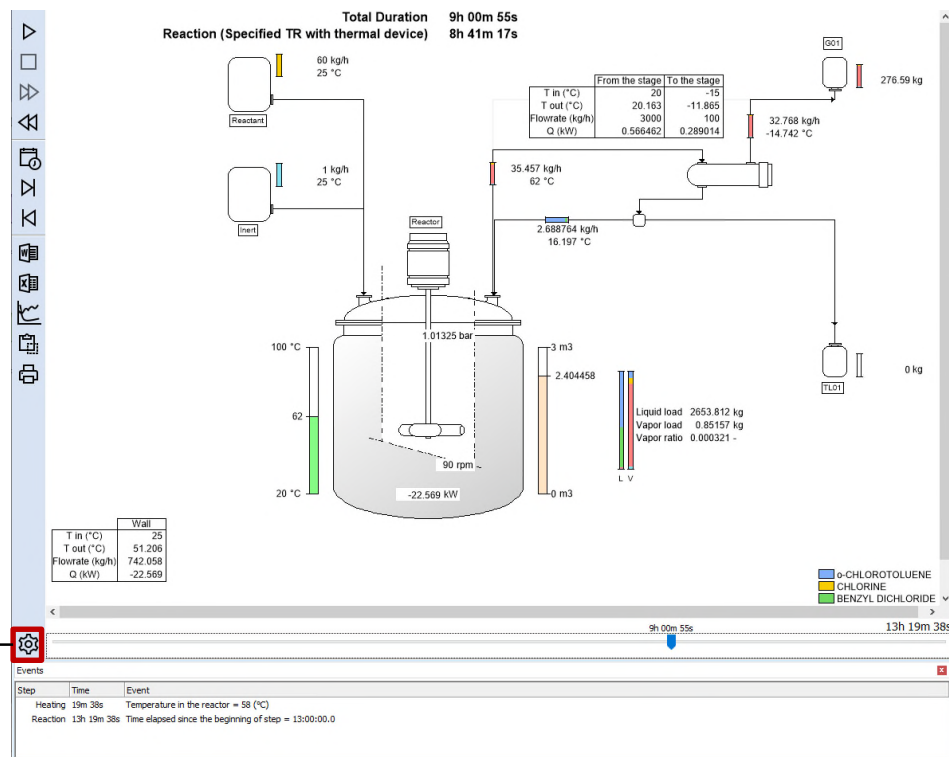
Toolbar that is used to pause, go to the next step, access the graphical settings, etc...

Operating parameters are displayed here (temperatures, pressures, flowrates, compositions, etc...)



# Step 6: Run the simulation

The following window displays in real time the process operating variables:



Click here to access the display options

### Display Options

- Reactor load
- Mixing device speed
- Feeds
- Internal streams
- Productions
- Heating systems
- Condenser
- Compounds legend

