

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.

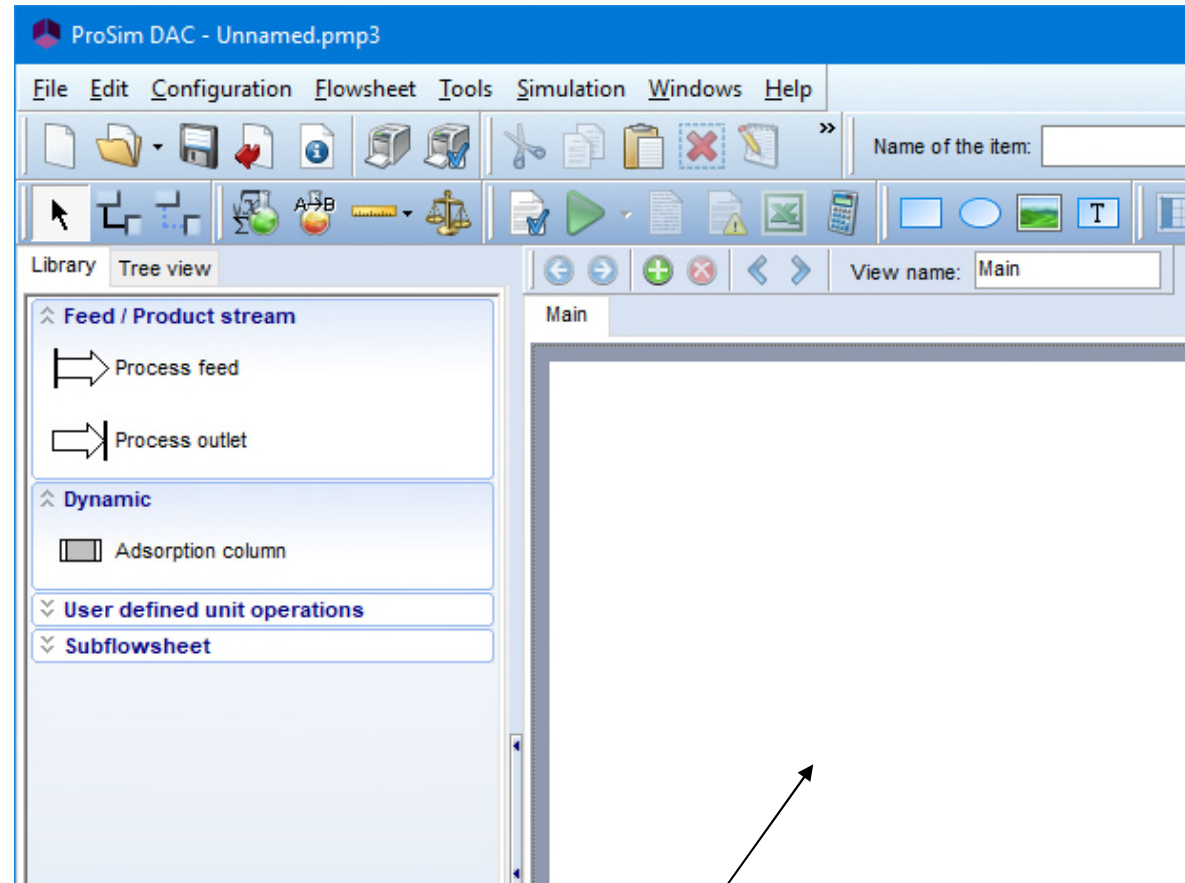
Before we start: Interface key functions

