Getting Started with ProSim DAC®

Use Case 1: Main features overview

Software & Services In Process Simulation

We guide You to efficiency

ProSim

Introduction

- This document presents a general overview of ProSim DAC, ProSim's gas adsorption column dynamic simulator.

- This step by step guide describes the different functions that are used to build a simulation of a gas-solid adsorption column. It is based on a TSA cycle to remove a VOC (dichloromethane) from a nitrogen stream. The adsorbent is an activated carbon.

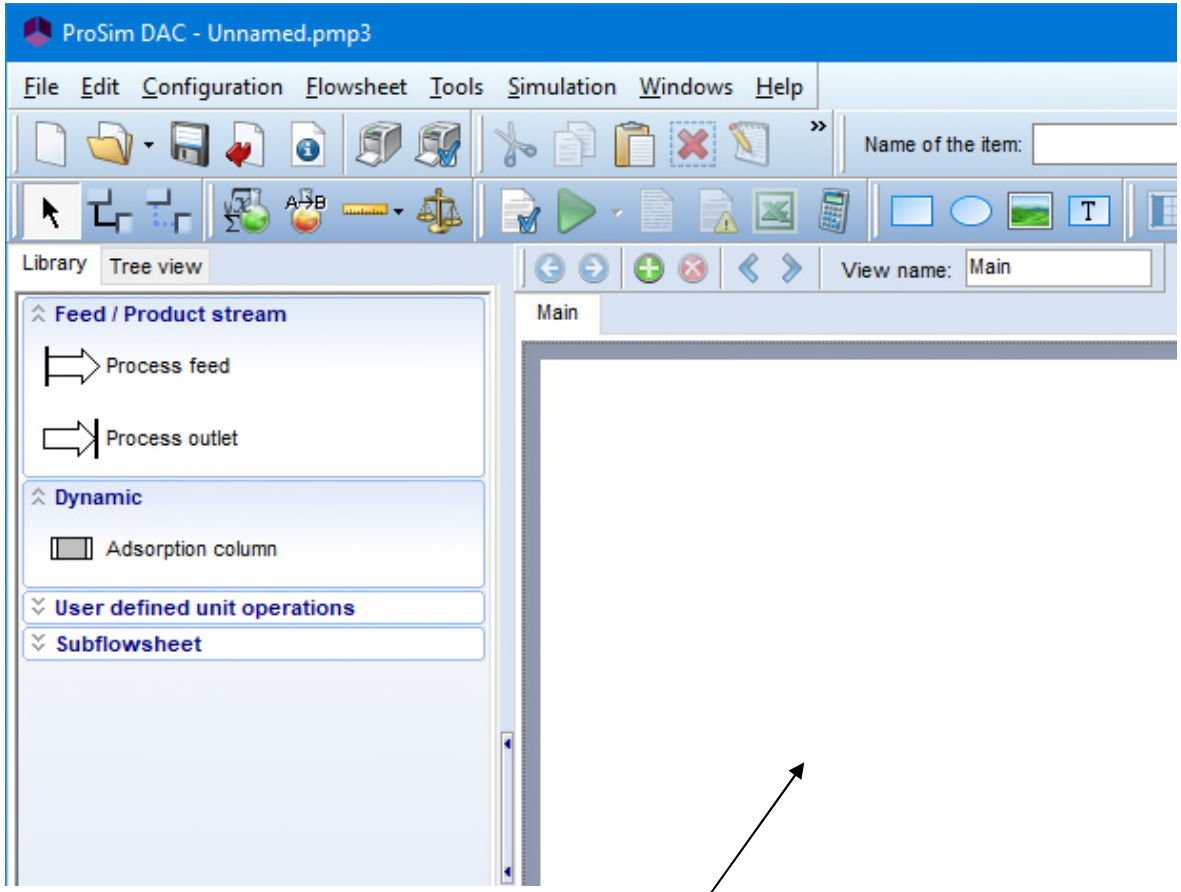
Before we start: Interface key functions

Menus bar

Tools bar

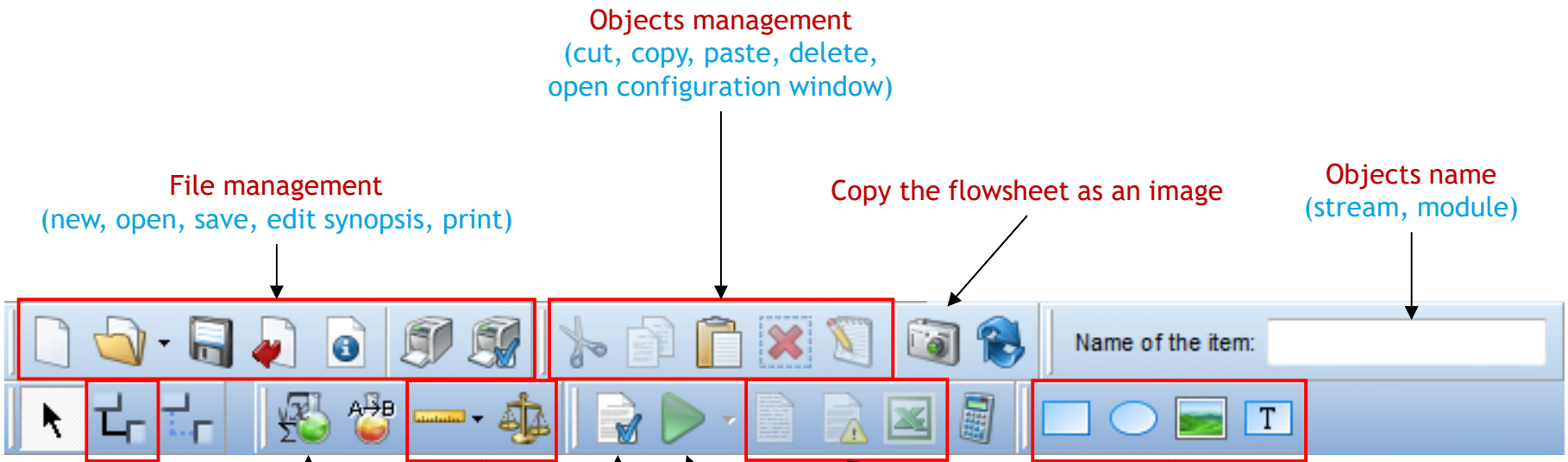
Categories list

Unit operations, within the selected categories



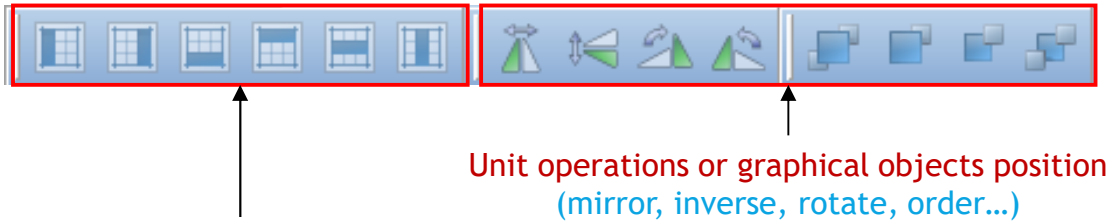
Drawing area

Before we start: Interface key functions



Before we start: Interface key functions

- Graphical object management

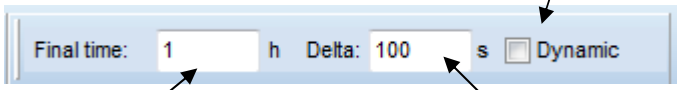


Arrange unit operations on the flowsheet
(align, center…)

Unit operations or graphical objects position
(mirror, inverse, rotate, order…)

Colors, borders, text content menus can be access any time by right-clicking on the object.

- Time management



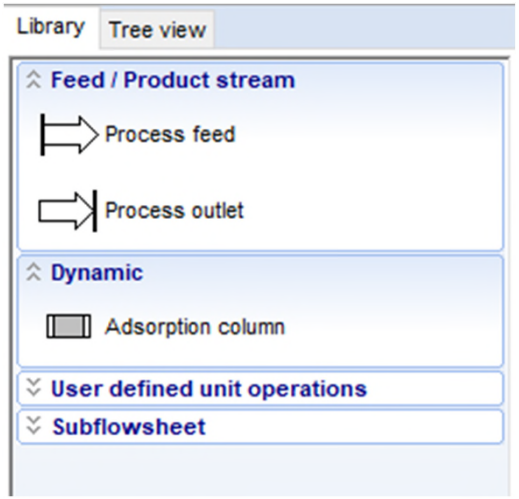
Check this box to allow a dynamic simulation

Simulation total duration

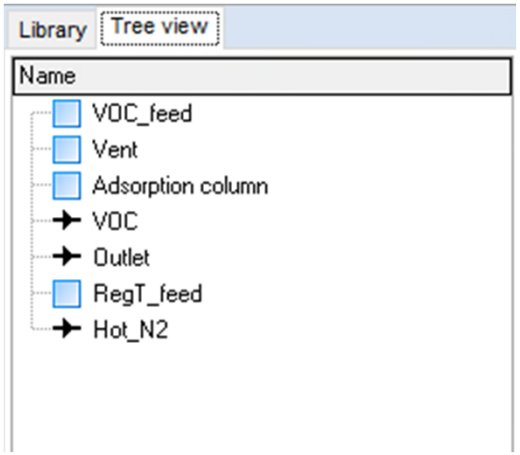
Simulation duration for a unit operation

Before we start: Interface key functions

- Unit operations library or tree view
  - Beside the Library View, which presents the unit operations available in ProSim DAC within categories, the Tree View lists the items (streams and unit operations) used in the flowsheet.
  - Selecting one (or several with the Ctrl button) item in the list selects the corresponding item in the flowsheet. Double clicking on the item in the list opens its configuration window.



Library view



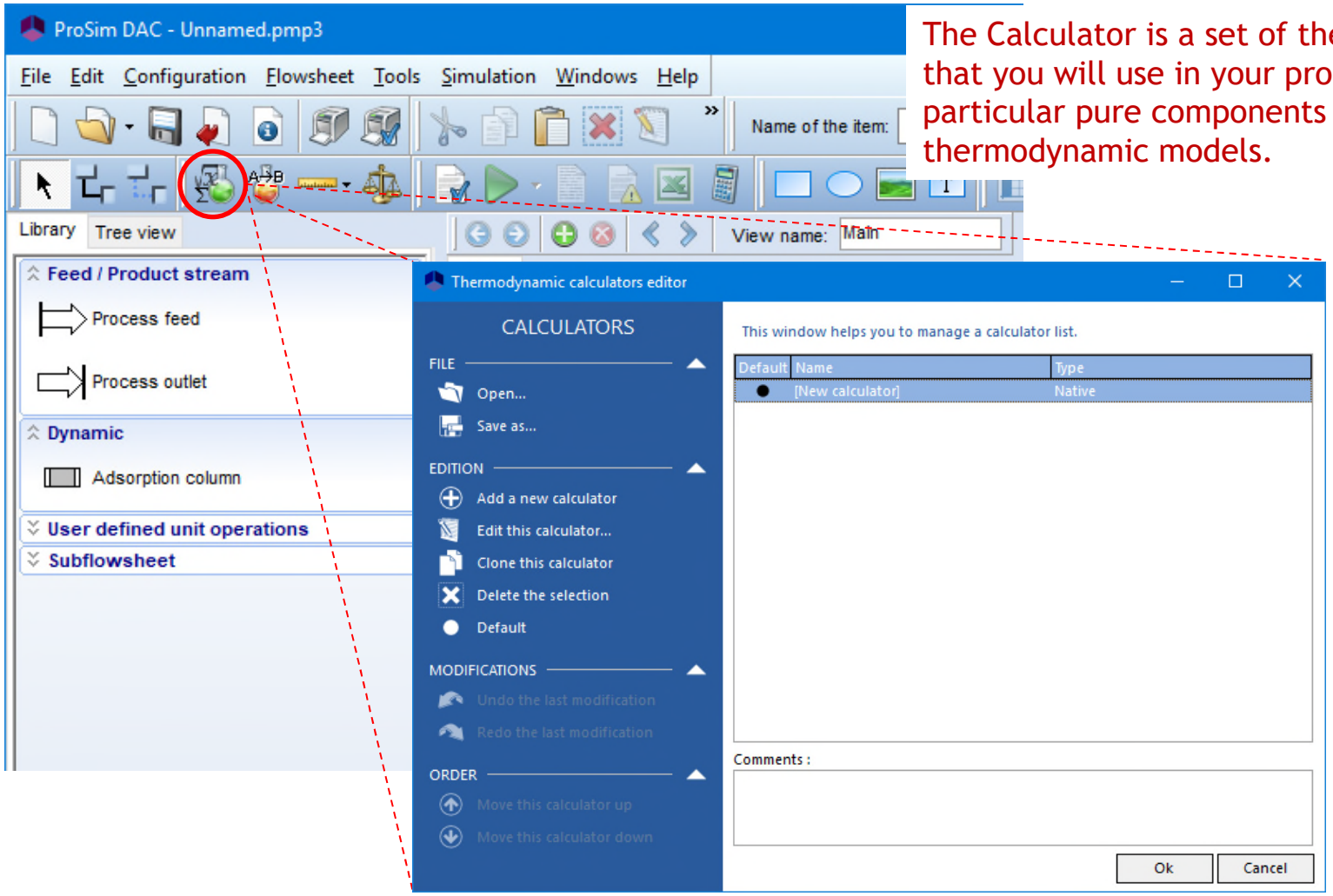
Tree view

Building the flowsheet

- The steps are the following:
  - Step 1: Select your components
  - Step 2: Select your thermodynamic profile
  - Step 3: Create your flowsheet
  - Step 4: Run the simulation
  - Step 5: Analyze the reports generated
  - Step 6: Share the simulation

Step 1: Select your components

The Calculator is a set of thermodynamic data that you will use in your process. It includes in particular pure components and thermodynamic models.

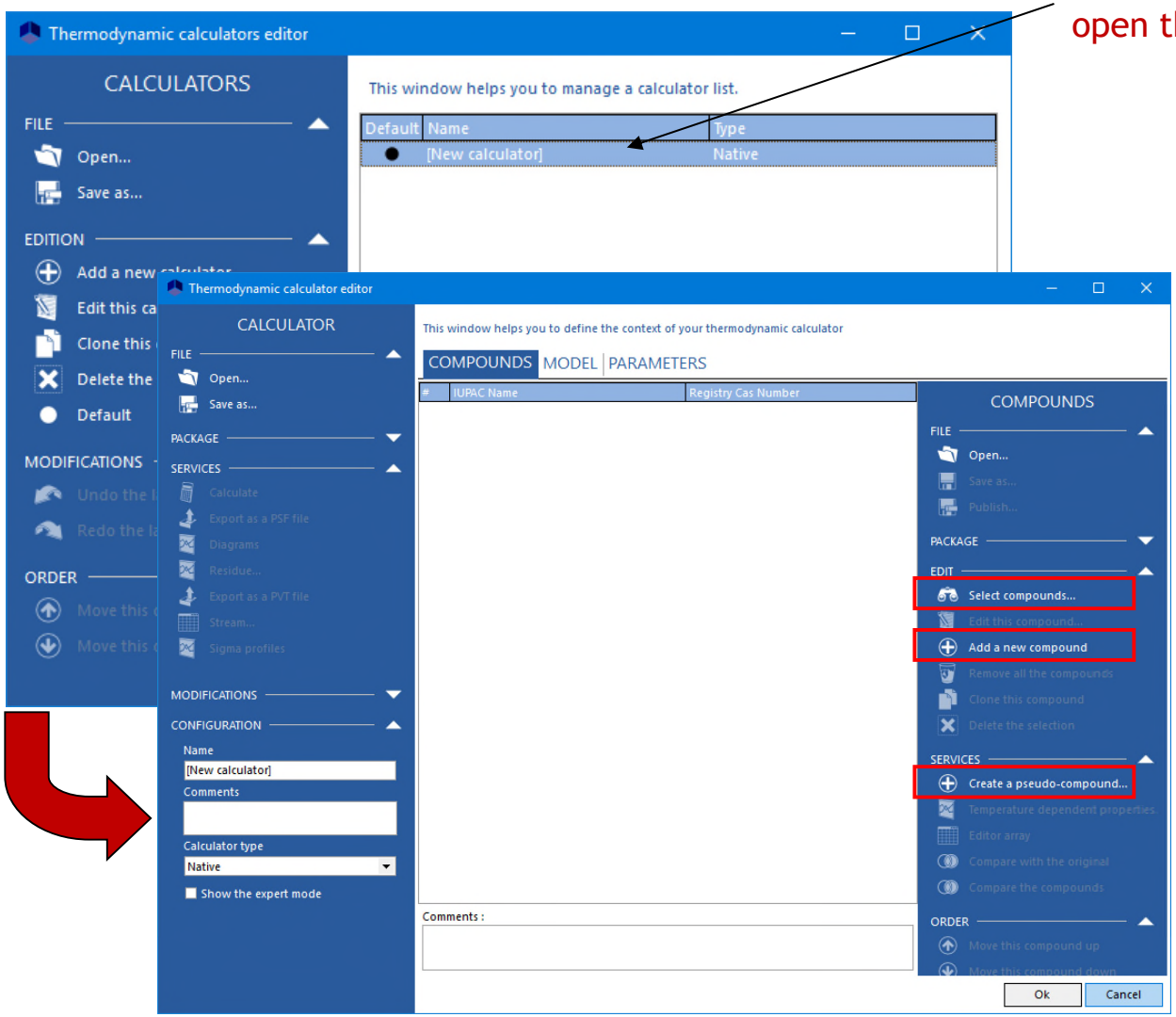


Click on the thermodynamic icon to open the calculators editor.

You can use several calculators in the same flowsheet.

Step 1: Select your components

Double click on the “New calculator” to open the calculator environment window.



To search for a component in one of the databases, click on “Select compounds”

To create a component “from scratch” with the properties that you have, click on “Add a new compound”

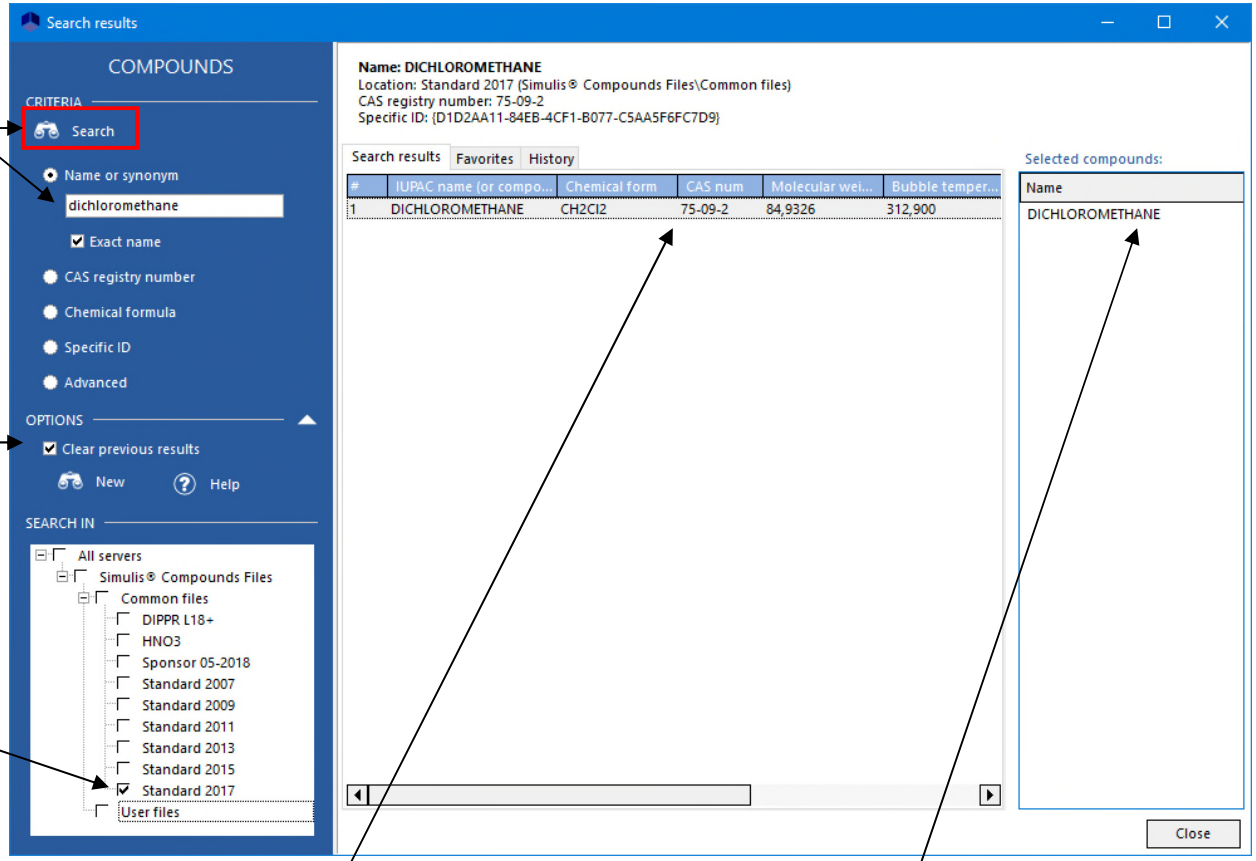
To create pseudo compounds, without lights ends, click on “Create pseudo-compounds”

Step 1: Select your components

Enter the name of the compound you are looking for or select another criteria. Once entered, press "Search"

Check this box to clear previous results

The databases registered on your computer are listed here. Select the last one (in date)



Search results are displayed in central window.