Right Bottom

---

Text size: Regular

Colors

---

Save as preferences

Apply preferences

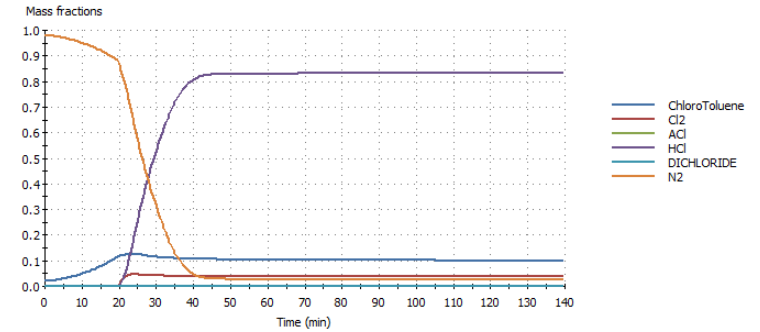
Restore    OK    Cancel

# Step 7: Analyze the simulation results

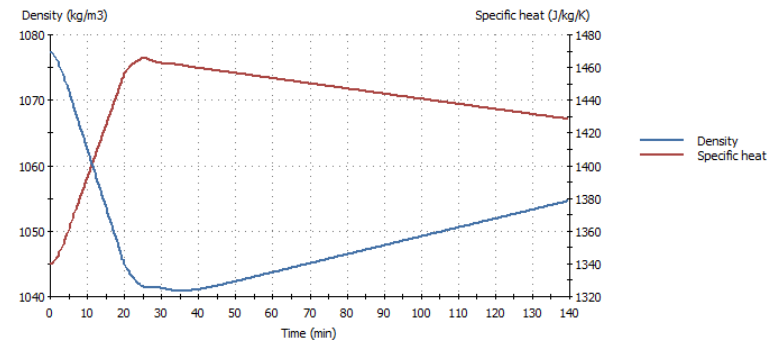
Once the simulation is complete, click on "Open the graph report" to analyze the evolution as a function of time of the variable parameters (pressure, temperature, flowrates, compositions, heat duties, physical properties, etc...)



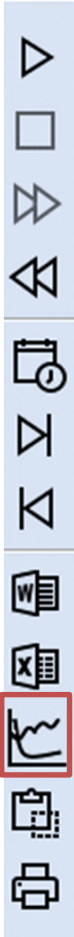
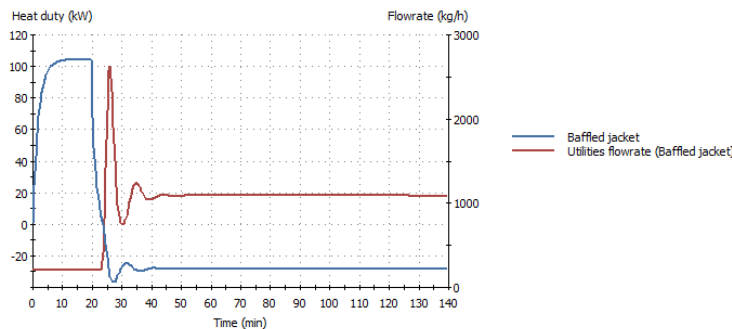
### Vapor mass fractions



### Physical properties



### Heat duty - Utilities flowrate



# Step 7: Analyze the simulation results

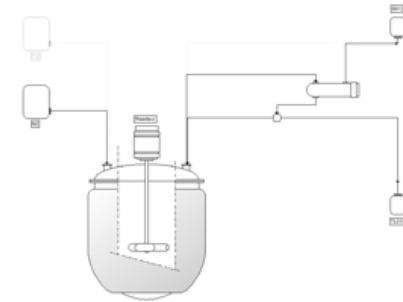
Click on "Open the report" to open the full simulation report in MS-Word format. It includes the input data (equipment and operating scenario) as well as the numerical and graphical results



Process.....	.....
Scenario.....	.....
Thermodynamic calculator.....	.....
.1 Model.....	.....
.2 Binary interaction parameters.....	.....
.3 Compounds.....	.....
.4 Reactions.....	.....
Feed streams.....	.....
.1 Cl2 - Reaction.....	.....
.2 N2 - Heating.....	.....
.3 N2 - Reaction.....	.....
<b>Step 1 - Heating.....</b>	<b>.....</b>
.1 Operating Mode.....	.....
.2 Vessel characteristics.....	.....
.2.1 Geometry.....	.....
.2.2 Material.....	.....
.3 Mixing characteristics.....	.....