Menus bar

Tools bar

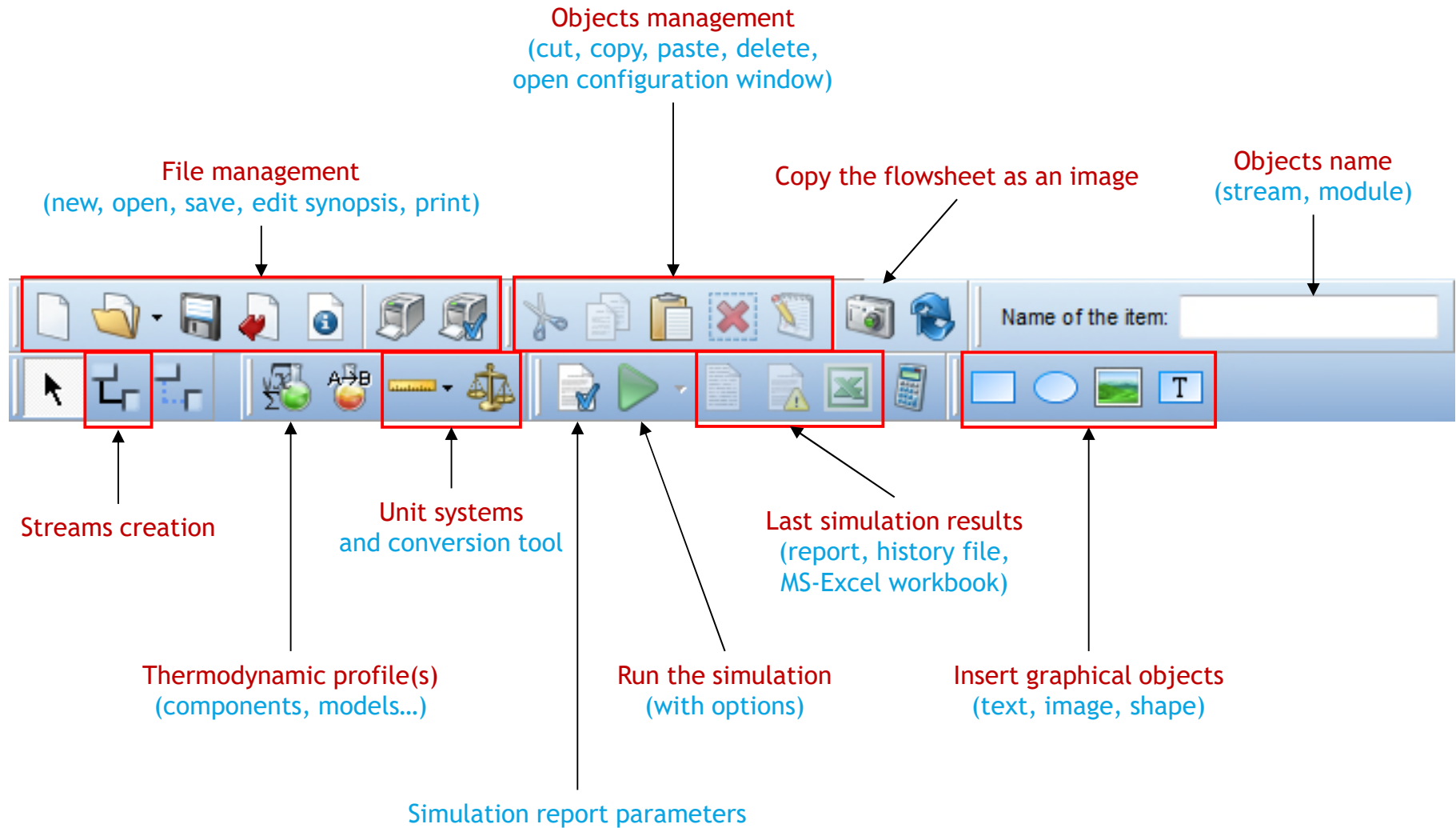
Categories list

Unit operations, within the selected categories



Drawing area

Before we start: Interface key functions



Before we start: Interface key functions

■ Graphical object management



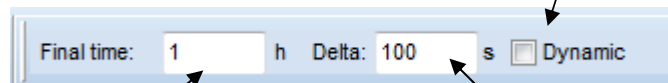
Arrange unit operations on the flowsheet
(align, center...)

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



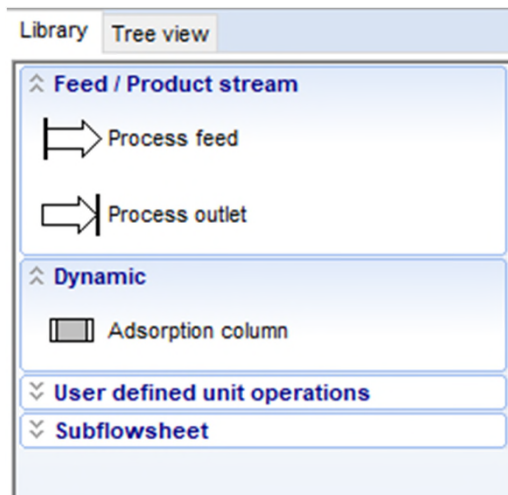
Simulation total duration

Simulation duration for a unit operation

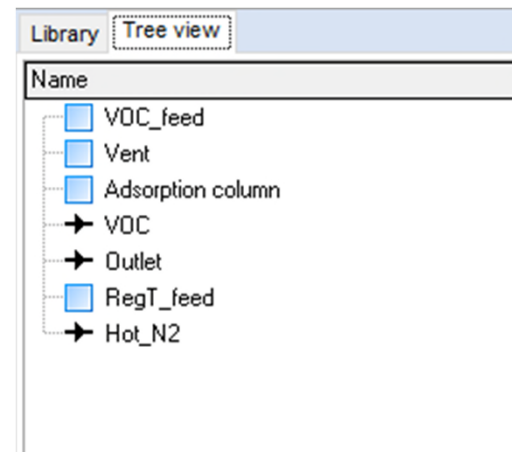
Check this box to allow a dynamic simulation