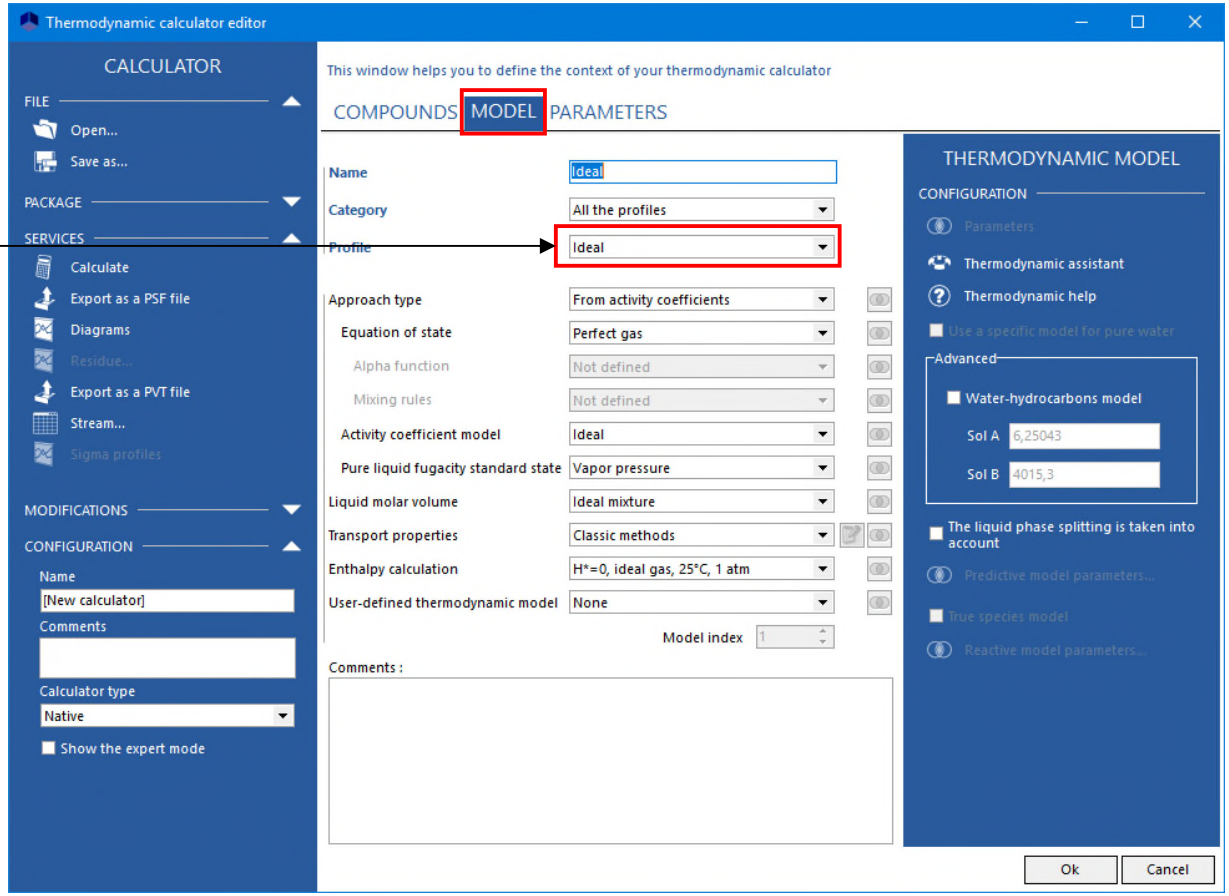
Double click on the compound you require to select it.
The selection will be displayed on the right window.

Repeat the operation to select all the components that you need.
For this simulation you will need dichloromethane and nitrogen.

Step 2: Select your thermodynamic profile

Once all components are selected, close the component search window to return to the Calculator edition environment.
Click on the “Model” tab to define the thermodynamic profile.

Select an appropriate thermodynamic profile using the pull down menu.
Here we use the “Ideal” thermodynamic profile.



Step 3: Create the flowsheet

A. Build the flowsheet

B. Connect all modules with material streams

C. Configure the inlets and the outlets

D. Configure the adsorption column

E. Configure the operating time

Step 3: Create the flowsheet
A- Build the flowsheet

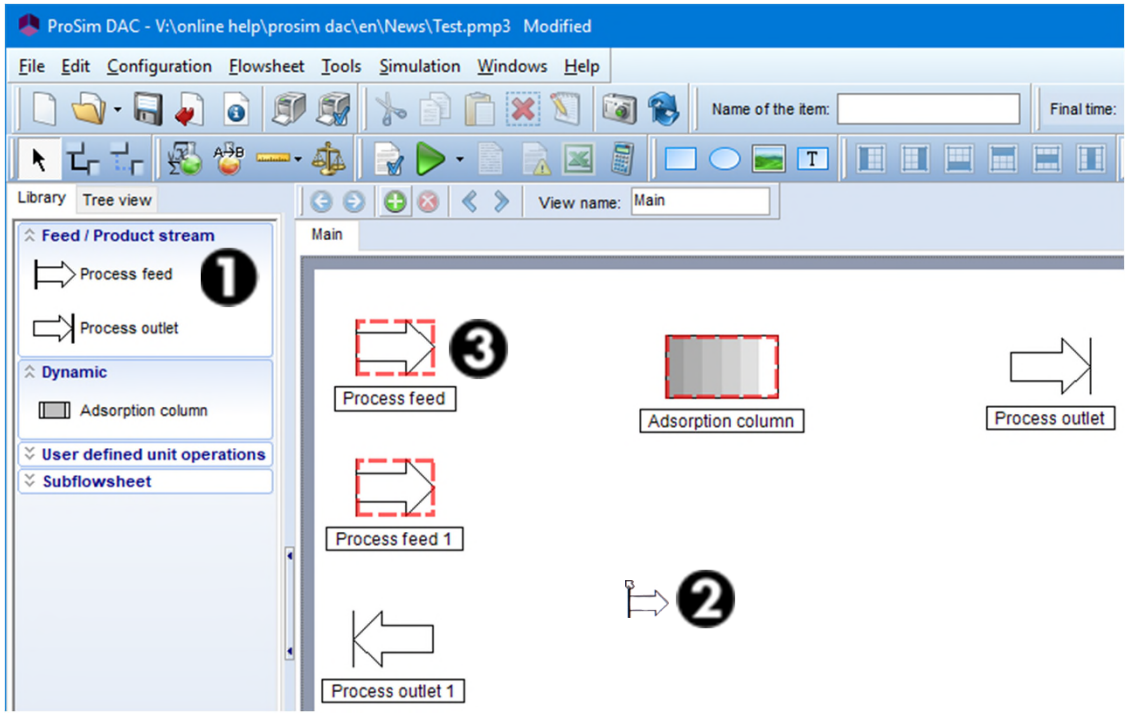
Two process feeds, two process outlets and one adsorption column are needed for this example.

1- Click on “Process feed” icon in the library category “Feed / Product stream” to select a process feed unit operation.

2- Move the mouse onto the drawing sheet and reach the desired position.

3- Click again, to release the unit.

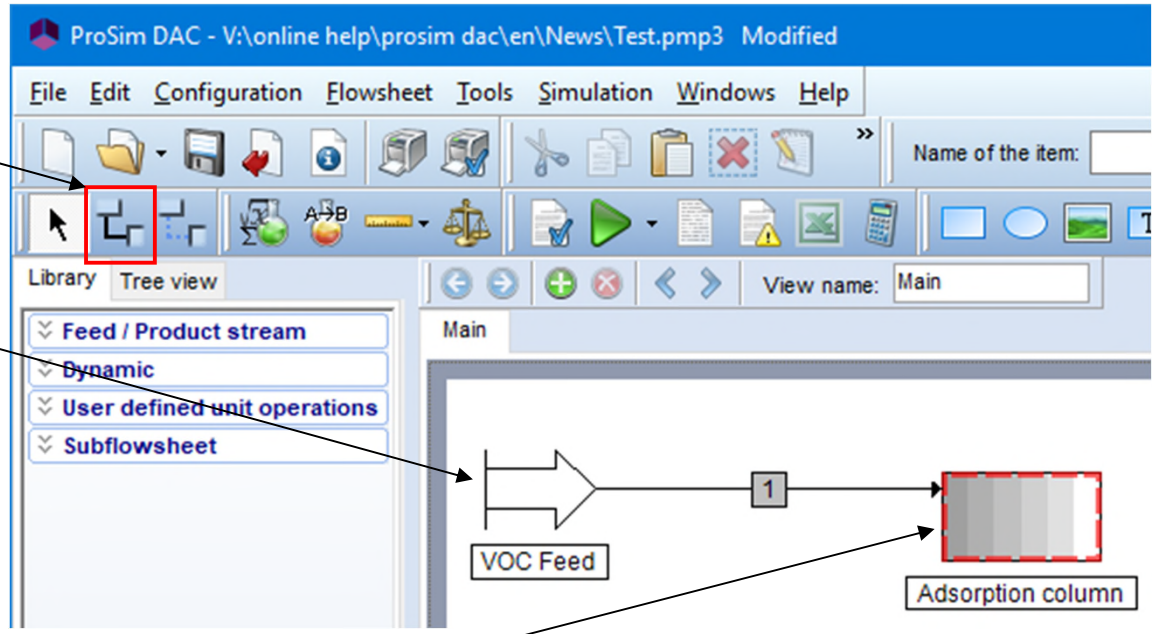
4- Repeat to add the second process feed, the two process outlets and the adsorption column.



Use the graphical object management toolbar to arrange the modules on the flowsheet

Step 3: Create the flowsheet
B- Connect the modules

1. Select the “Create a material stream” icon
2. Select the first unit operation (source) by clicking on it
3. Select the connected unit operation (target) by clicking on it as well



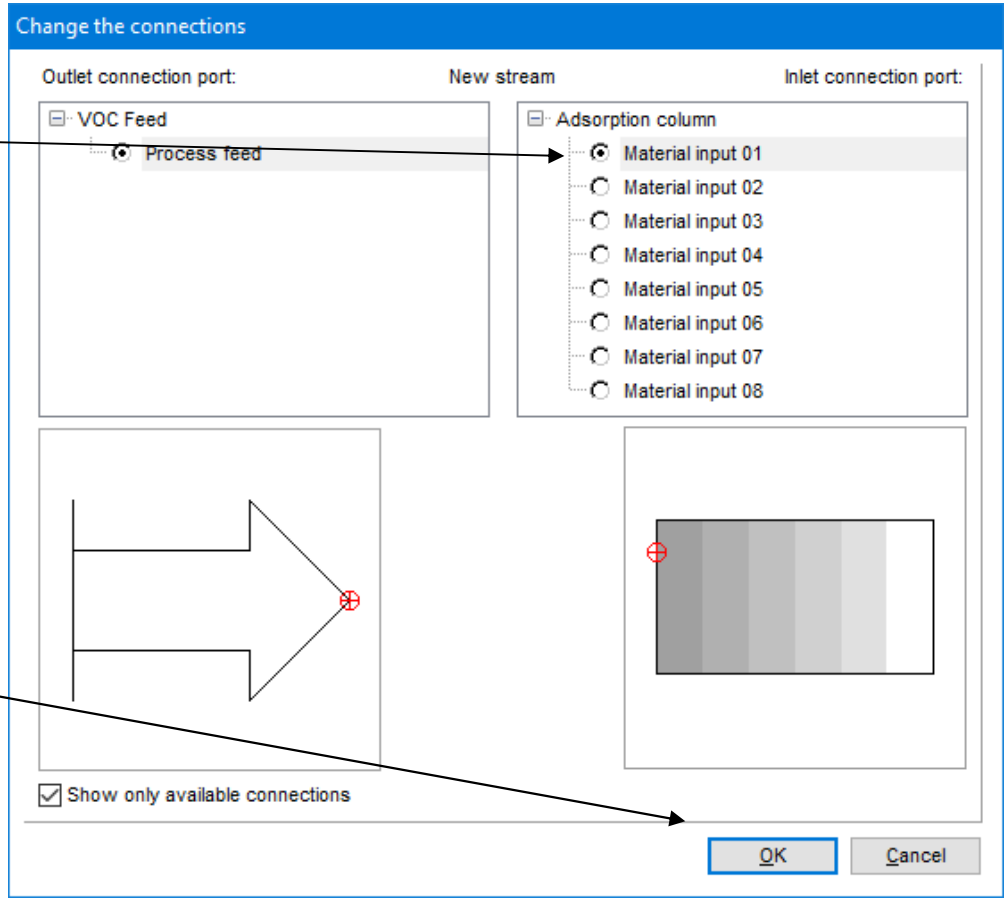
Step 3: Create the flowsheet
B- Connect the modules

Several options for connection are available for the inlets and the outlets of the adsorption column module

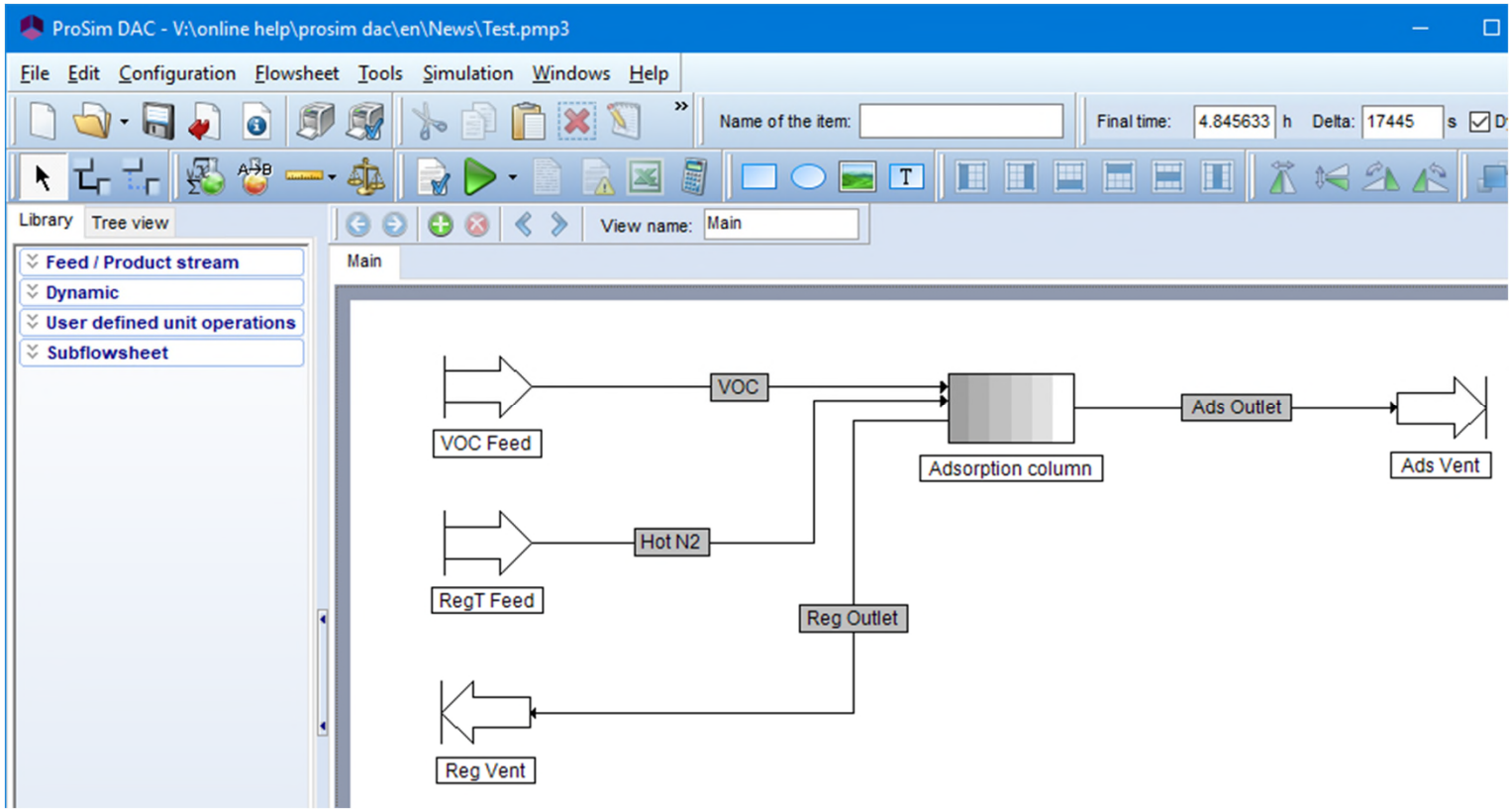
1. Select the inlet, here the “Material input 01”. This choice is used only for graphical display.