BatchReactor BR\_G501\_EN-Chlorotoluene-chloration 3/18/2019

## 5. STEP 1 - HEATING



ibuprofen Calculator [New calculator]

Input stream	Output streams
- N2	- TL01
	- G01

### 5.1. OPERATING MODE

Operating Mode:	Variable heat
Pressure (PR)	1.00000 <b>atm</b>



The detailed table of content provides a convenient access to the results

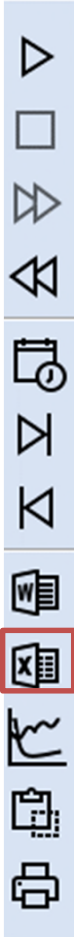


# Step 7: Analyze the simulation results

Click here to access the simulation report in MS-Excel format. It includes the evolution of the process variables as a function of time



	Time (h)	Liquid volume (m3)	Feed flowrate (kg/h)	Liquid sidestream (kg/h)	Vapor sidestream (kg/h)	Vapor distillate (kg/h)	liquid distillate (kg/h)	Reflux (kg/h)
2413								
2414	1.67E-04	2.2278891	1	0	0	1.0052927	0	2.00E-02
2415	1.67E-02	2.2286754	1	0	0	1.3371409	0	2.73E-02
2416	3.33E-02	2.230627	1	0	0	1.5397891	0	3.36E-02
2417	5.00E-02	2.2332999	1	0	0	1.6559845	0	3.94E-02
2418	6.67E-02	2.2364167	1	0	0	1.7185781	0	4.53E-02
2419	8.33E-02	2.239802	1	0	0	1.7493801	0	5.13E-02
2420	0.1	2.243351	1	0	0	1.7614792	0	5.76E-02
2421	0.116667	2.2470044	1	0	0	1.7625298	0	6.43E-02
2422	0.133333	2.2507285	1	0	0	1.757826	0	7.16E-02
2423	0.15	2.2544892	1	0	0	1.7492106	0	7.94E-02
2424	0.166667	2.2582715	1	0	0	1.7412496	0	8.80E-02
2425	0.183333	2.2620693	1	0	0	1.7278169	0	9.70E-02
2426	0.2	2.2658796	1	0	0	1.7193188	0	0.10702215
2427	0.216667	2.2697004	1	0	0	1.7098734	0	0.11781666
2428	0.233333	2.2735296	1	0	0	1.7007094	0	0.12949264
2429	0.25	2.2773661	1	0	0	1.6923622	0	0.14214939
2430	0.266667	2.2812092	1	0	0	1.6844712	0	0.15582606
2431	0.283333	2.2850585	1	0	0	1.6773023	0	0.17061809
2432	0.3	2.2889139	1	0	0	1.6706803	0	0.18658742
2433	0.316667	2.2927754	1	0	0	1.6645653	0	0.20381152



# Step 7: Analyze the simulation results

Multiple different files are created in the folder where the simulation file is stored, in particular:

- The simulation file (\*.pbpr)
- The simulation report in MS-Word format (\*.docx)
- The simulation report in MS-Excel format (\*.csv)