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

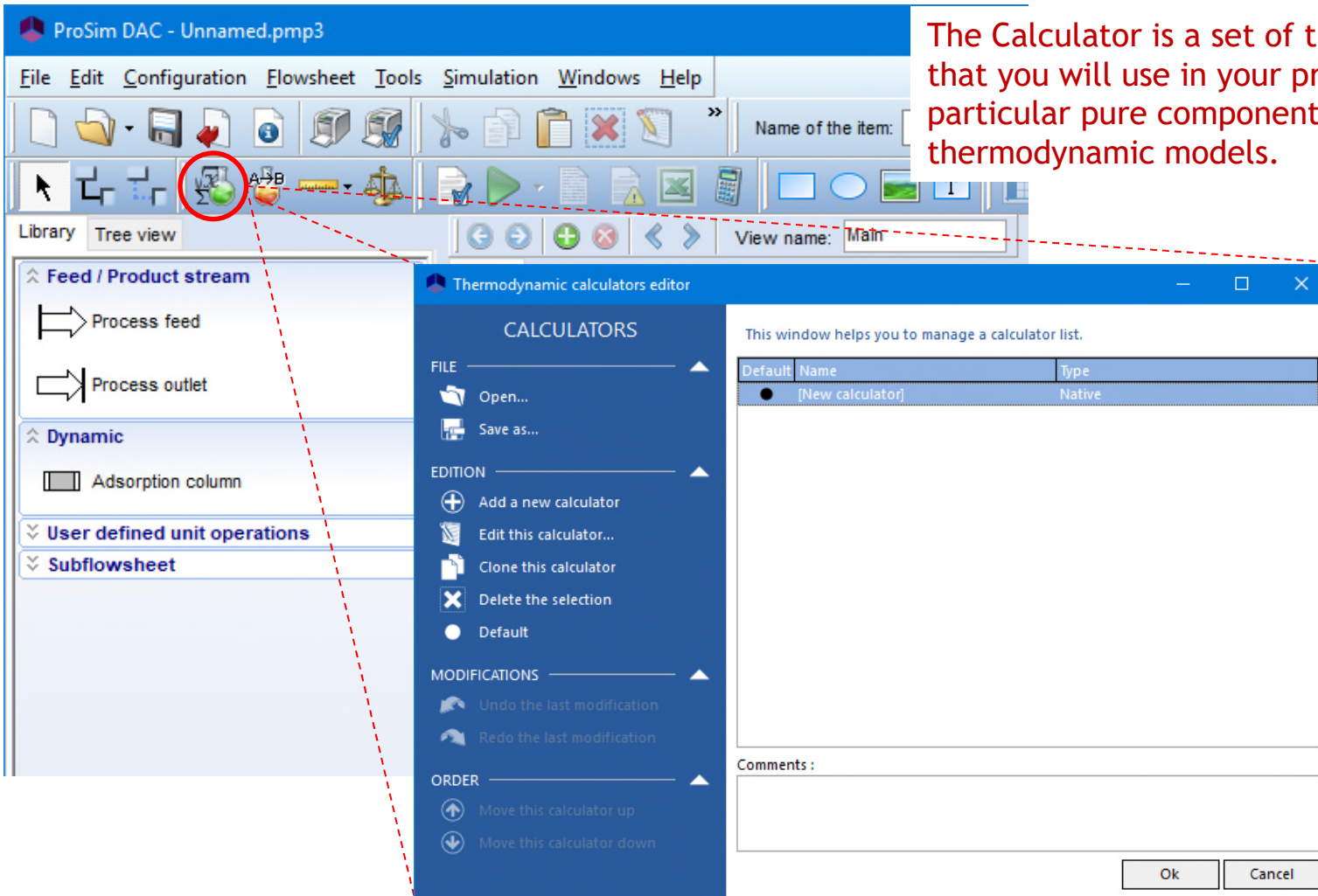


Tree view

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.

Thermodynamic calculators editor

This window helps you to manage a calculator list.