2. Confirm by clicking on “OK”.

3. Repeat for the different material streams needed.



Step 3: Create the flowsheet
B- Connect the modules



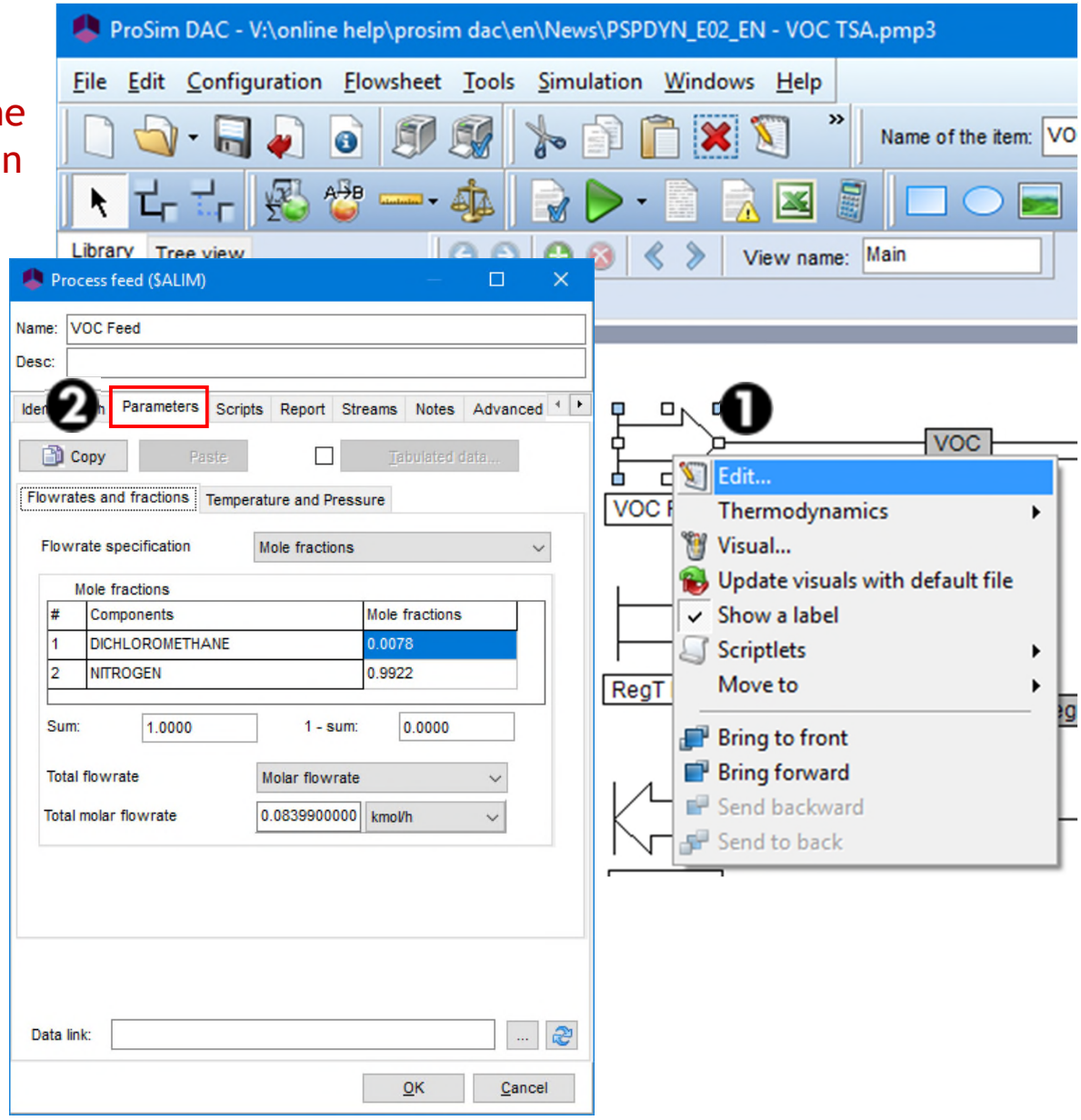
Material streams can be colored in order to ease the reading of the flowsheet. Simply right click on the stream to access the option.

Step 3: Create the flowsheet
C- Inlets and outlets

To configure a process feed:

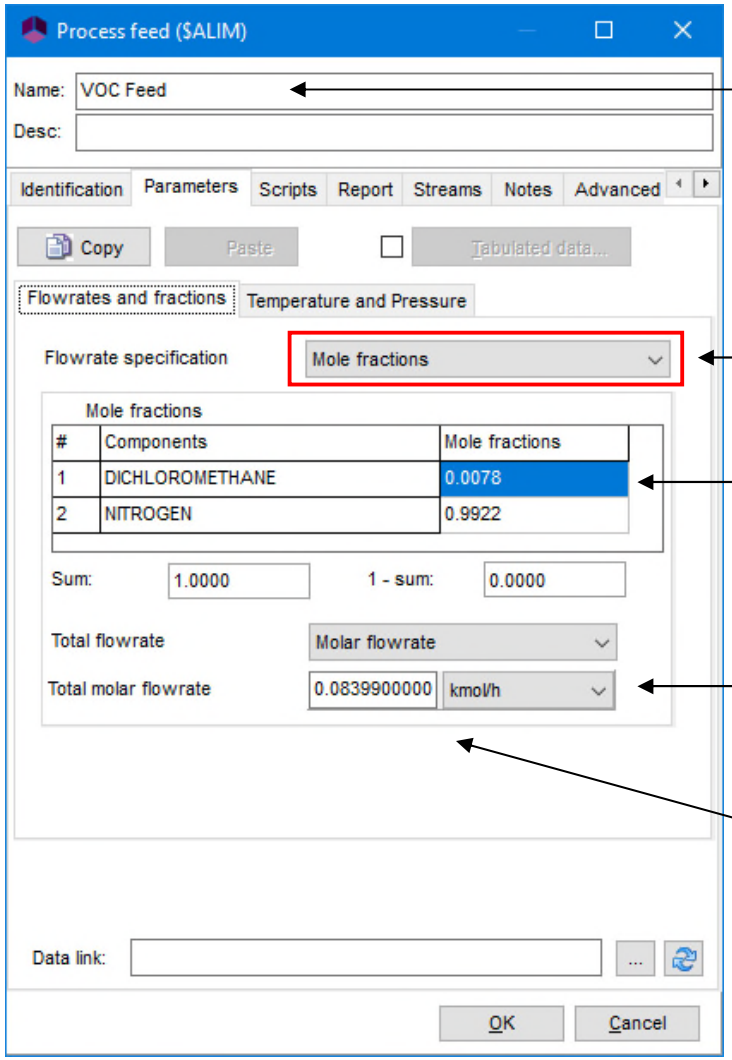
1. Double-click on its icon on the flowsheet or select “Edit…” in the contextual menu.

2. Press the “Parameters” tab.



Step 3: Create the flowsheet
C- Inlets and outlets

- VOC stream inlet characteristics



Change the default name (option)

Select “Mole fractions”

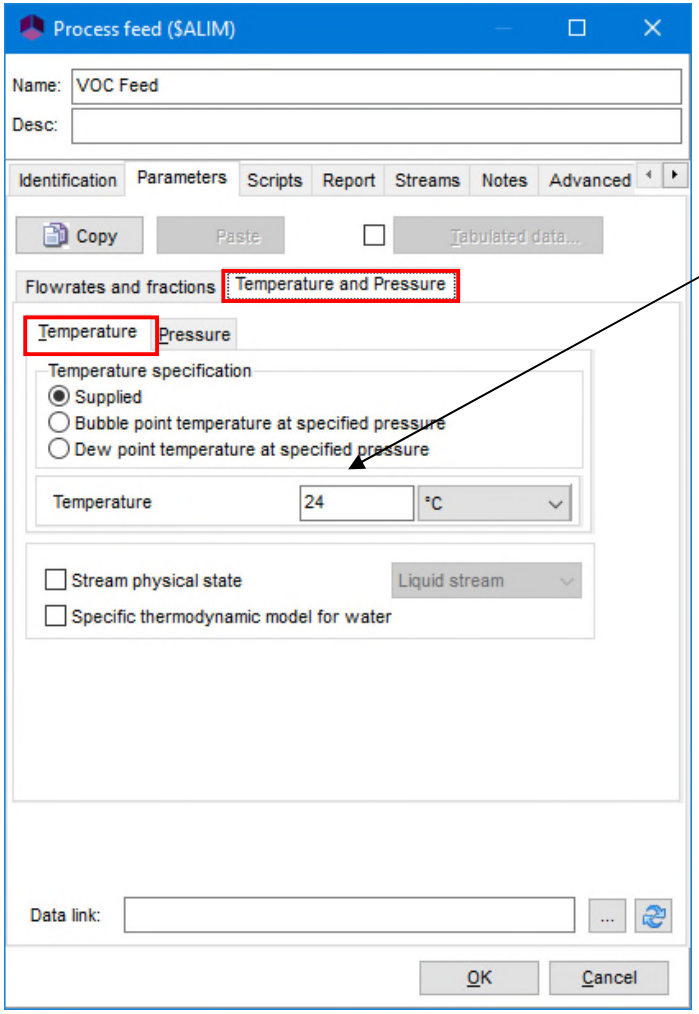
Fill in the mole fractions

Select “Molar flowrate”

Fill in the molar flow rate

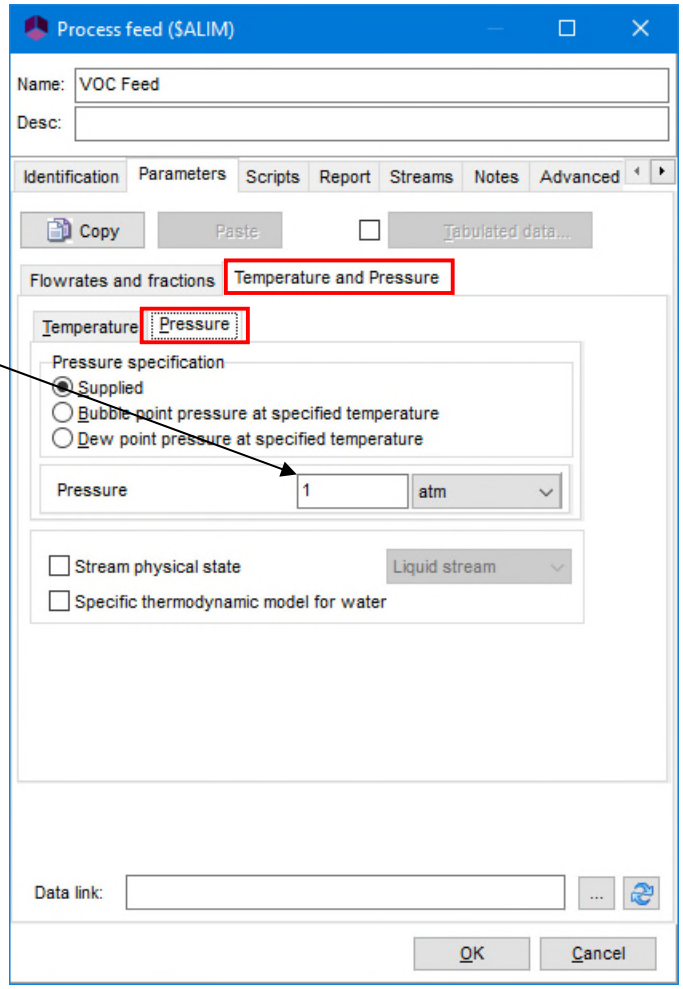
Step 3: Create the flowsheet
C- Inlets and outlets

- VOC stream inlet characteristics



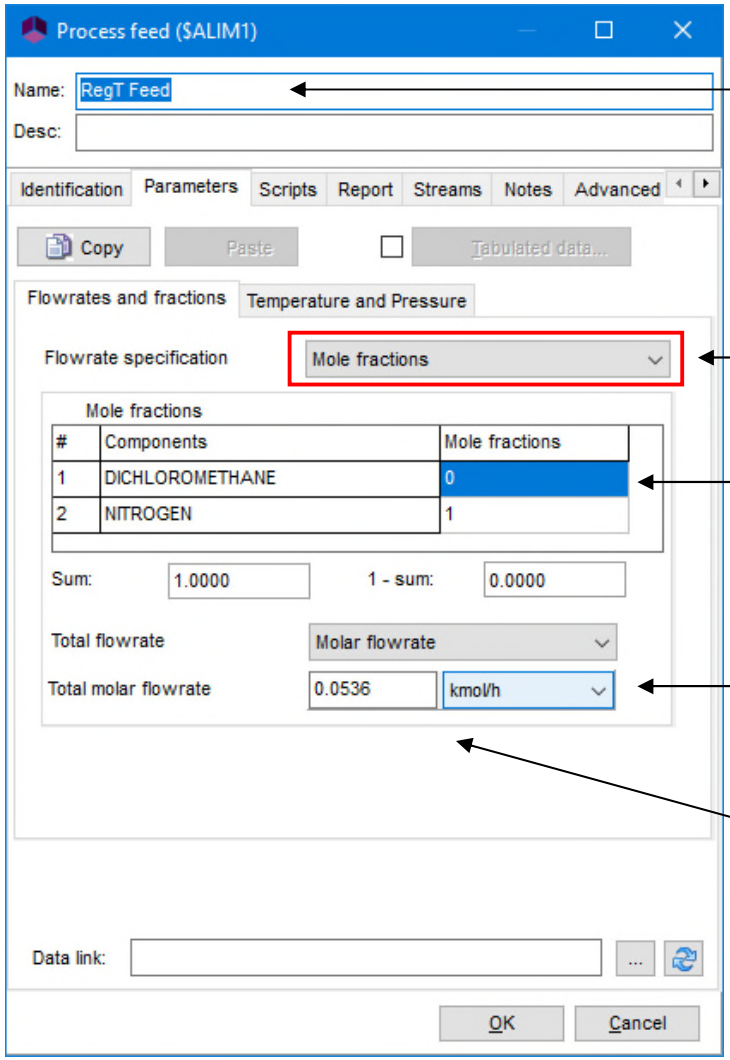
Specify the temperature

Specify the pressure



Step 3: Create the flowsheet
C- Inlets and outlets

- Hot nitrogen stream (for regeneration) inlet characteristics



Change the default name (option)

Select “Mole fractions”

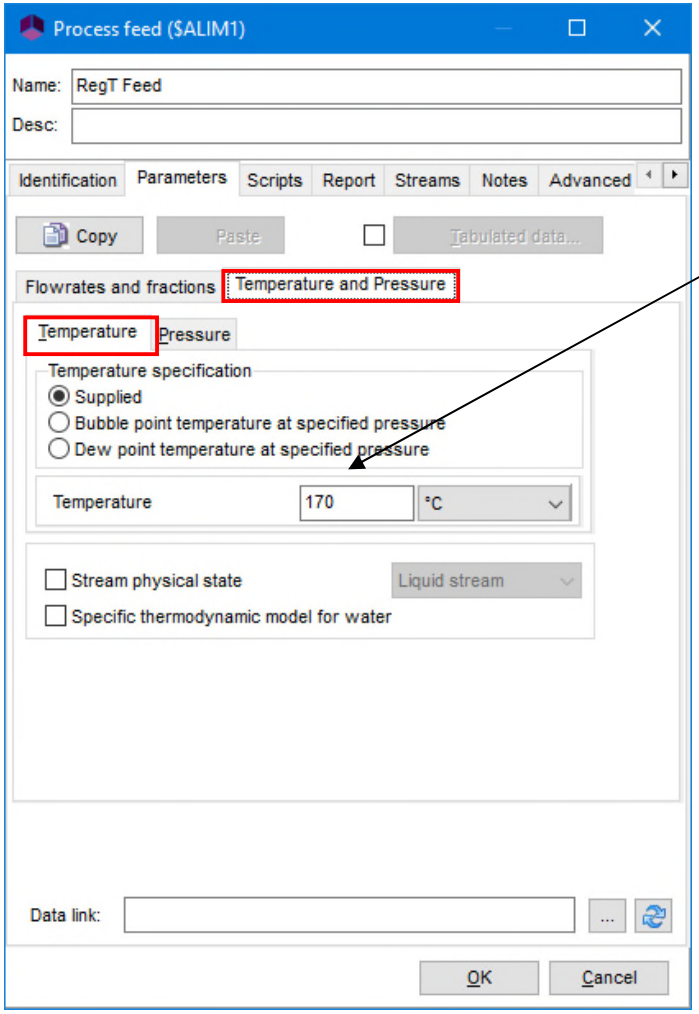
Fill in the mole fractions

Select “Molar flowrate”

Fill in the molar flow rate

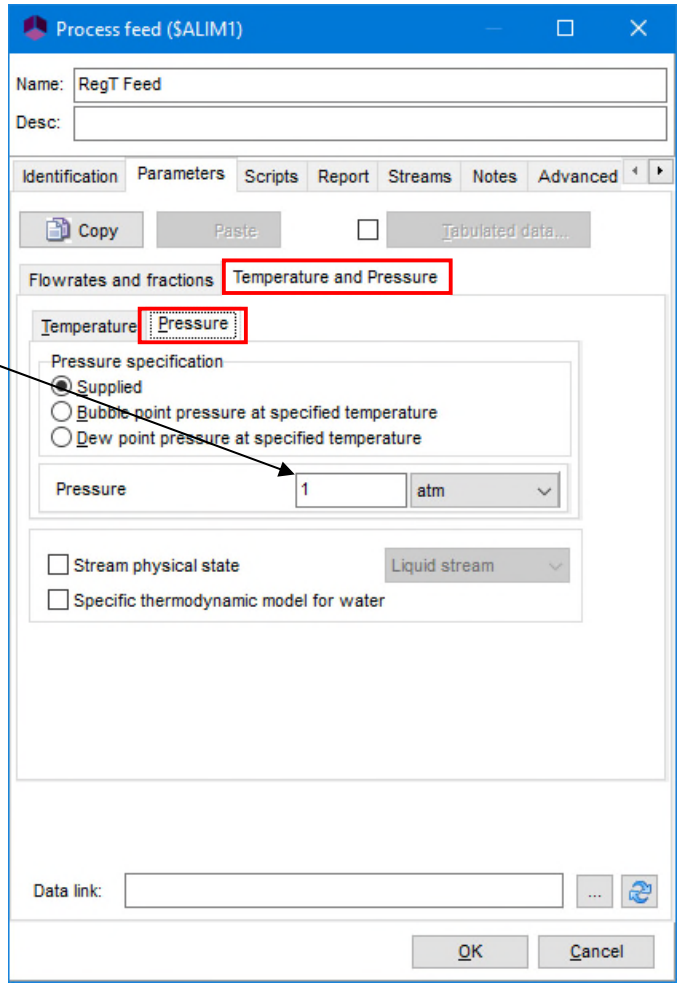
Step 3: Create the flowsheet
C- Inlets and outlets