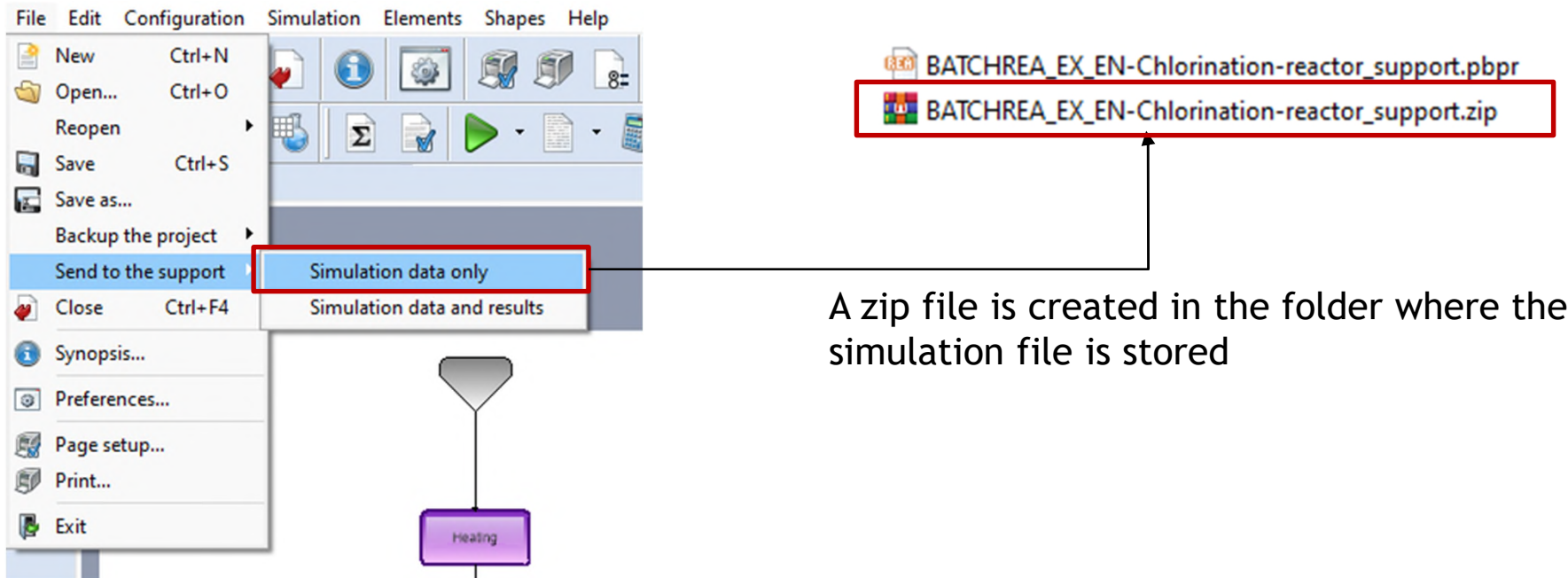
Nom	Modifié le	Type	Taille
BATCHREA_EX_EN-Chlorination-reactor files	03/08/2022 18:26	Dossier de fichiers	
BATCHREA_EX_EN-Chlorination-reactor.csv	03/08/2022 18:26	Fichier CSV Micro...	1 144 Ko
BATCHREA_EX_EN-Chlorination-reactor.docx	03/08/2022 18:26	Document Micros...	778 Ko
BATCHREA_EX_EN-Chlorination-reactor.don	03/08/2022 18:24	Fichier DON	6 Ko
BATCHREA_EX_EN-Chlorination-reactor.his	03/08/2022 18:26	Document texte	33 Ko
BATCHREA_EX_EN-Chlorination-reactor.log	03/08/2022 18:26	Document texte	1 Ko
BATCHREA_EX_EN-Chlorination-reactor.pbpr	03/08/2022 18:23	Fichier PBPR	6 513 Ko
BATCHREA_EX_EN-Chlorination-reactor.res	03/08/2022 18:26	Compiled Resourc...	1 255 Ko
BATCHREA_EX_EN-Chlorination-reactor.xyg	03/08/2022 18:26	Fichier XYG	1 155 Ko

# Step 7: Analyze the simulation results

For any questions, please contact ProSim technical support by sending an email to [support@prosim.net](mailto:support@prosim.net), with:

- The objectives of your simulation
- Your simulation file

To facilitate the sending of the simulation file by email, a zip file can be automatically generated by clicking on “send to support”



The screenshot displays the ProSim software interface. The 'File' menu is open, and the 'Send to the support' option is highlighted. A red box highlights the 'Send to the support' menu item, and another red box highlights the 'Simulation data only' sub-option. An arrow points from the 'Simulation data only' option to a file explorer window showing two files: 'BATCHREA\_EX\_EN-Chlorination-reactor\_support.pbpr' and 'BATCHREA\_EX\_EN-Chlorination-reactor\_support.zip'. The zip file is highlighted with a red box. Below the menu, a diagram shows a funnel-shaped reactor with a 'Heating' block connected to its bottom.

A zip file is created in the folder where the simulation file is stored



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# ProSim

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