Default	Name	Type
<input checked="" type="radio"/>	[New calculator]	Native

Comments :

Ok Cancel

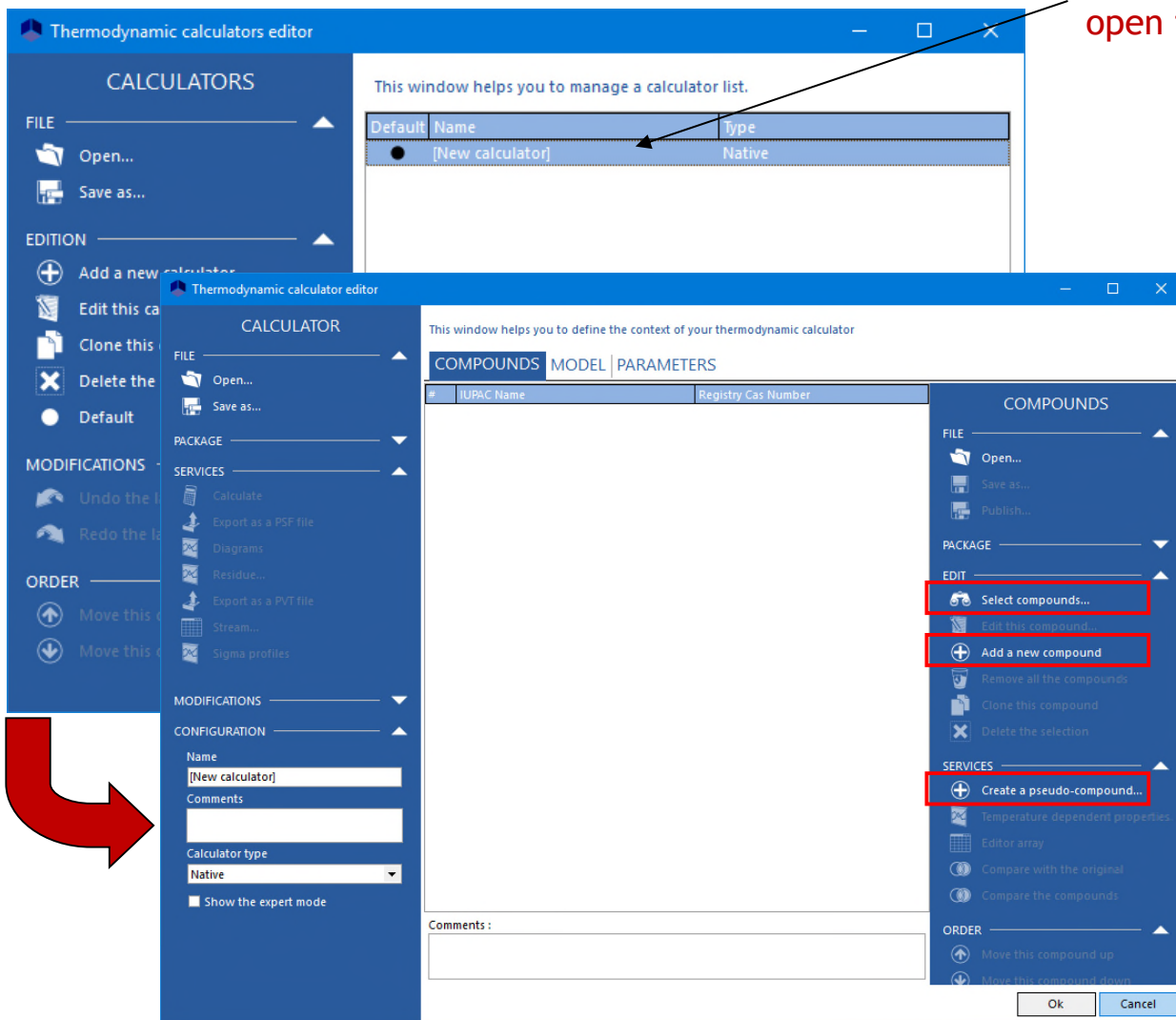
Click on the thermodynamic icon to open the calculators editor.



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

COMPOUNDS

CRITERIA

Search

☐ Name or synonym

☐ CAS registry number

☐ Chemical formula

☐ Specific ID

☐ Advanced

☒ Exact name

OPTIONS

☒ Clear previous results

New Help

SEARCH IN

- All servers
 - Simulis® Compounds Files
 - Common files
 - DIPPR L18+
 - HNO3
 - Sponsor 05-2018
 - Standard 2007
 - Standard 2009
 - Standard 2011
 - Standard 2013
 - Standard 2015
 - ☒ Standard 2017
 - User files

Name: DICHLOROMETHANE
 Location: Standard 2017 (Simulis® Compounds Files\Common files)
 CAS registry number: 75-09-2
 Specific ID: [D1D2AA11-84EB-4CF1-B077-C5AA5F6FC7D9]

Search results Favorites History

#	IUPAC name (or compo...	Chemical form	CAS num	Molecular wet...	Bubble temper...
1	DICHLOROMETHANE	CH2Cl2	75-09-2	84,9326	312,900

Selected compounds:

Name

DICHLOROMETHANE

Close

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.