- Hot nitrogen stream (for regeneration) inlet characteristics



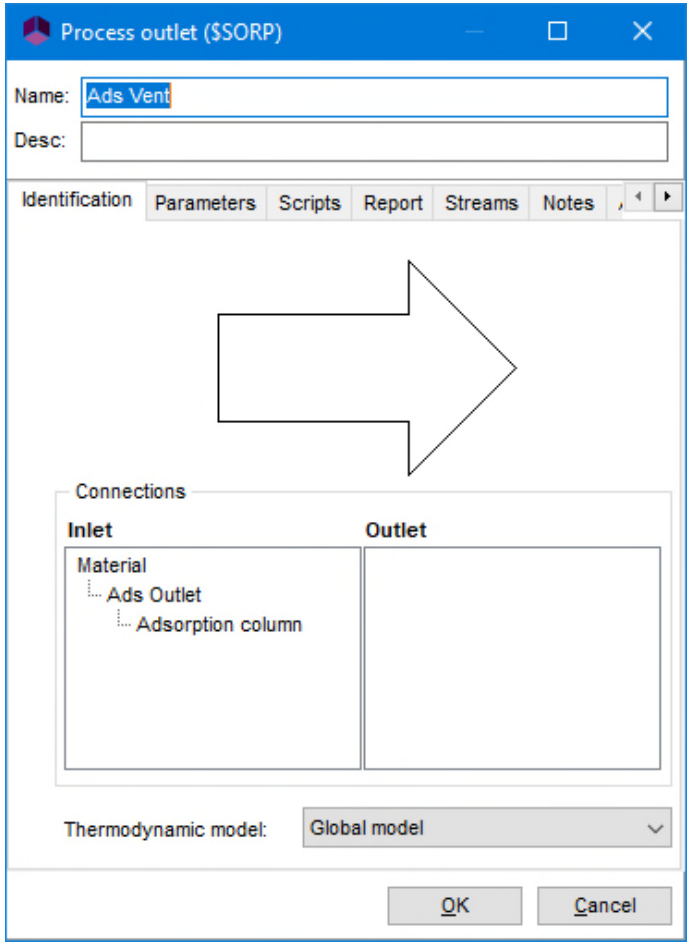
Specify the temperature

Specify the pressure



Step 3: Create the flowsheet
C- Inlets and outlets

- Process outlets
  - No parameters are needed for process outlets

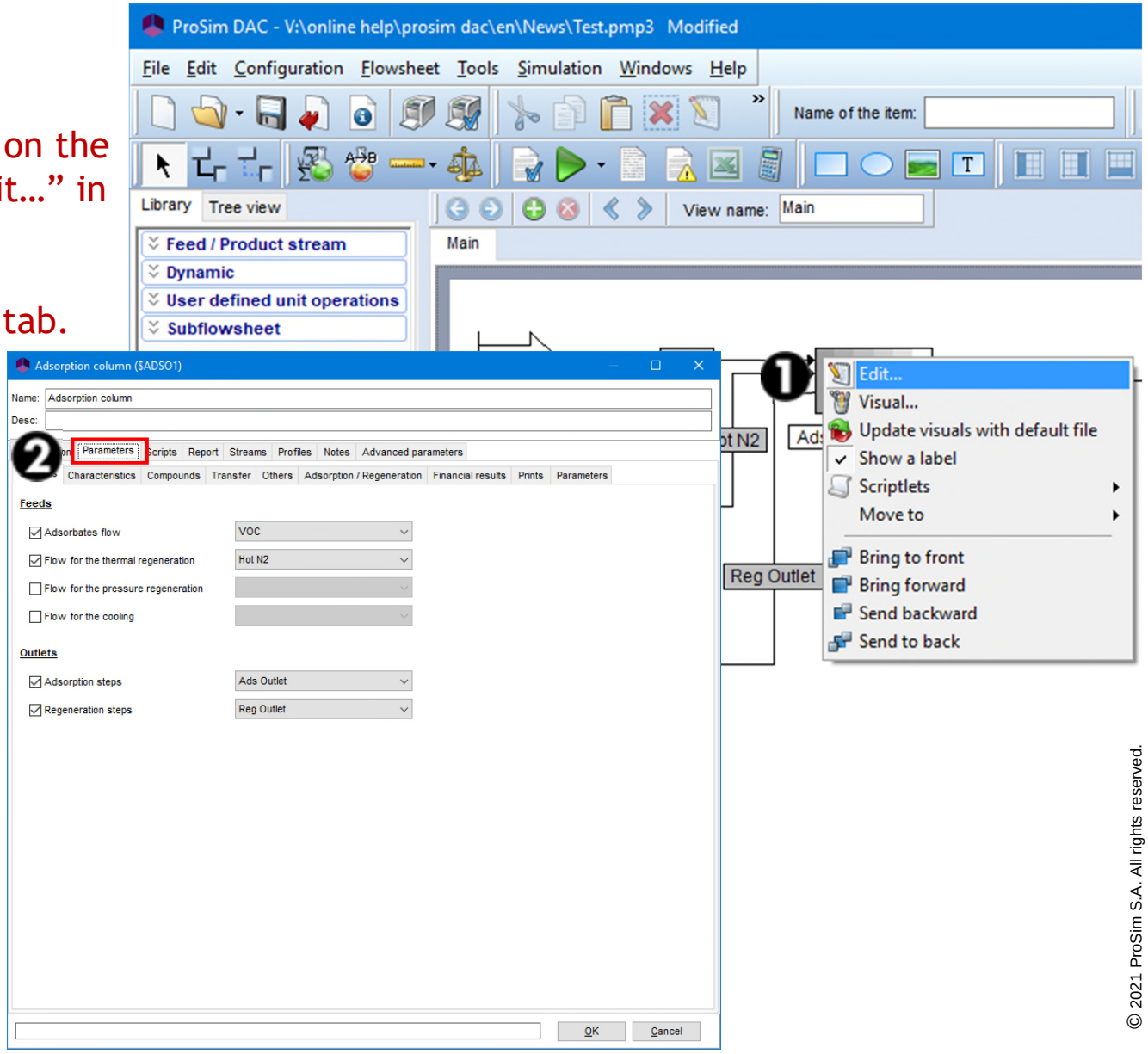


Step 3: Create the flowsheet
D- Adsorption column

To configure the adsorption column:

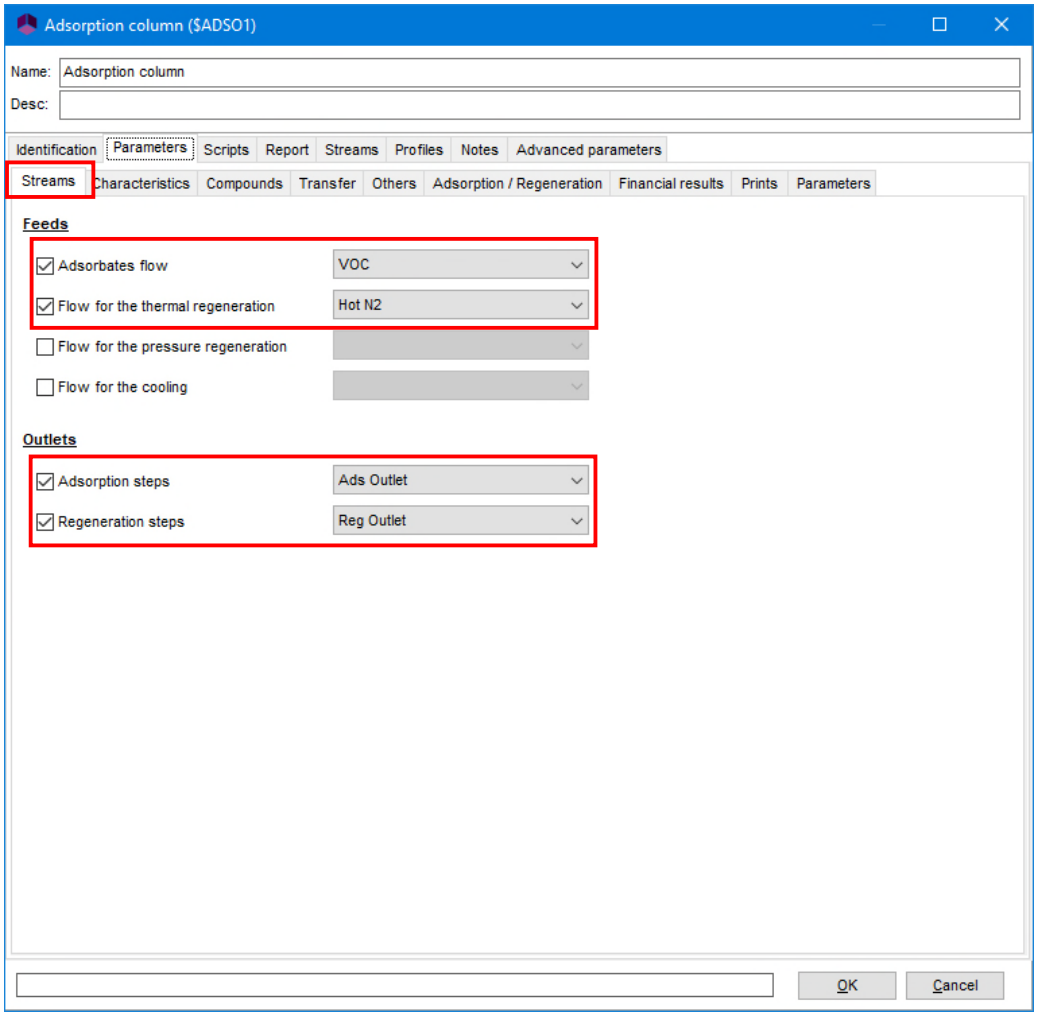
1. Double-click on its icon on the flowsheet or select “Edit…” in the contextual menu.

2. Press the “Parameters” tab.



Step 3: Create the flowsheet
D- Adsorption column

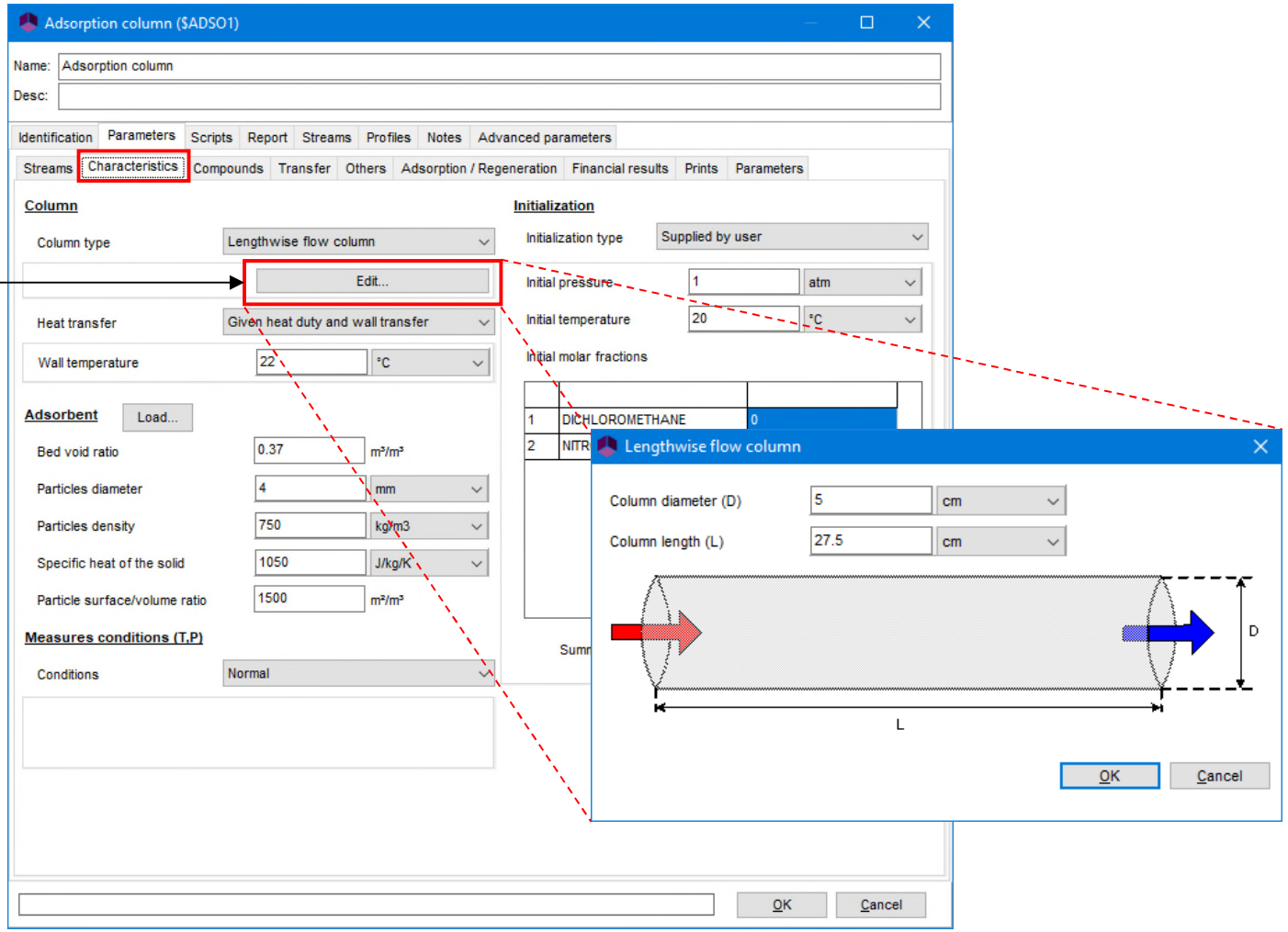
- "Streams" tab
  - Identify the streams for each use



Step 3: Create the flowsheet
D- Adsorption column

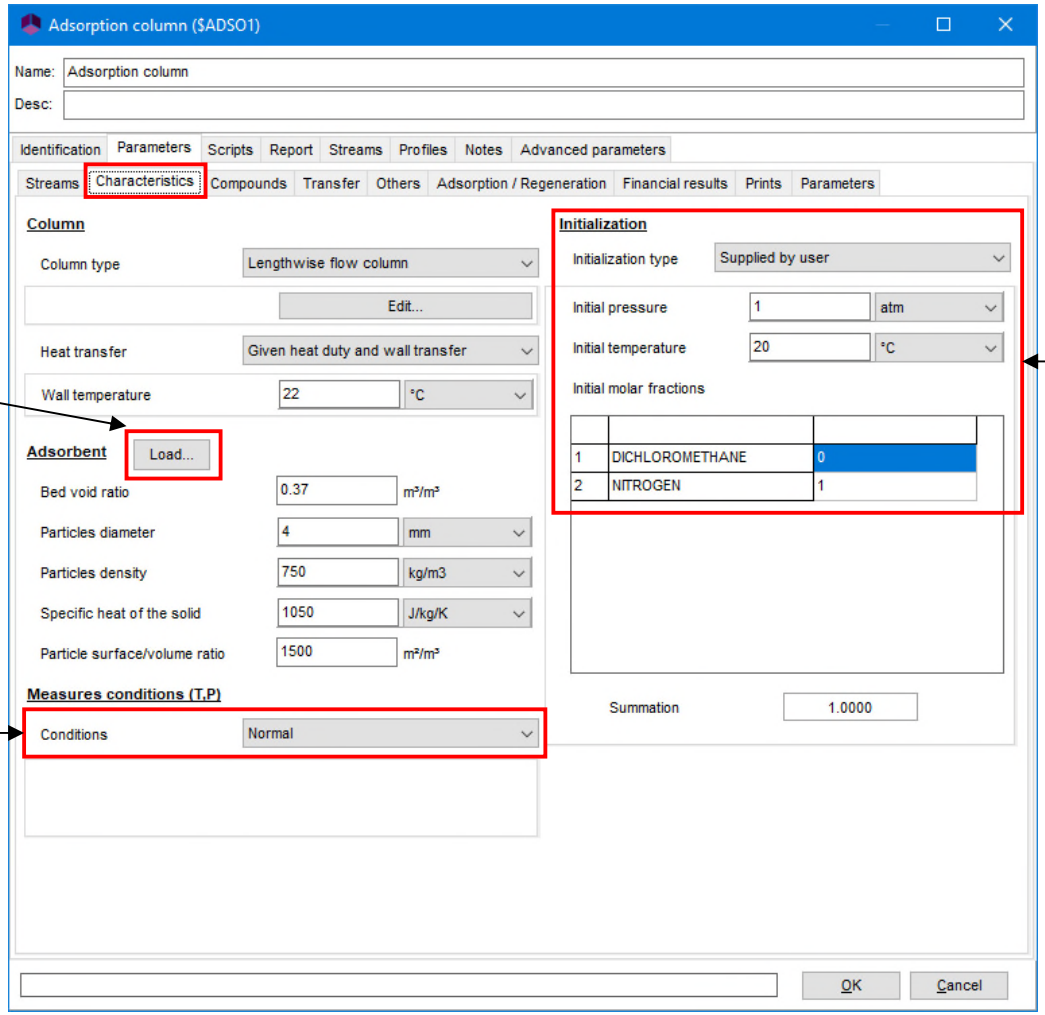
- "Characteristics" tab
  - Fill in the main characteristics of the column

Size of the bed



Step 3: Create the flowsheet
D- Adsorption column

- "Characteristics" tab
  - Fill in the main characteristics of the column



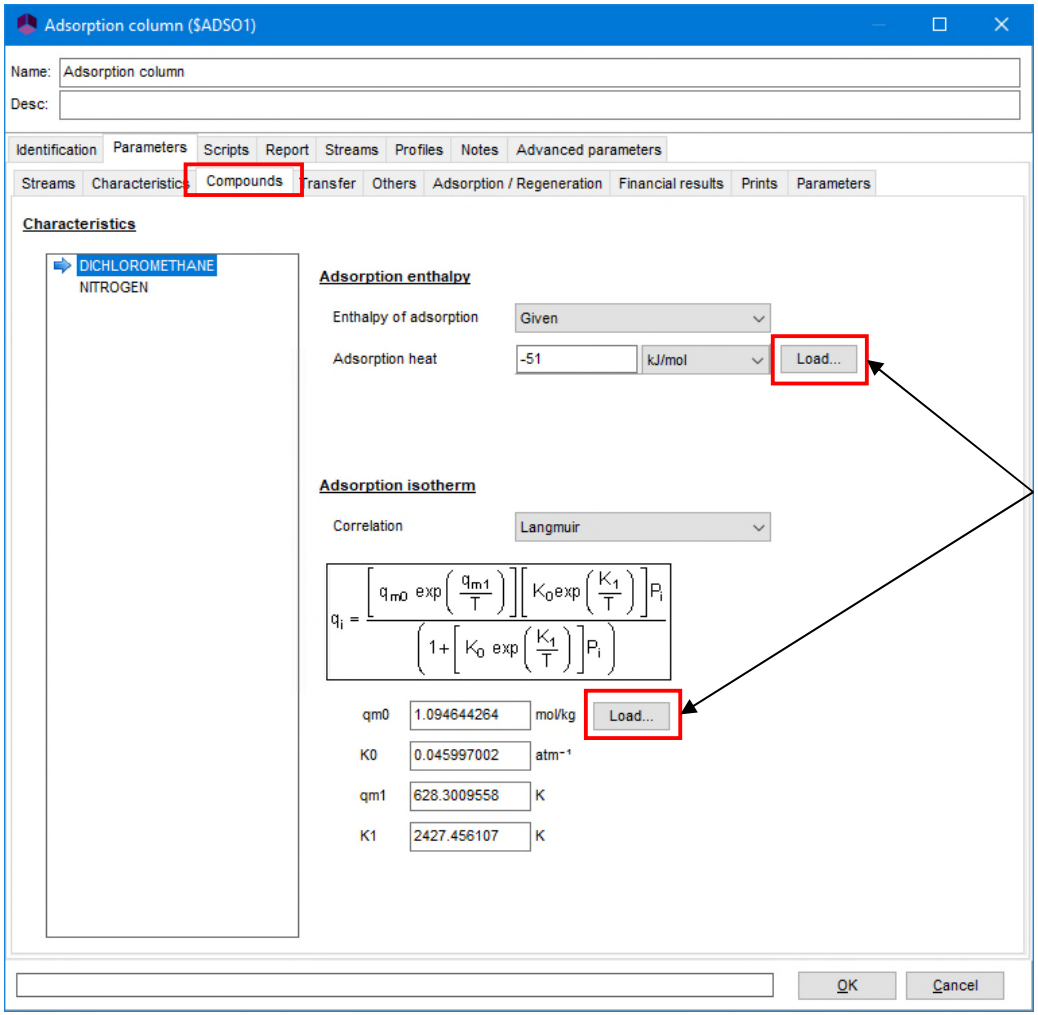
Adsorbent data base

T, P reference for the concentrations

State of the column before the first adsorption

Step 3: Create the flowsheet
D- Adsorption column

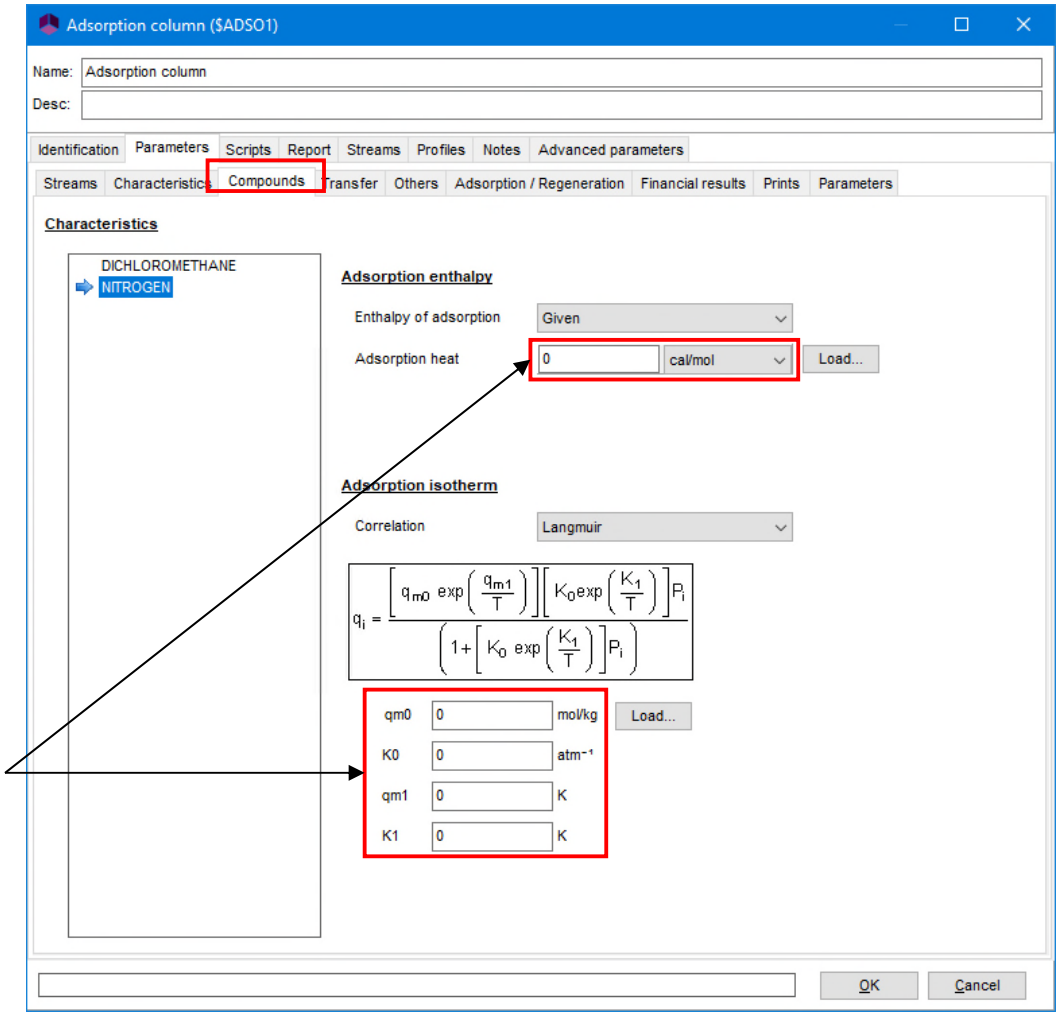
- "Compounds" tab
  - Fill in the dichloromethane adsorption isotherm and its adsorption enthalpy