The screenshot shows the 'Thermodynamic calculator editor' window. The 'MODEL' tab is selected in the top navigation bar. The 'Profile' dropdown menu is set to 'Ideal'. The 'THERMODYNAMIC MODEL' panel on the right shows the 'Water-hydrocarbons model' with Sol A and Sol B values.

Thermodynamic calculator editor

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

COMPOUNDS **MODEL** PARAMETERS

Name: Ideal

Category: All the profiles

Profile: Ideal

Approach type: From activity coefficients

Equation of state: Perfect gas

Alpha function: Not defined

Mixing rules: Not defined

Activity coefficient model: Ideal

Pure liquid fugacity standard state: Vapor pressure

Liquid molar volume: Ideal mixture

Transport properties: Classic methods

Enthalpy calculation: $H^*=0$, ideal gas, 25°C, 1 atm

User-defined thermodynamic model: None

Model index: 1

Comments:

THERMODYNAMIC MODEL

CONFIGURATION

Parameters

Thermodynamic assistant

Thermodynamic help

Use a specific model for pure water

Advanced:

Water-hydrocarbons model

Sol A: 6,25043

Sol B: 4015,3

The liquid phase splitting is taken into account

Predictive model parameters...

True species model

Reactive model parameters...

Ok Cancel

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

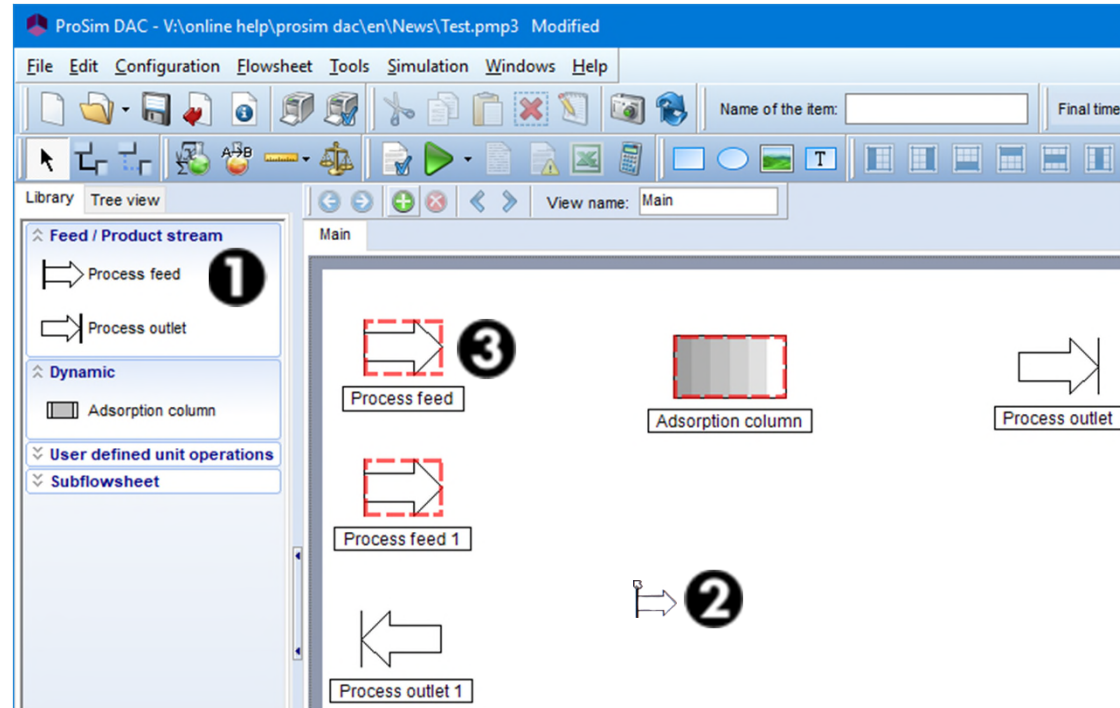
Two process feeds, two process outlets and one adsorption column are needed for this example.

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.

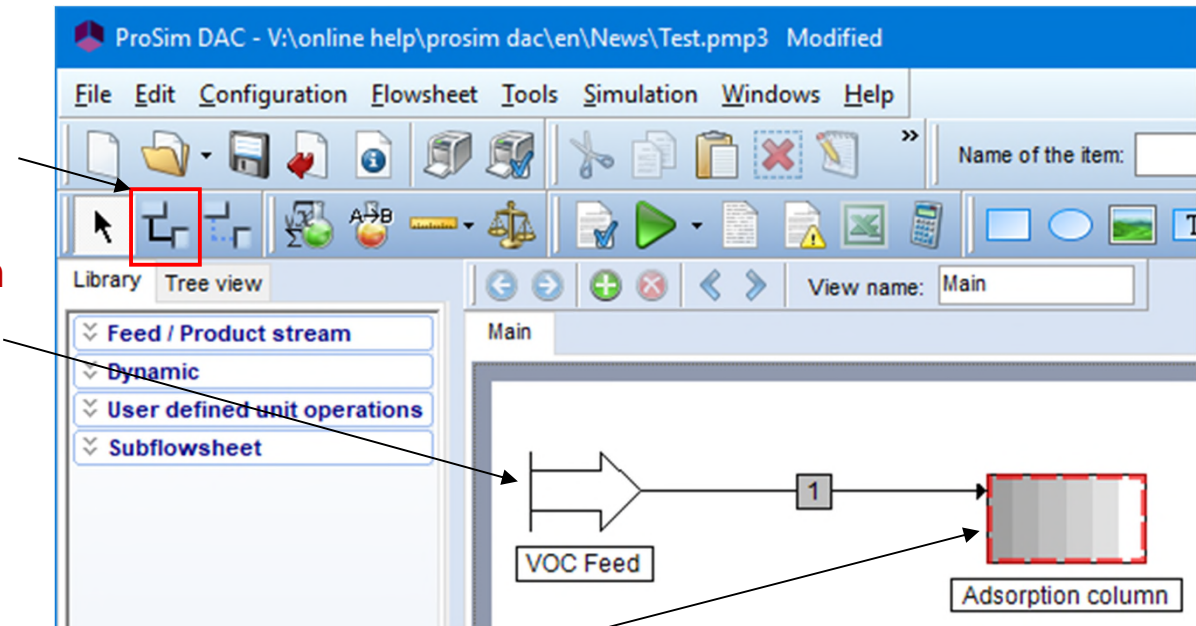


Use the graphical object management toolbar to arrange the modules on the flowsheet

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

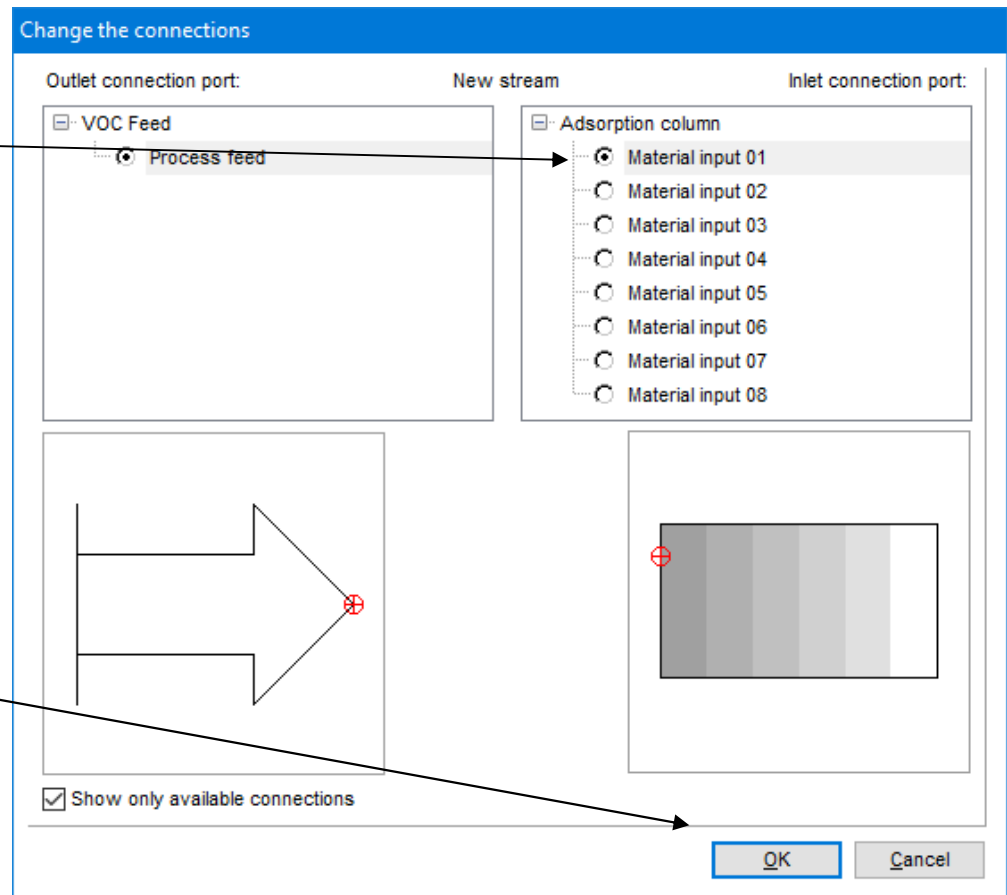
B- Connect the modules

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”.