Adsorption enthalpy and isotherm databases

Step 3: Create the flowsheet
D- Adsorption column

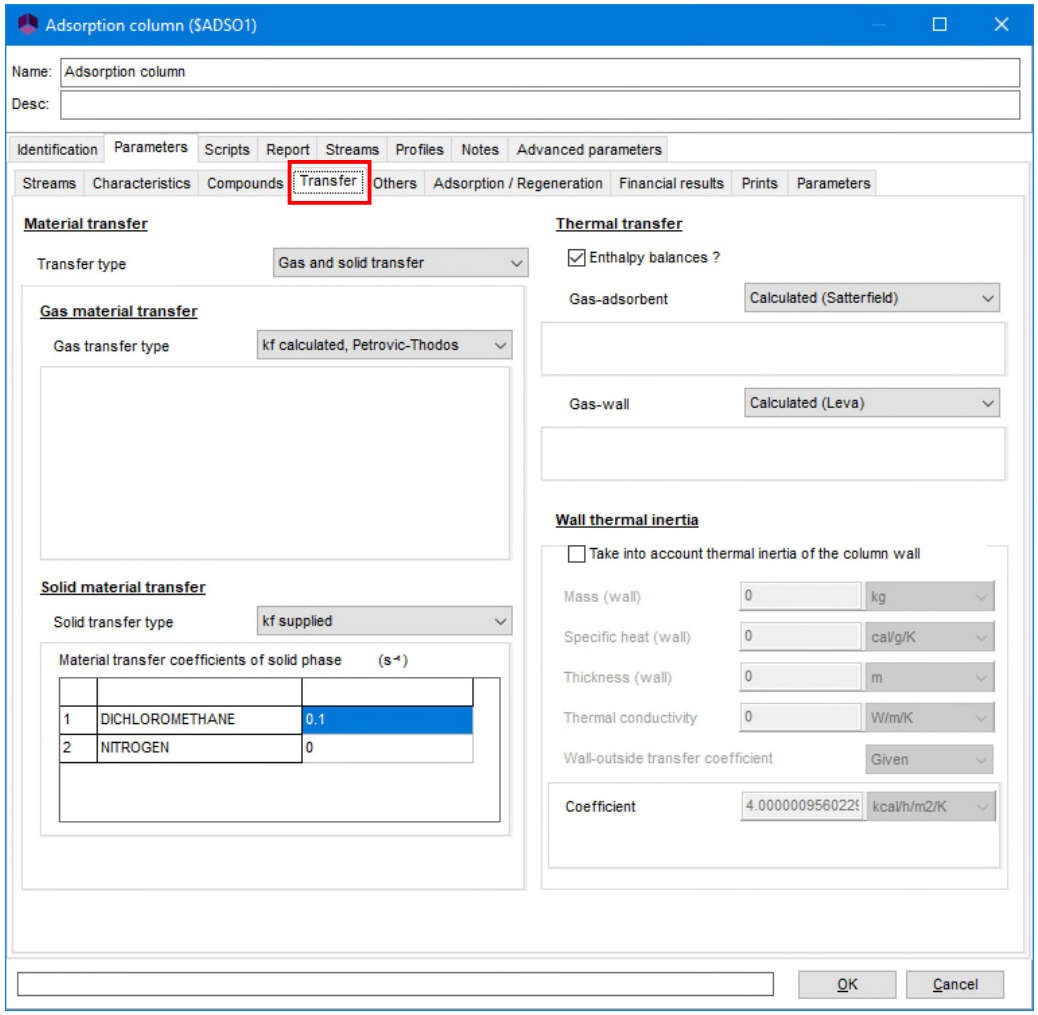
- "Compounds" tab
  - Fill in the dichloromethane adsorption isotherm and its adsorption enthalpy



The nitrogen is assumes to be an inert (i.e. no adsorption)

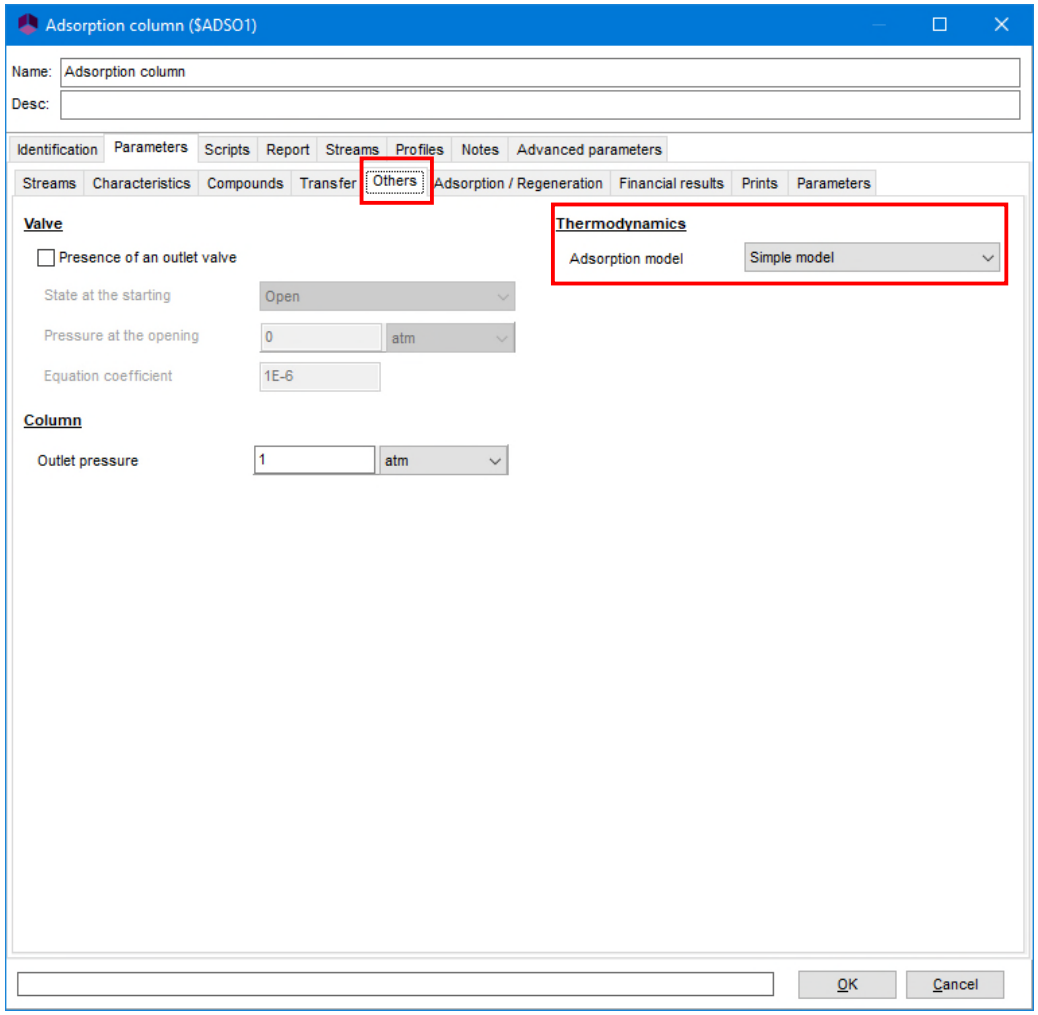
Step 3: Create the flowsheet
D- Adsorption column

- "Transfer" tab
  - Select the models for the mass and mass transfer models



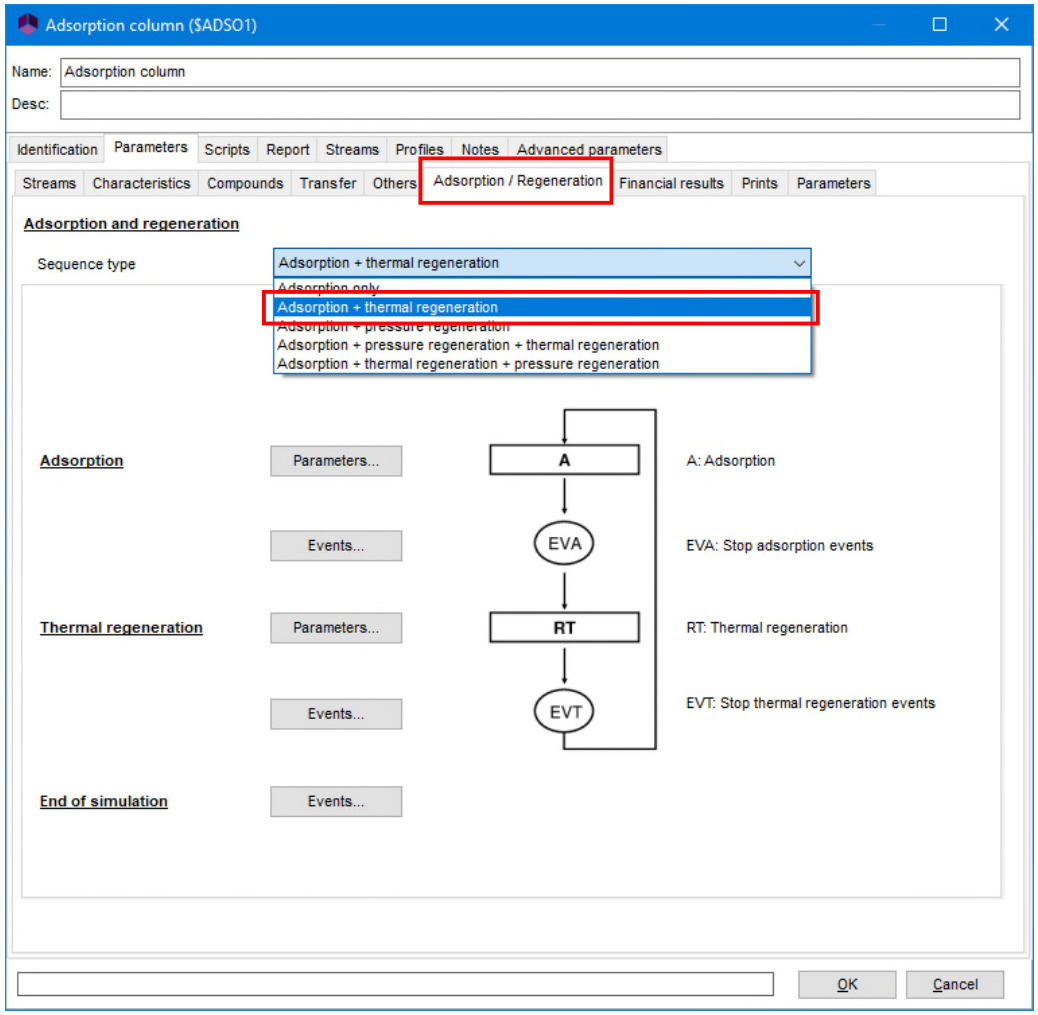
Step 3: Create the flowsheet
D- Adsorption column

- "Others" tab
  - Select the thermodynamic adsorption model



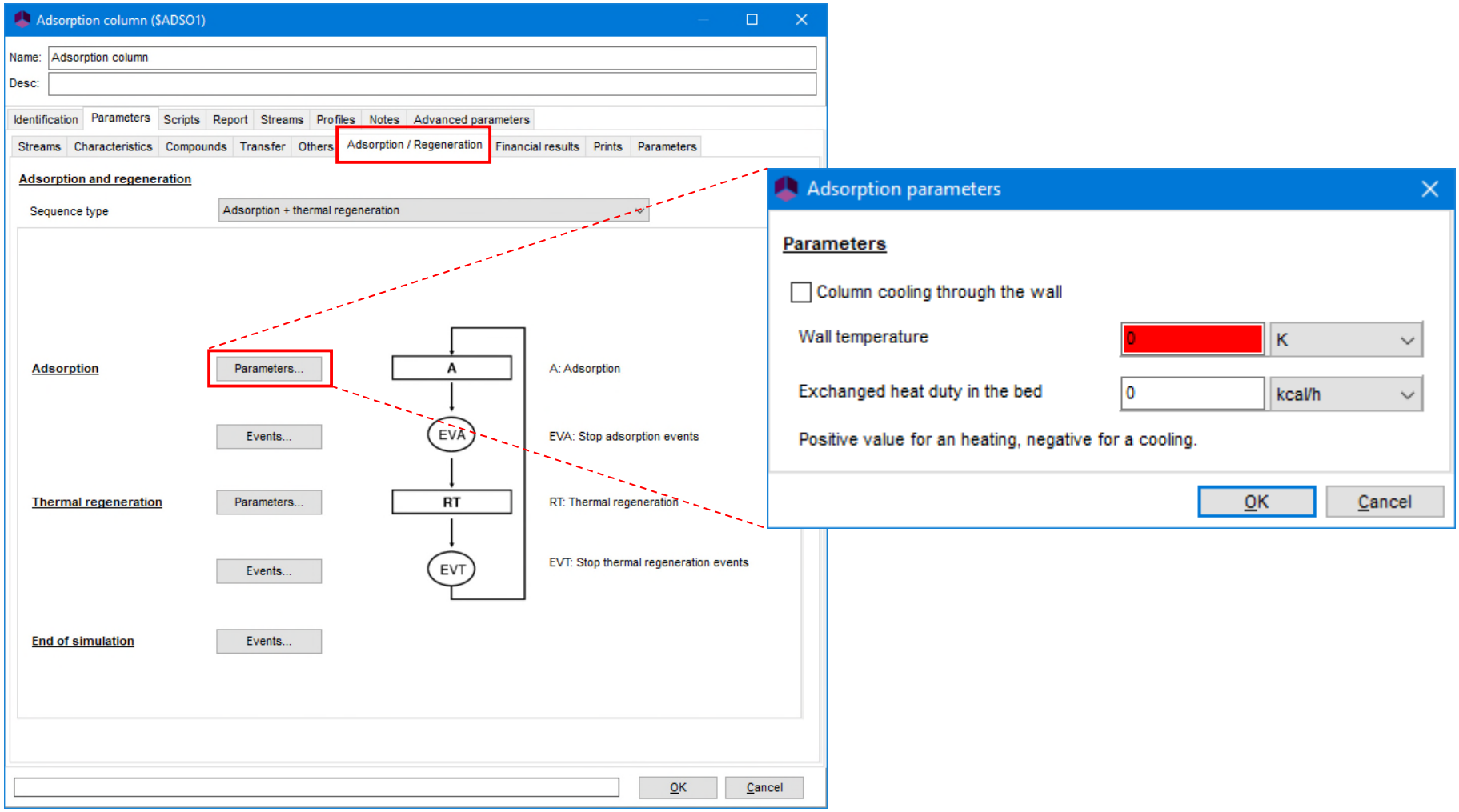
Step 3: Create the flowsheet
D- Adsorption column

- "Adsorption / Regeneration" tab
  - Select the TSA cycle (Adsorption + thermal regeneration)



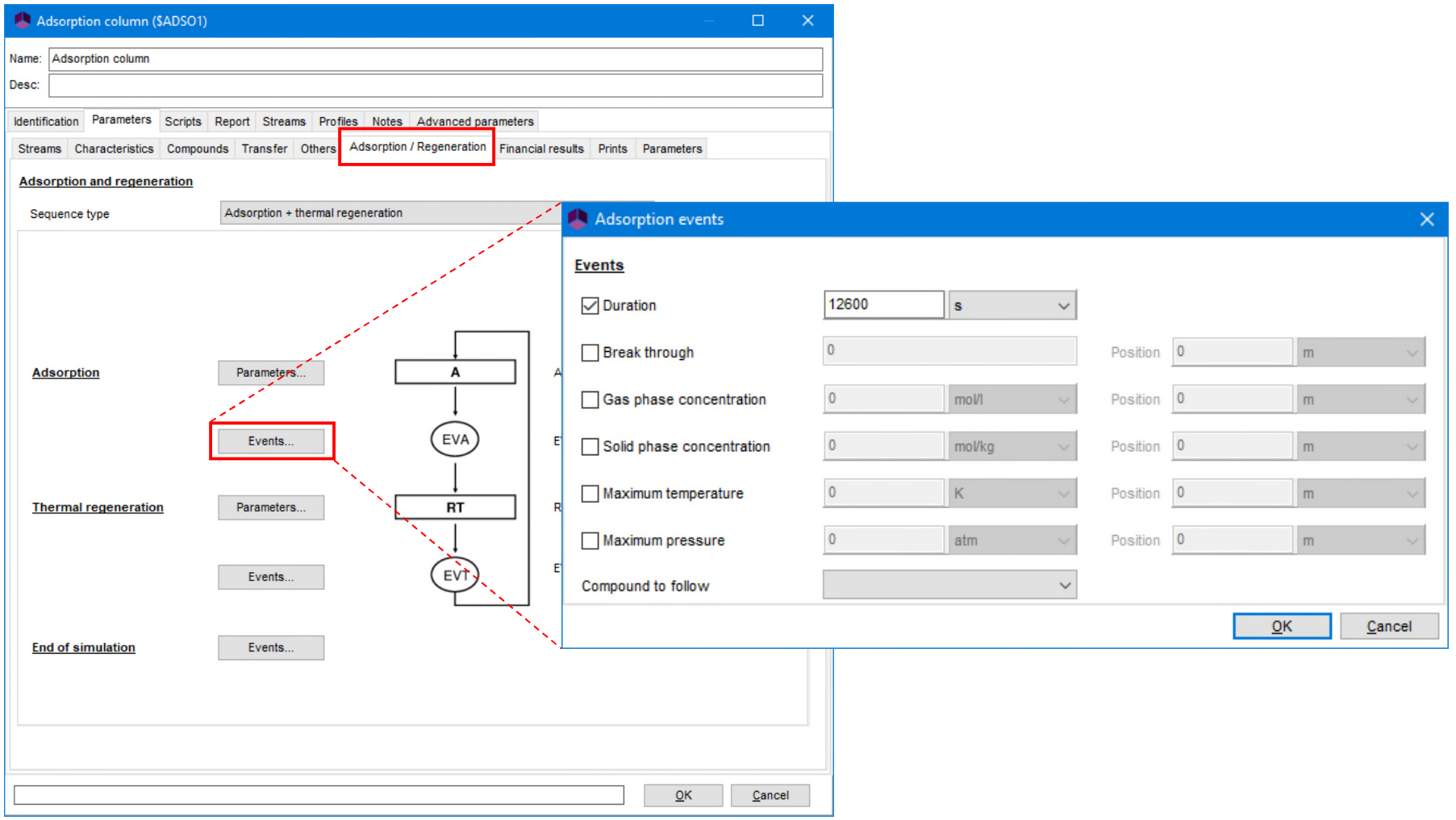
Step 3: Create the flowsheet
D- Adsorption column