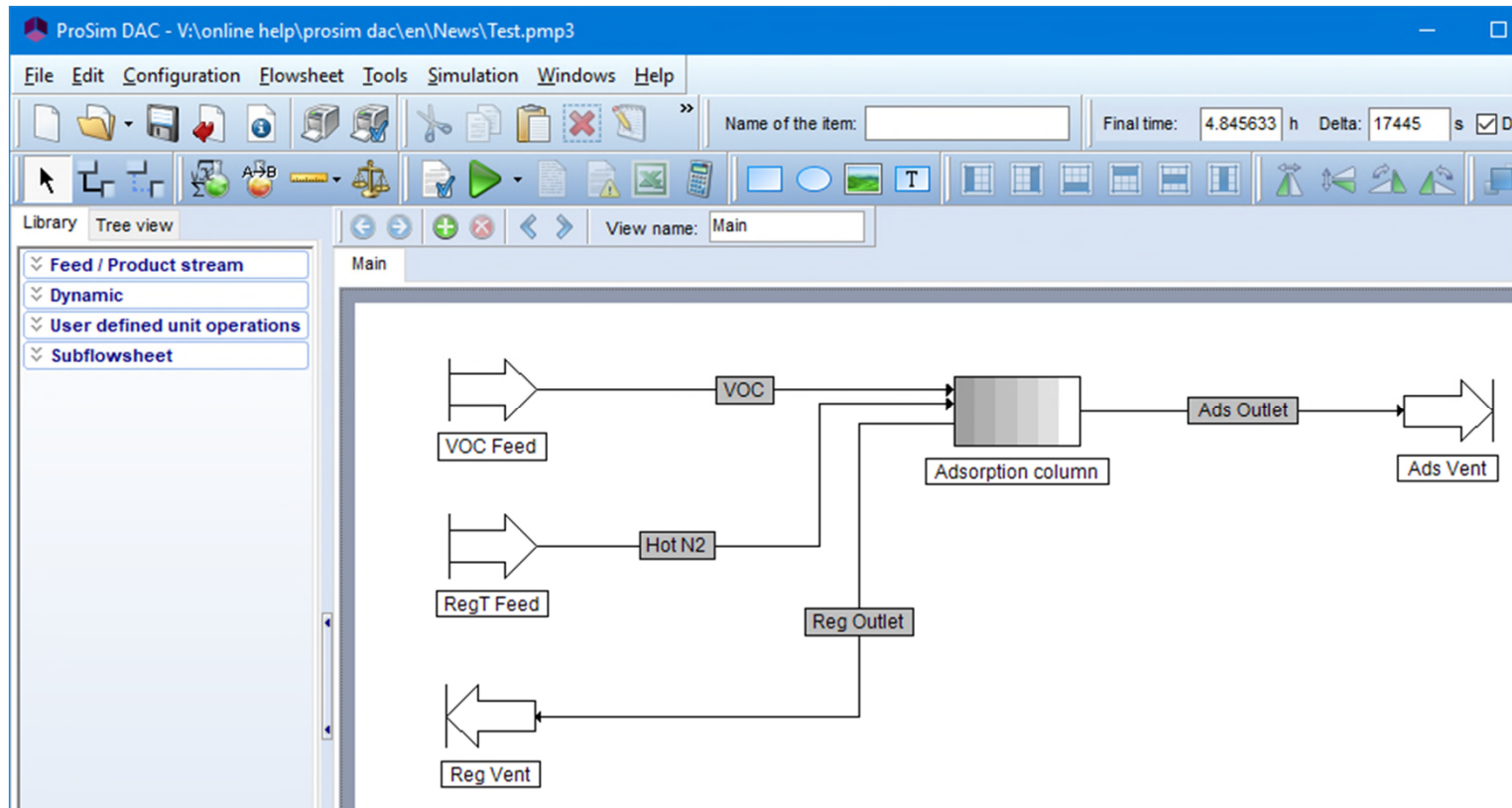
3. Repeat for the different material streams needed.



Step 3: Create the flowsheet

B- Connect the modules

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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.