- "Adsorption / Regeneration" tab
  - Fill in the parameters of the adsorption step



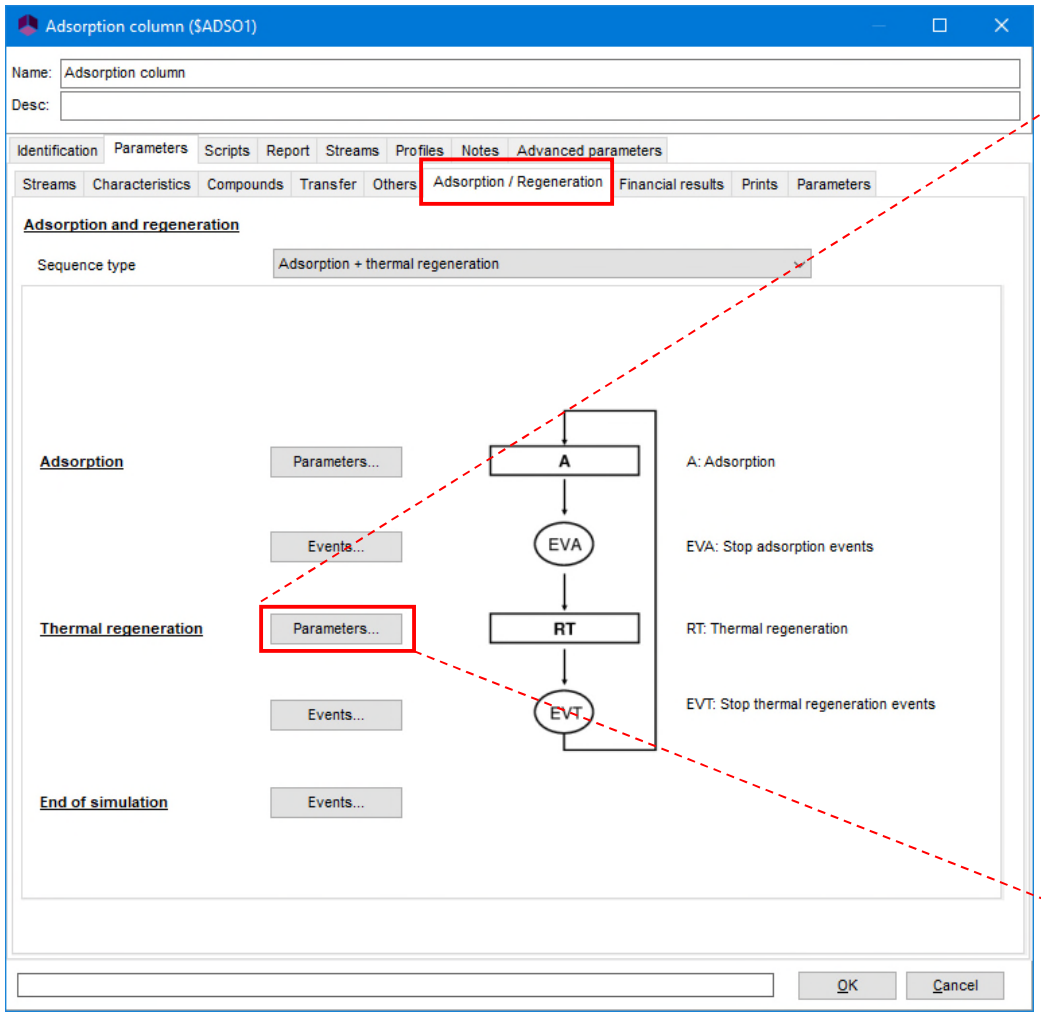
Step 3: Create the flowsheet
D- Adsorption column

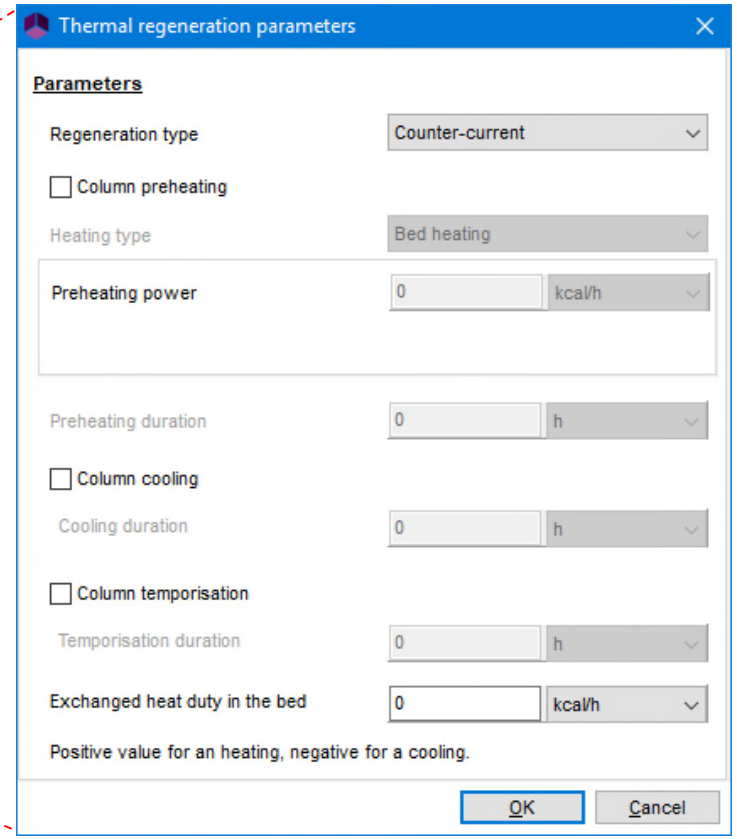
- "Adsorption / Regeneration" tab
  - Fill in the parameters of the event which stops the adsorption step



Step 3: Create the flowsheet
D- Adsorption column

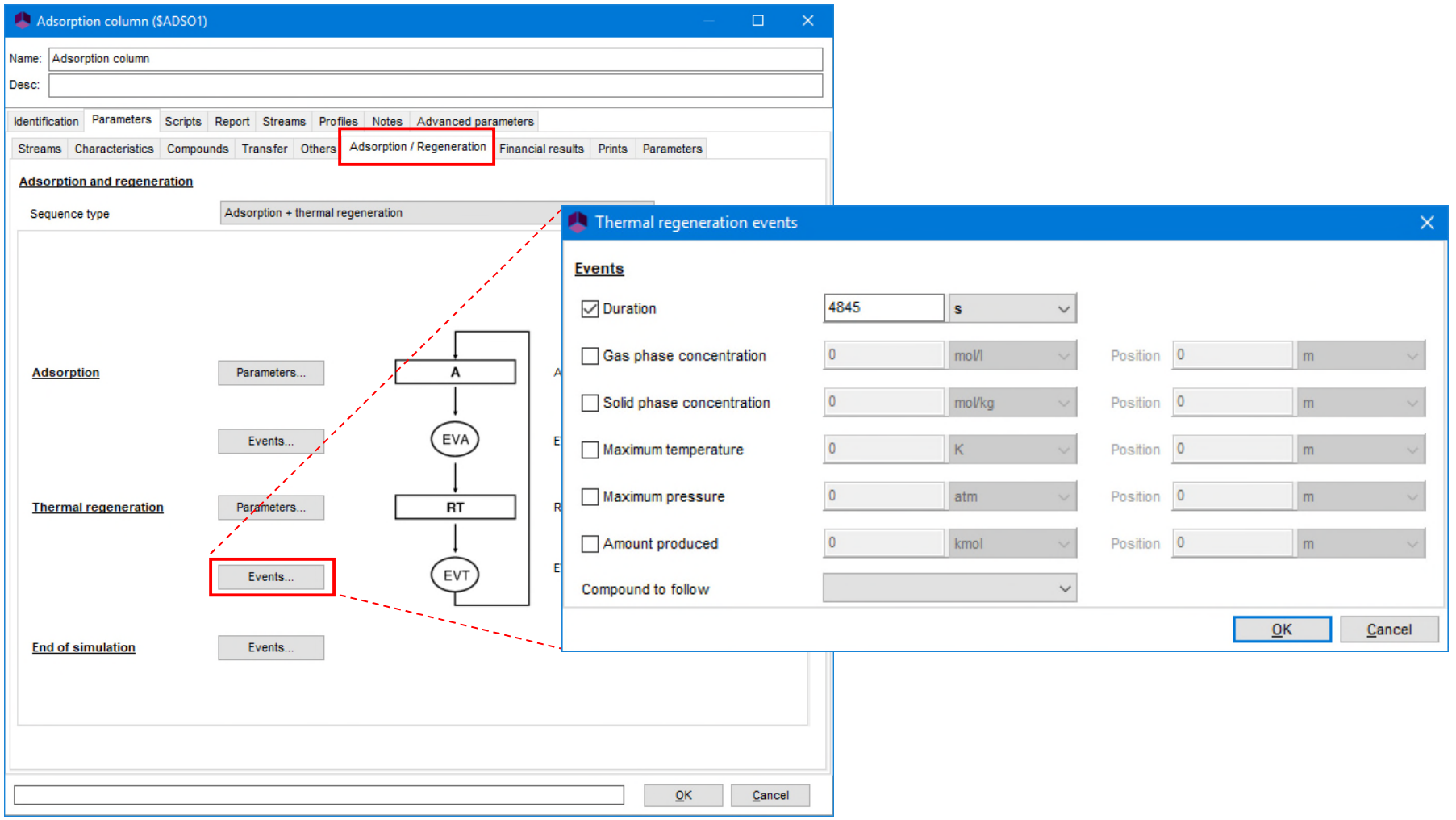
- "Adsorption / Regeneration" tab
  - Fill in the parameters of the thermal regeneration step





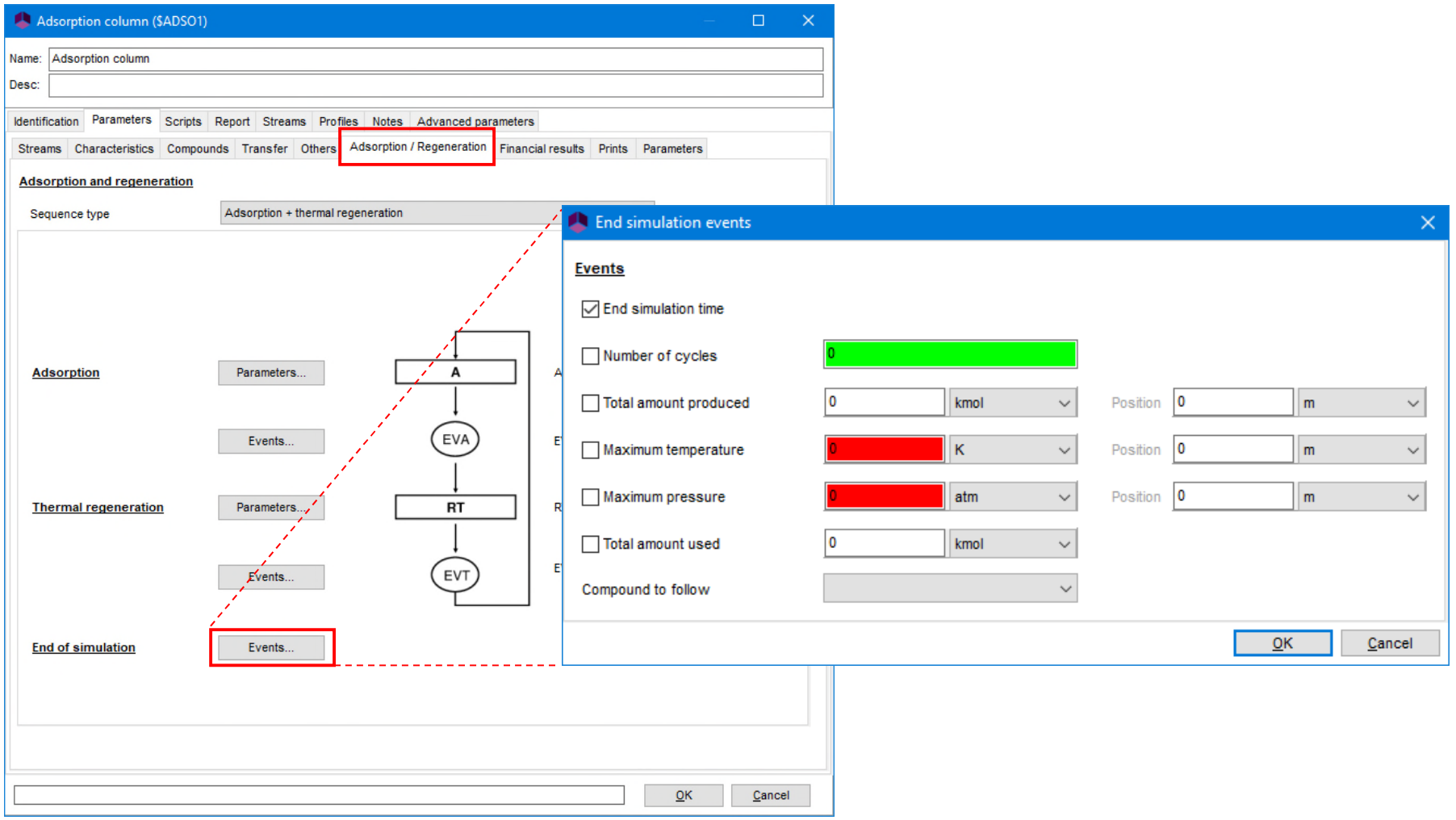
Step 3: Create the flowsheet
D- Adsorption column

- "Adsorption / Regeneration" tab
  - Fill in the parameters of the event which stops the thermal regeneration step



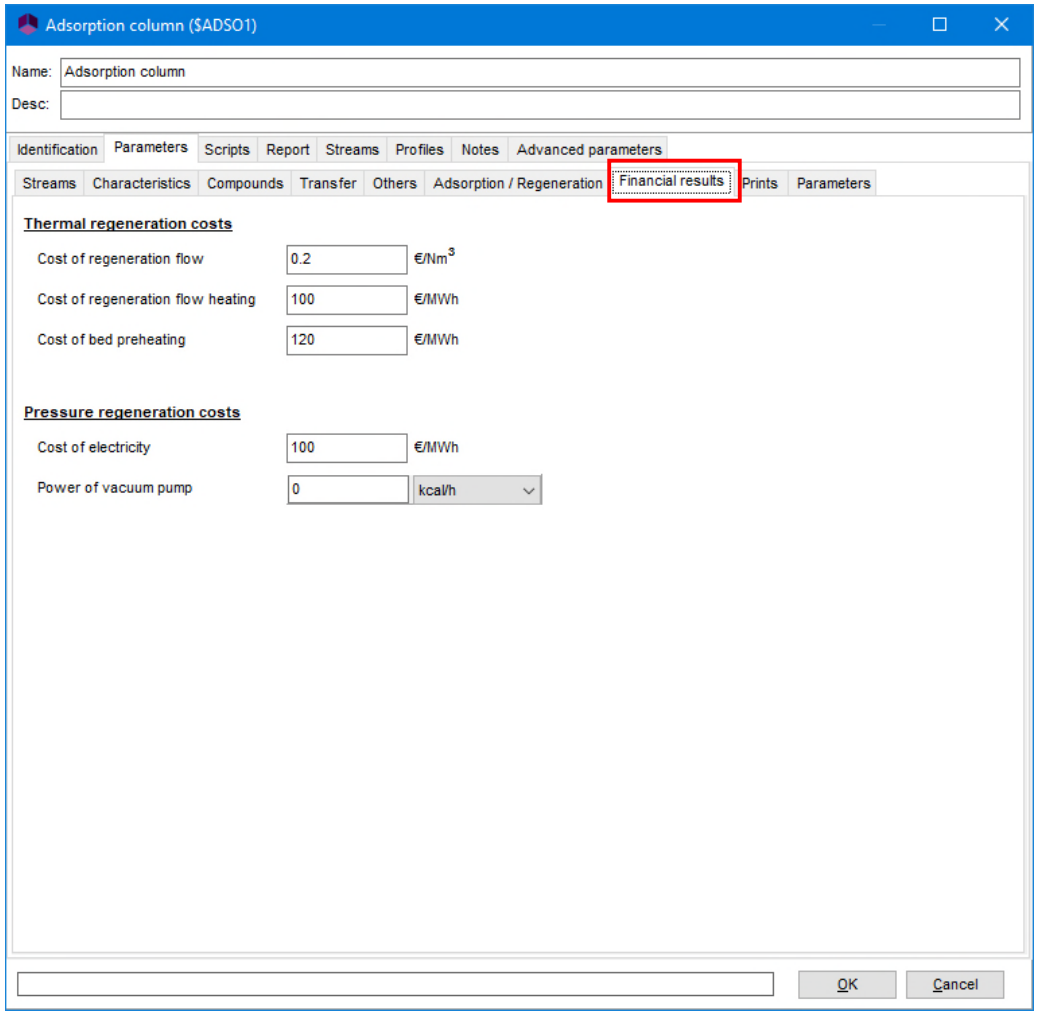
Step 3: Create the flowsheet
D- Adsorption column

- "Adsorption / Regeneration" tab
  - Fill in the parameters of the event which stops the simulation



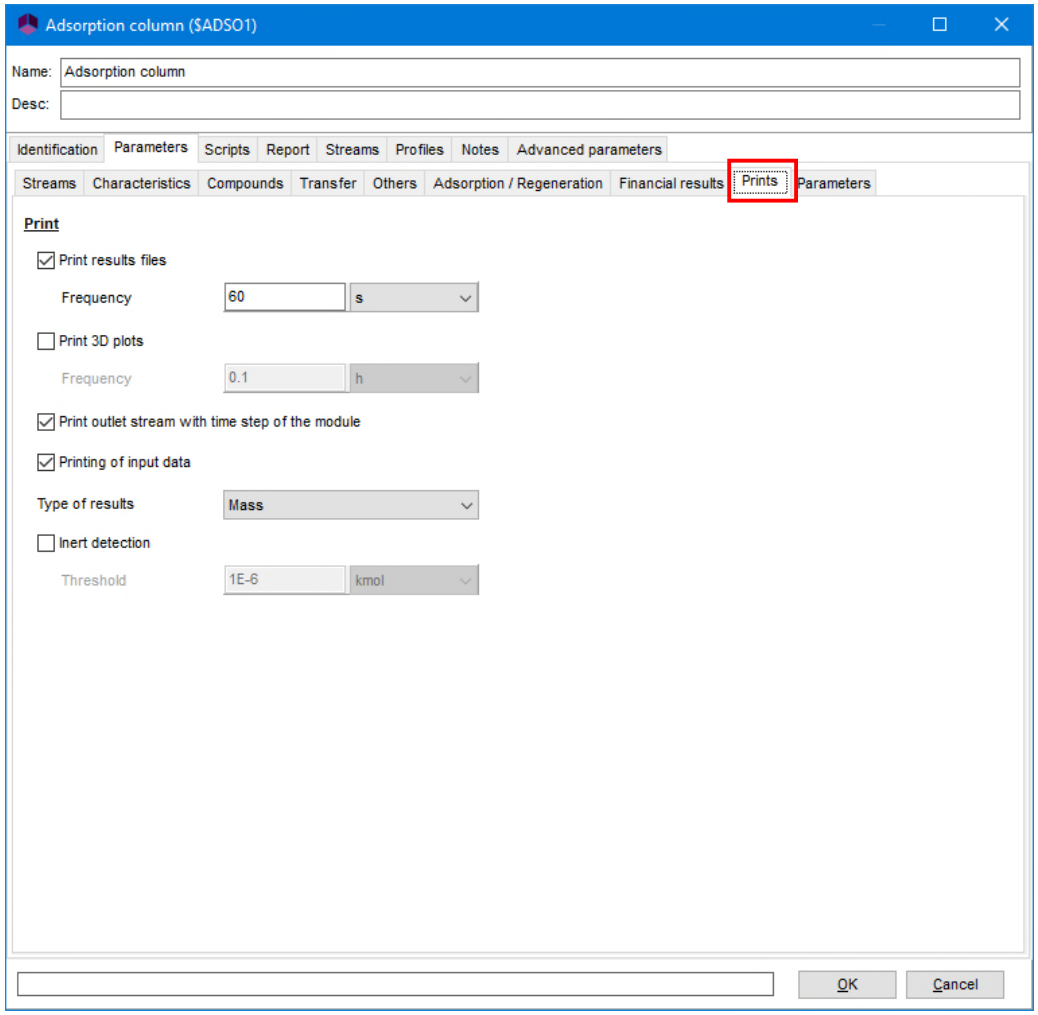
Step 3: Create the flowsheet
D- Adsorption column

- "Financial results" tab
  - Fill in the parameters used by the financial balance on the regeneration steps



Step 3: Create the flowsheet
D- Adsorption column

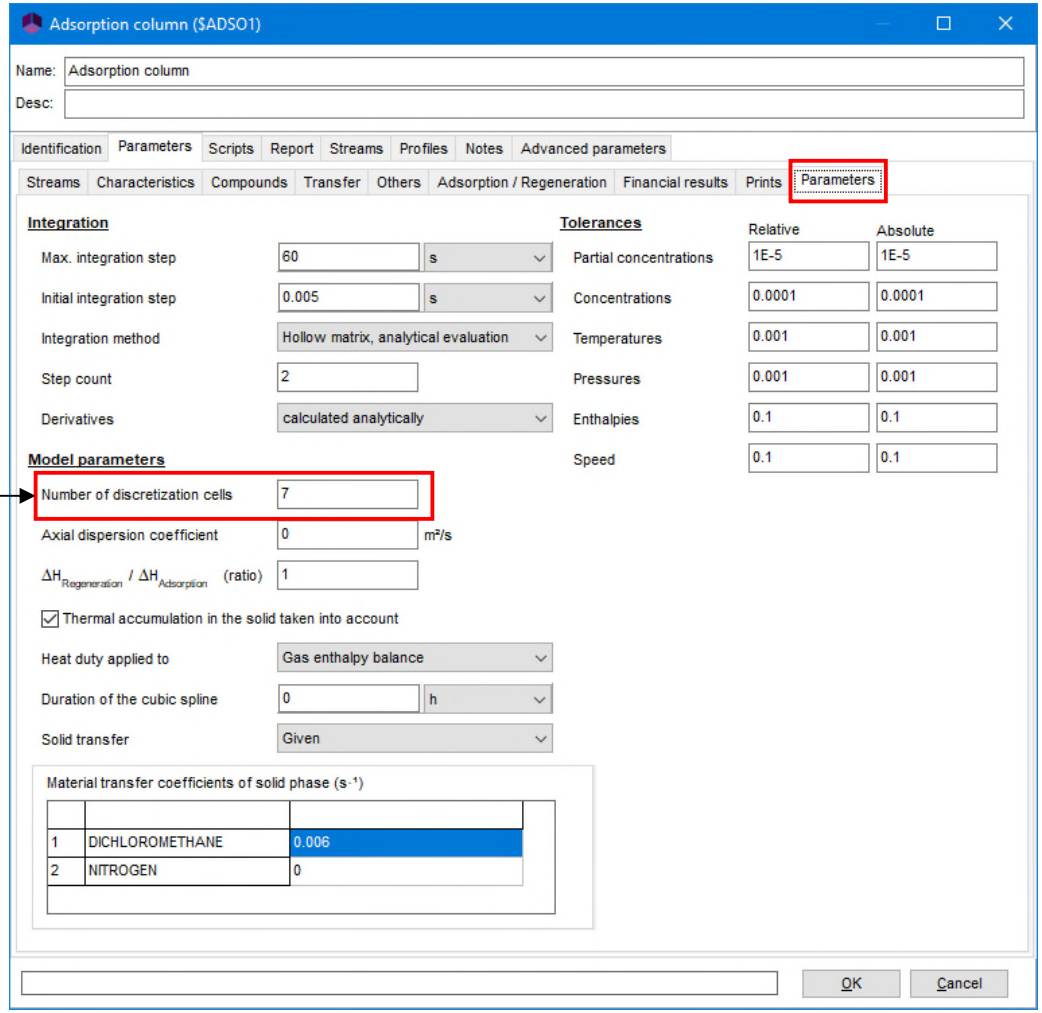
- "Prints" tab
  - Fill in the parameters of the reports (time dependent results)



Step 3: Create the flowsheet
D- Adsorption column

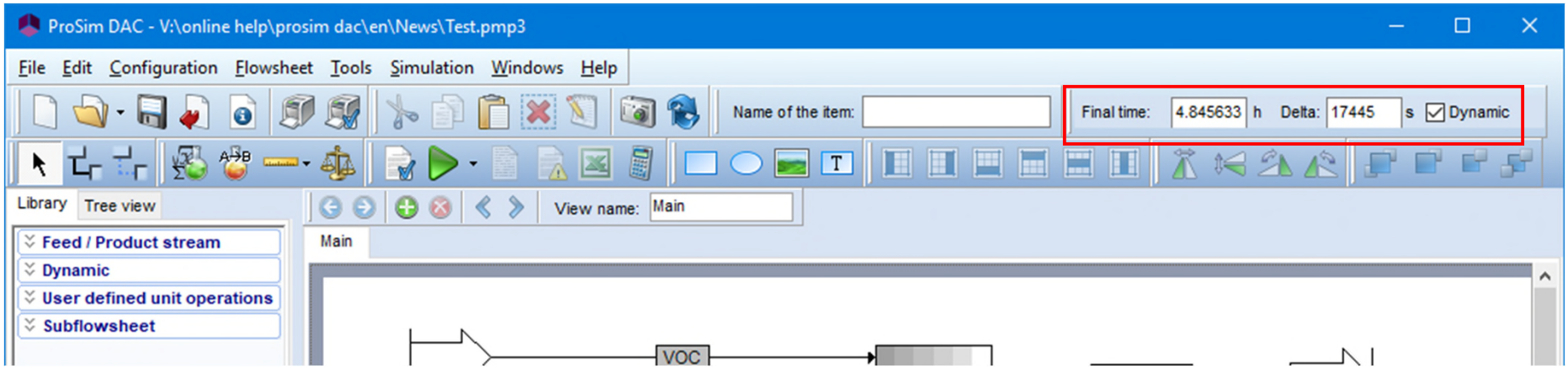
- "Parameters" tab
  - Fill in the numerical parameters and the model parameters

Number of longitudinal discretization cells

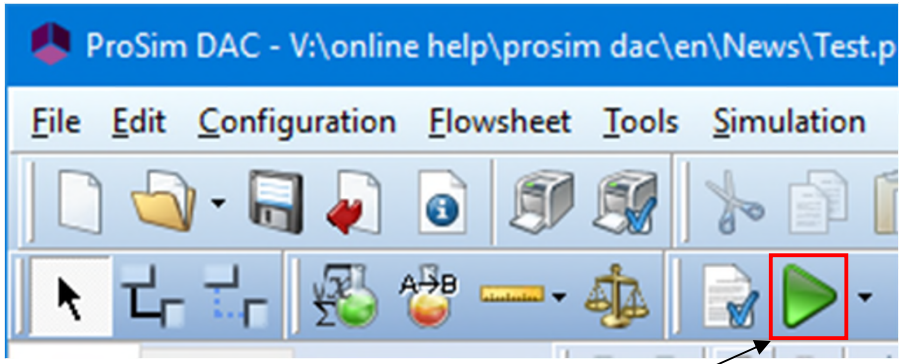


Step 3: Create the flowsheet
D- Operating time

- Define the total operating time
  - In ProSim DAC the final time and the “Delta” has to be the same

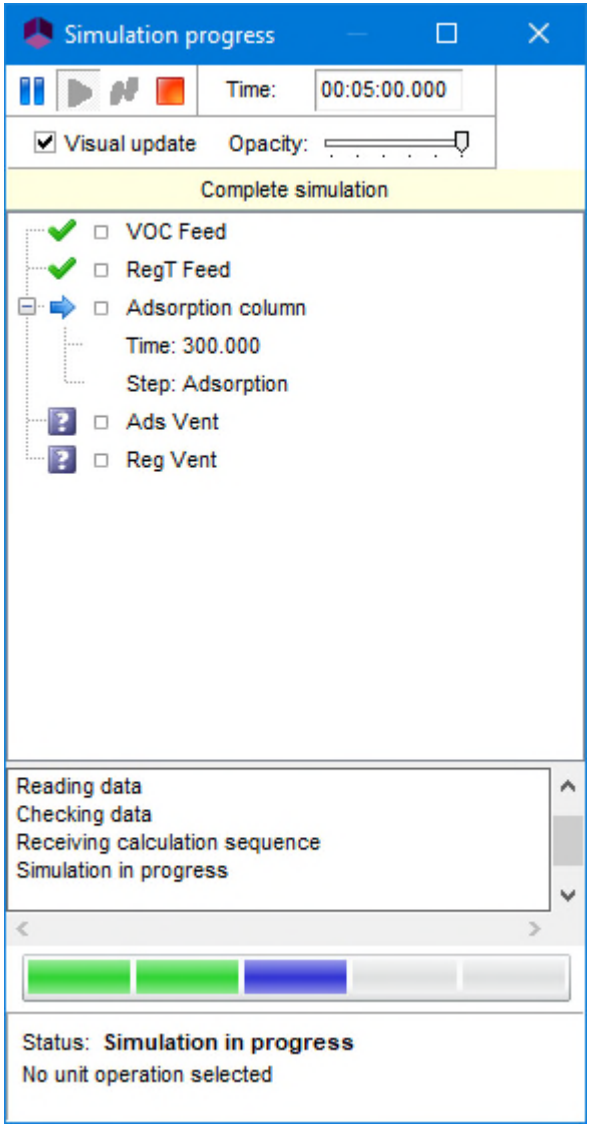


Step 4: Running the simulation



Click on the green arrow to start the simulation

When the simulation starts,
the “Simulation progress” window opens.

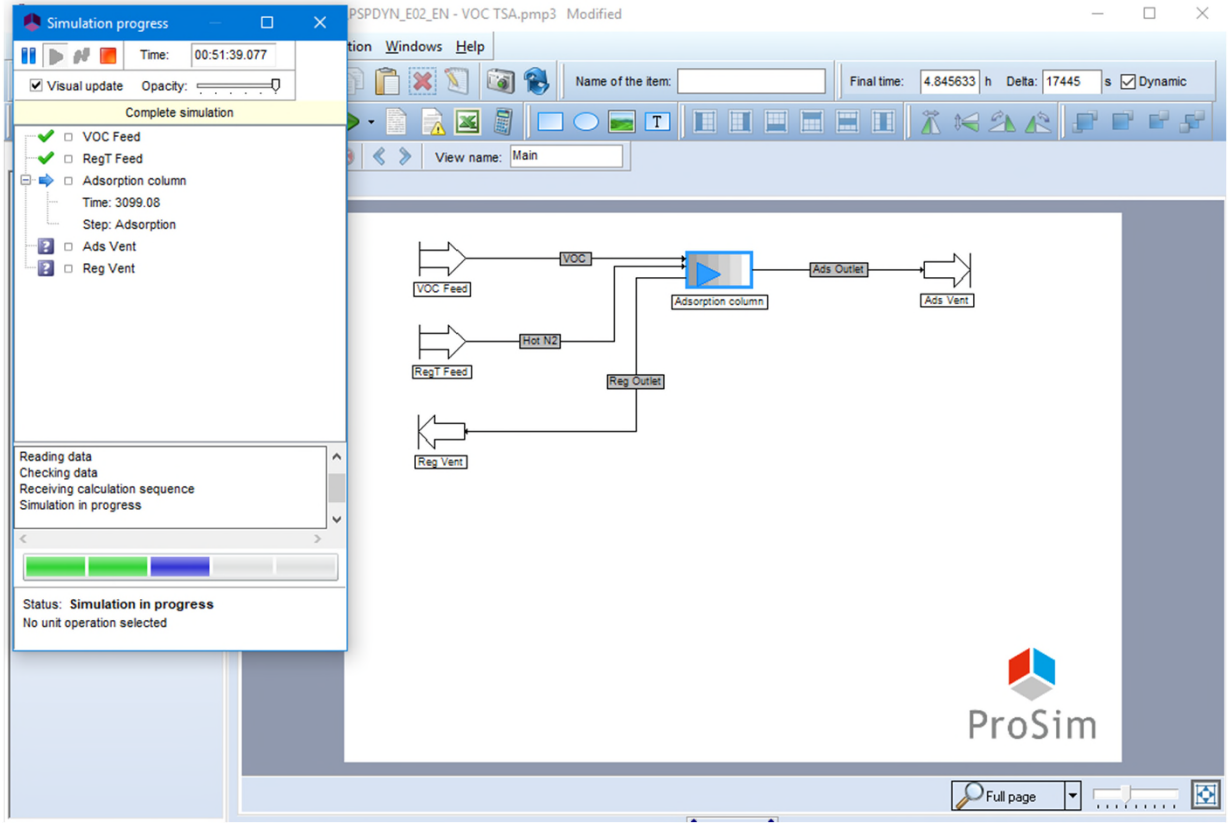


Step 4: Running the simulation

During the calculation, different symbols and indications will appear and disappear in the "Simulation progress" window and in the drawing area.

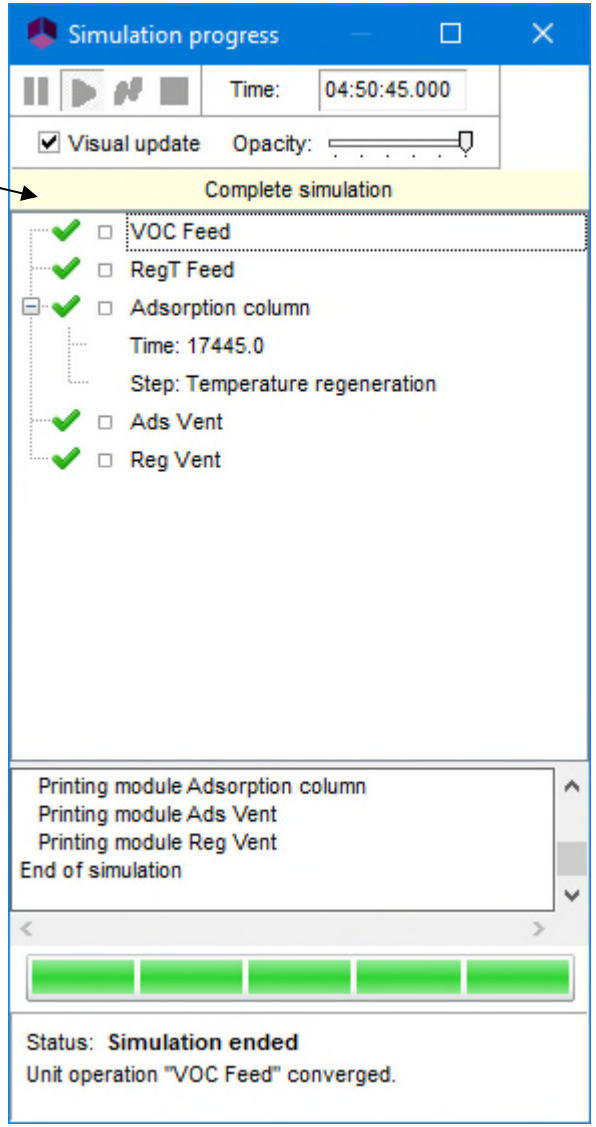
- A green validation mark indicates that the module has been correctly calculated
- A blue arrow indicates that calculation is in progress
- A blue question mark indicates that the module has not been calculated yet

- A red cross indicates a convergence error



Step 4: Running the simulation

When all the modules have been properly calculated, all the marks are in green. Your simulation is successful.



Closing the “Simulation progress” window will, by default, automatically open the simulation report (this option cab be changed in the “Preferences” of the software).

Step 5: Simulation reports

A. Global report

B. Adsorption column report and profiles

C. Outlet streams profiles

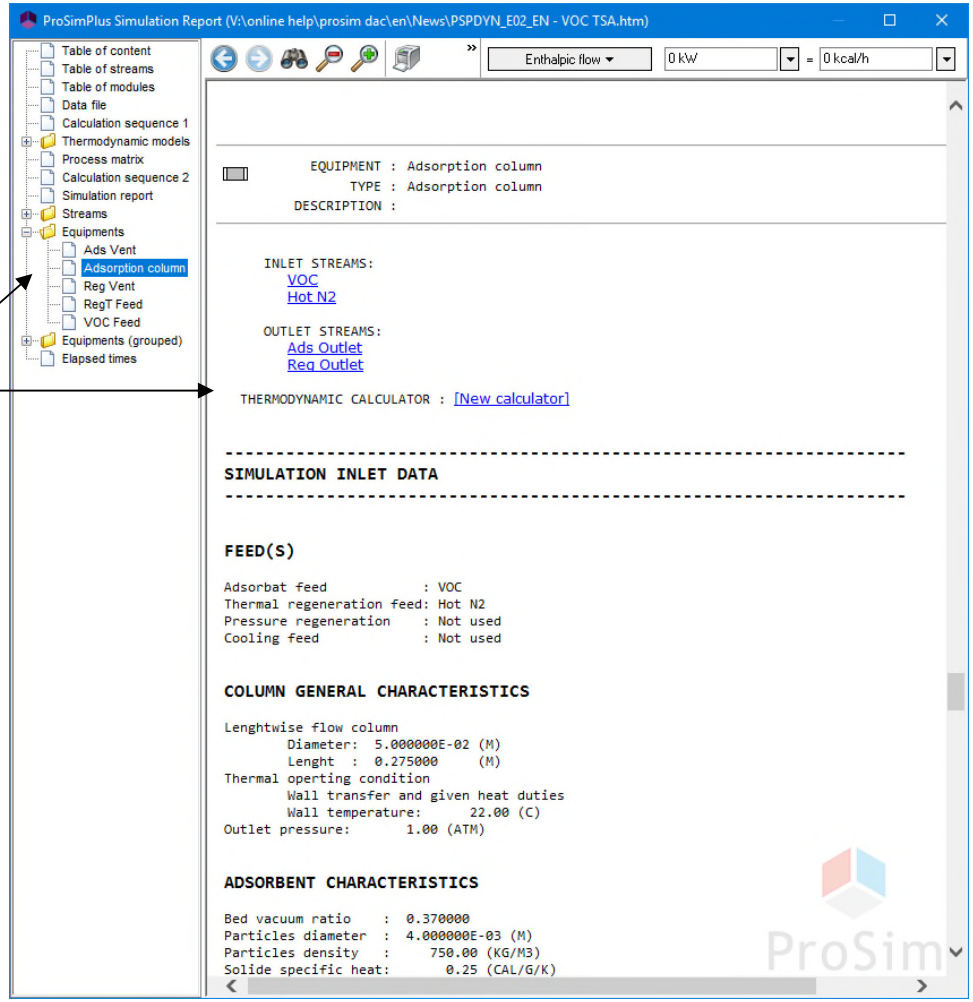
Step 5: Simulation reports
A- Global report

The HTML report is automatically displayed after each run

It provides information about:

- Pure component properties and thermodynamic models
- List of equipment calculation
- Process streams characteristics
- Results for each process equipment
- Convergence and constraints

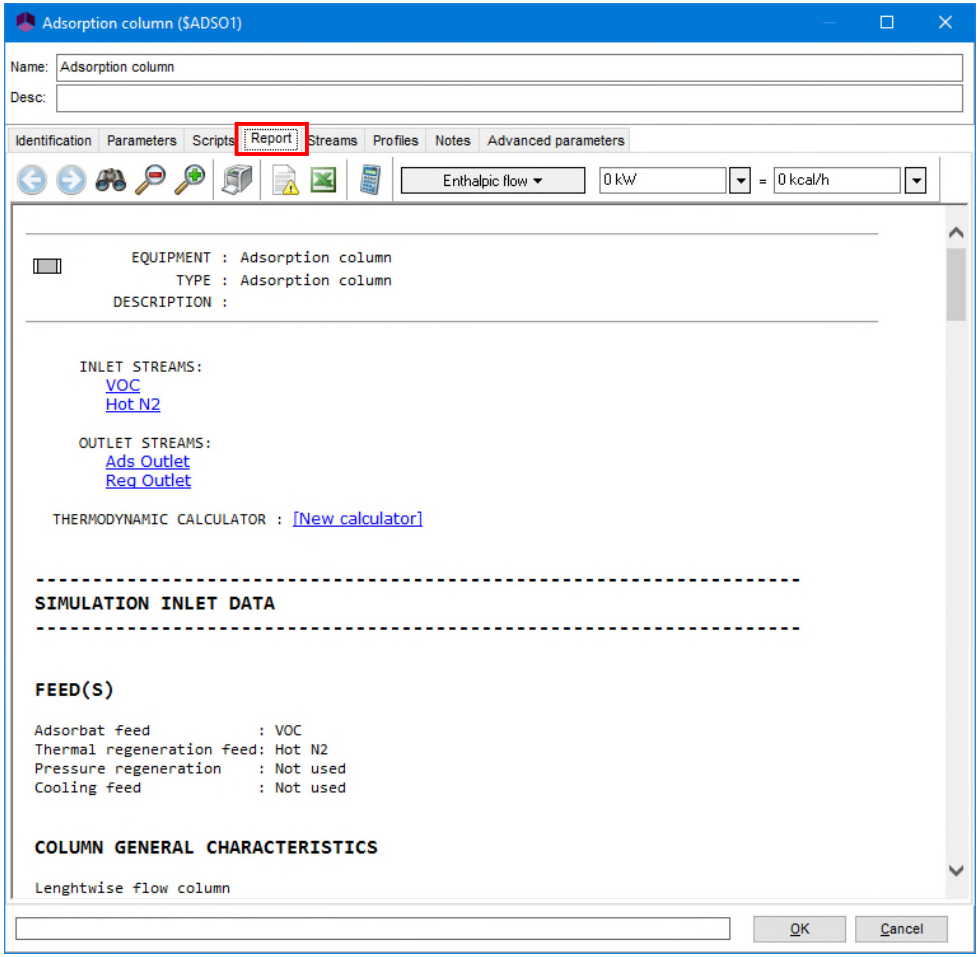
Hyperlinks give you direct access to detailed information on initial configuration, unit operations, calculation sequence and results.



All the reports are created in the project folder.

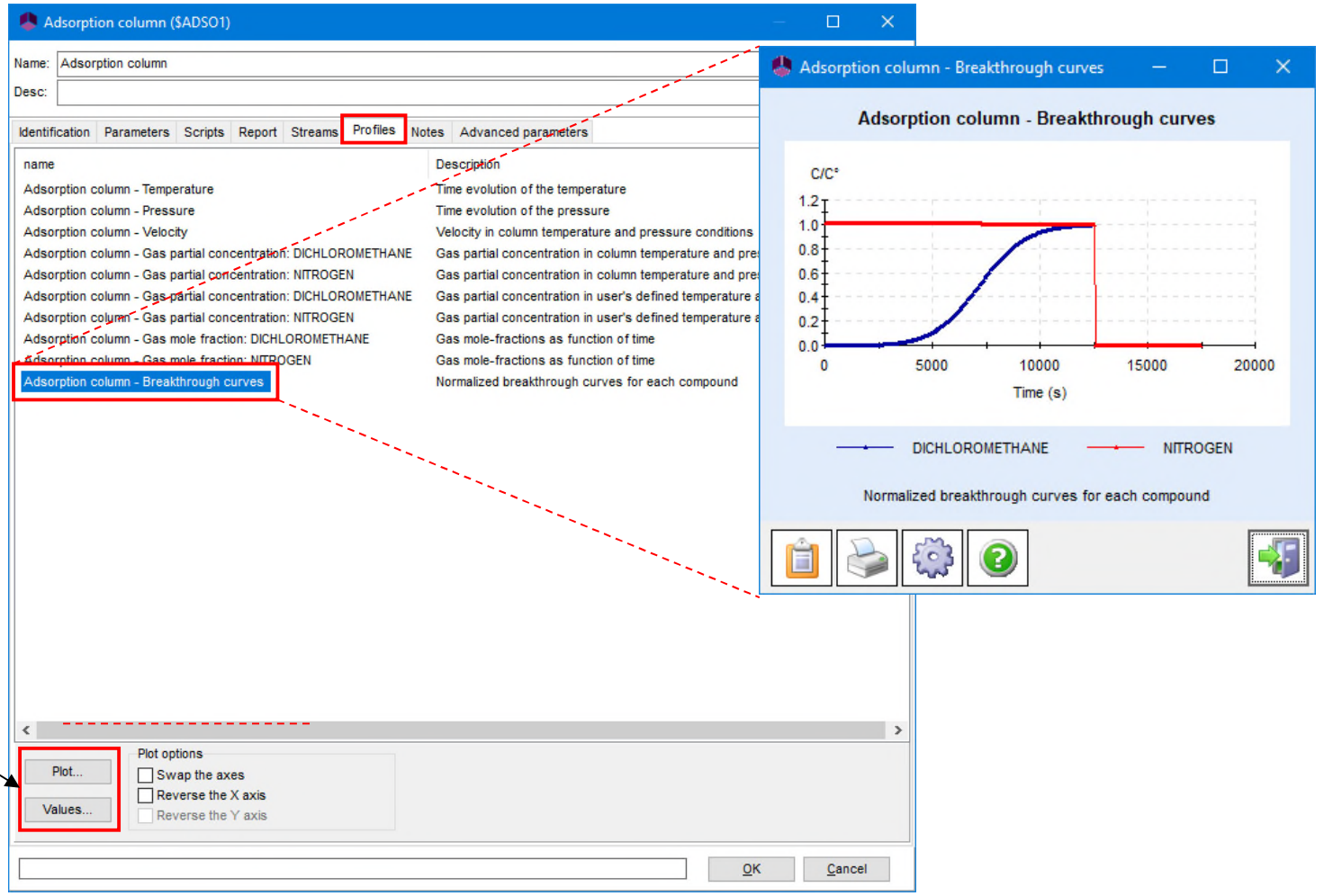
Step 5: Simulation reports
B- Adsorption column report and profiles

- Tabulated results are also available in the “Report” tab of the adsorption column module
  - Adsorbed quantities, regenerated quantities, etc.



Step 5: Simulation reports
B- Adsorption column report and profiles

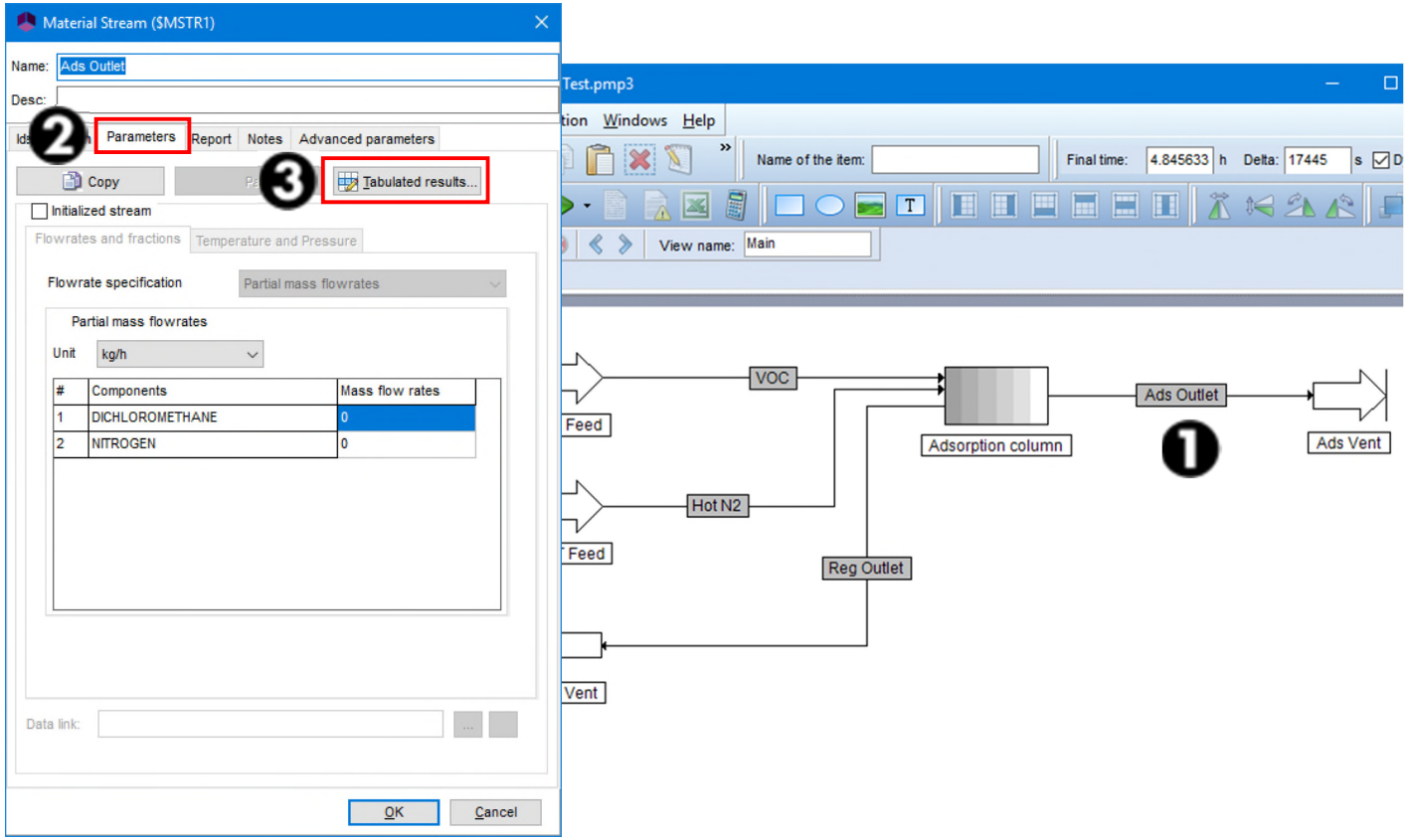
- Profiles are available in the “Report” tab of the adsorption column module
  - Temperature, concentrations, breakthrough curve, etc.



Plot the graph or display the values

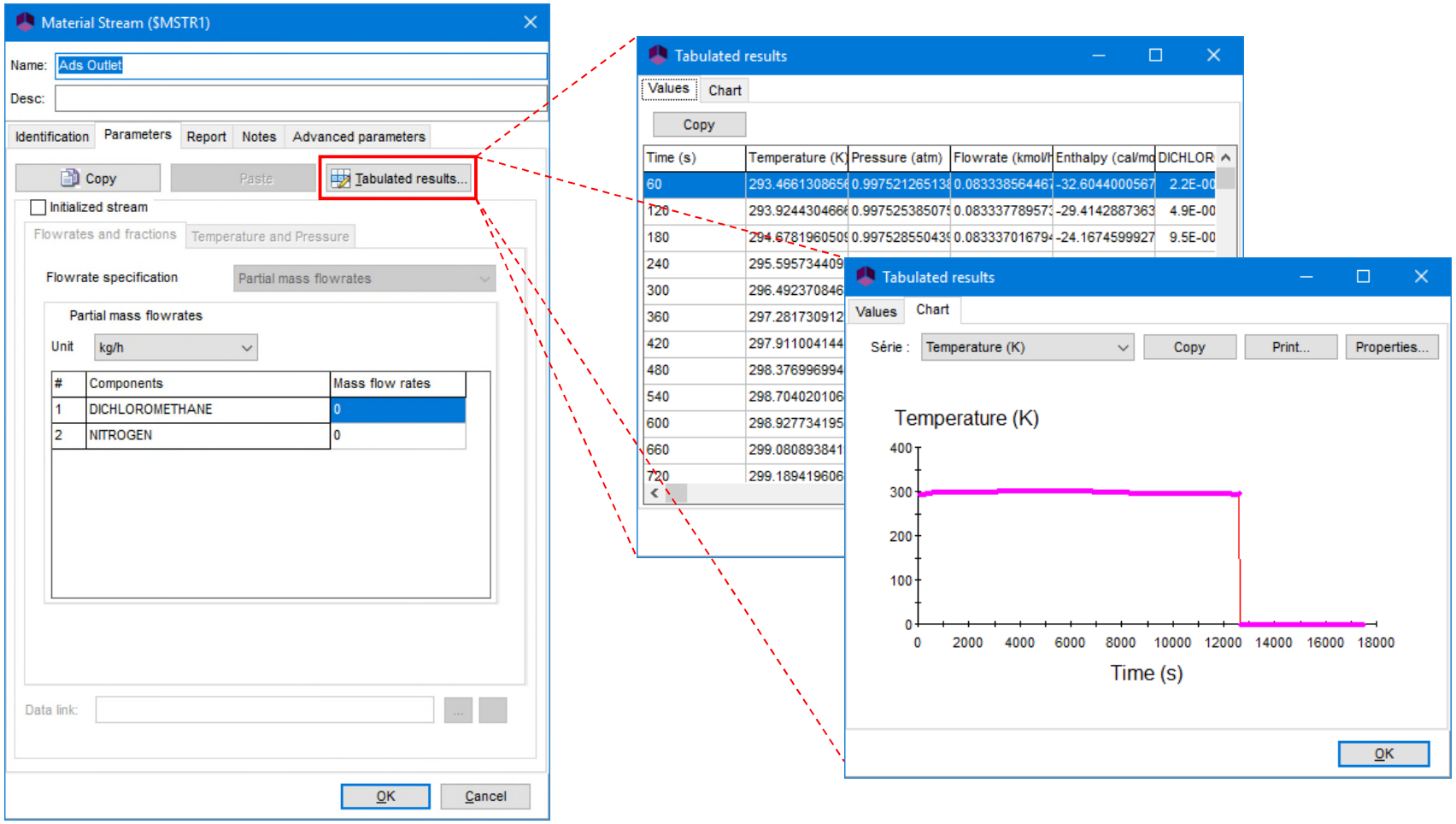
Step 5: Simulation reports
C- Outlet streams profiles

- Profiles are available in outlet streams
  1. Double-click on the outlet stream to open its edition windows
  2. Go on the “Parameters” tab
  3. Click on “Tabulated results…” button



Step 5: Simulation reports
C- Outlet streams profiles

- Profiles are available in outlet streams
  - Temperature, compositions, etc. profiles of the outlet of the column

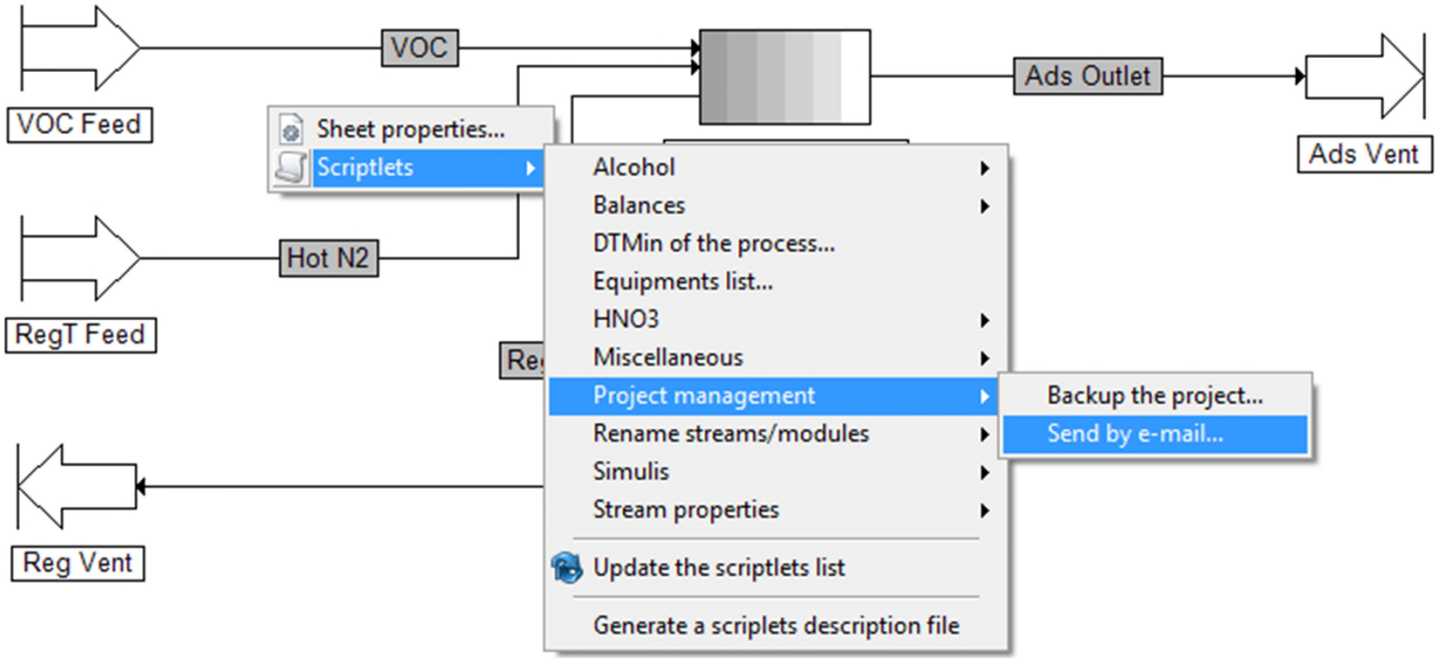


Step 6: Sharing the simulation

When you need to send the simulation to someone else, simply right click anywhere on the flowsheet, and select the Scriptlet “Send by e-mail…”.

This action will automatically create a zip file that will include among other:

- ✓ The “.pmp3” file (ProSim DAC file)
- ✓ The “.htm.” file (simulation report file)
- ✓ …



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