ProSim DAC - V:\online help\prosim dac\en\News\PSPDYN_E02_EN - VOC TSA.pmp3

File Edit Configuration Flowsheet Tools Simulation Windows Help

Name of the item: VO

View name: Main

Process feed (\$ALIM)

Name: VOC Feed

Desc:

Parameters Scripts Report Streams Notes Advanced

Copy Paste Tabulated data...

Flowrates and fractions Temperature and Pressure

Flowrate specification Mole fractions

#	Components	Mole fractions
1	DICHLOROMETHANE	0.0078
2	NITROGEN	0.9922

Sum: 1.0000 1 - sum: 0.0000

Total flowrate Molar flowrate

Total molar flowrate 0.0839900000 kmol/h

Data link:

OK Cancel

1 Edit...

Thermodynamics

Visual...

Update visuals with default file

✓ Show a label

Scriptlets

Move to

Bring to front

Bring forward

Send backward

Send to back

Step 3: Create the flowsheet

C- Inlets and outlets

- VOC stream inlet characteristics

Process feed (\$ALIM)

Name: VOC Feed

Desc:

Identification Parameters Scripts Report Streams Notes Advanced

Copy Paste ☐ Tabulated data...

Flowrates and fractions Temperature and Pressure

Flowrate specification Mole fractions

#	Components	Mole fractions
1	DICHLOROMETHANE	0.0078
2	NITROGEN	0.9922

Sum: 1.0000 1 - sum: 0.0000

Total flowrate Molar flowrate

Total molar flowrate 0.0839900000 kmol/h

Data link: ...

OK Cancel

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

Process feed (\$ALIM)

Name: VOC Feed

Desc:

Identification Parameters Scripts Report Streams Notes Advanced

Copy Paste Tabulated data...

Flowrates and fractions Temperature and Pressure

Temperature Pressure

Temperature specification

☒ Supplied

☐ Bubble point temperature at specified pressure

☐ Dew point temperature at specified pressure

Temperature 24 °C

☐ Stream physical state Liquid stream

☐ Specific thermodynamic model for water

Data link:

OK Cancel

Specify the
temperature

Specify the
pressure

Process feed (\$ALIM)

Name: VOC Feed

Desc:

Identification Parameters Scripts Report Streams Notes Advanced

Copy Paste Tabulated data...

Flowrates and fractions Temperature and Pressure

Temperature Pressure

Pressure specification

☒ Supplied

☐ Bubble point pressure at specified temperature

☐ Dew point pressure at specified temperature

Pressure 1 atm

☐ Stream physical state Liquid stream

☐ Specific thermodynamic model for water

Data link:

OK Cancel

Step 3: Create the flowsheet

C- Inlets and outlets

- Hot nitrogen stream (for regeneration) inlet characteristics

Process feed (\$ALIM1)

Name:

Desc:

Identification Parameters Scripts Report Streams Notes Advanced

Copy Paste ☐ Tabulated data...

Flowrates and fractions Temperature and Pressure

Flowrate specification Mole fractions

#	Components	Mole fractions
1	DICHLOROMETHANE	0
2	NITROGEN	1

Sum: 1 - sum:

Total flowrate Molar flowrate

Total molar flowrate kmol/h

Data link: ...

OK Cancel

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

Process feed (\$ALIM1)

Name: RegT Feed

Desc:

Identification Parameters Scripts Report Streams Notes Advanced

Copy Paste Tabulated data...

Flowrates and fractions **Temperature and Pressure**

Temperature Pressure

Temperature specification

☒ Supplied

☐ Bubble point temperature at specified pressure

☐ Dew point temperature at specified pressure

Temperature 170 °C

☐ Stream physical state Liquid stream

☐ Specific thermodynamic model for water

Data link:

OK Cancel

Specify the temperature

Specify the pressure

Process feed (\$ALIM1)

Name: RegT Feed

Desc:

Identification Parameters Scripts Report Streams Notes Advanced

Copy Paste Tabulated data...

Flowrates and fractions **Temperature and Pressure**

Temperature **Pressure**

Pressure specification

☒ Supplied

☐ Bubble point pressure at specified temperature

☐ Dew point pressure at specified temperature

Pressure 1 atm

☐ Stream physical state Liquid stream

☐ Specific thermodynamic model for water

Data link:

OK Cancel

Step 3: Create the flowsheet C- Inlets and outlets

- Process outlets
 - No parameters are needed for process outlets

Process outlet (\$SORP)

Name:

Desc:

Identification Parameters Scripts Report Streams Notes

→

Connections

Inlet	Outlet
Material ... Ads Outlet ... Adsorption column	

Thermodynamic model:

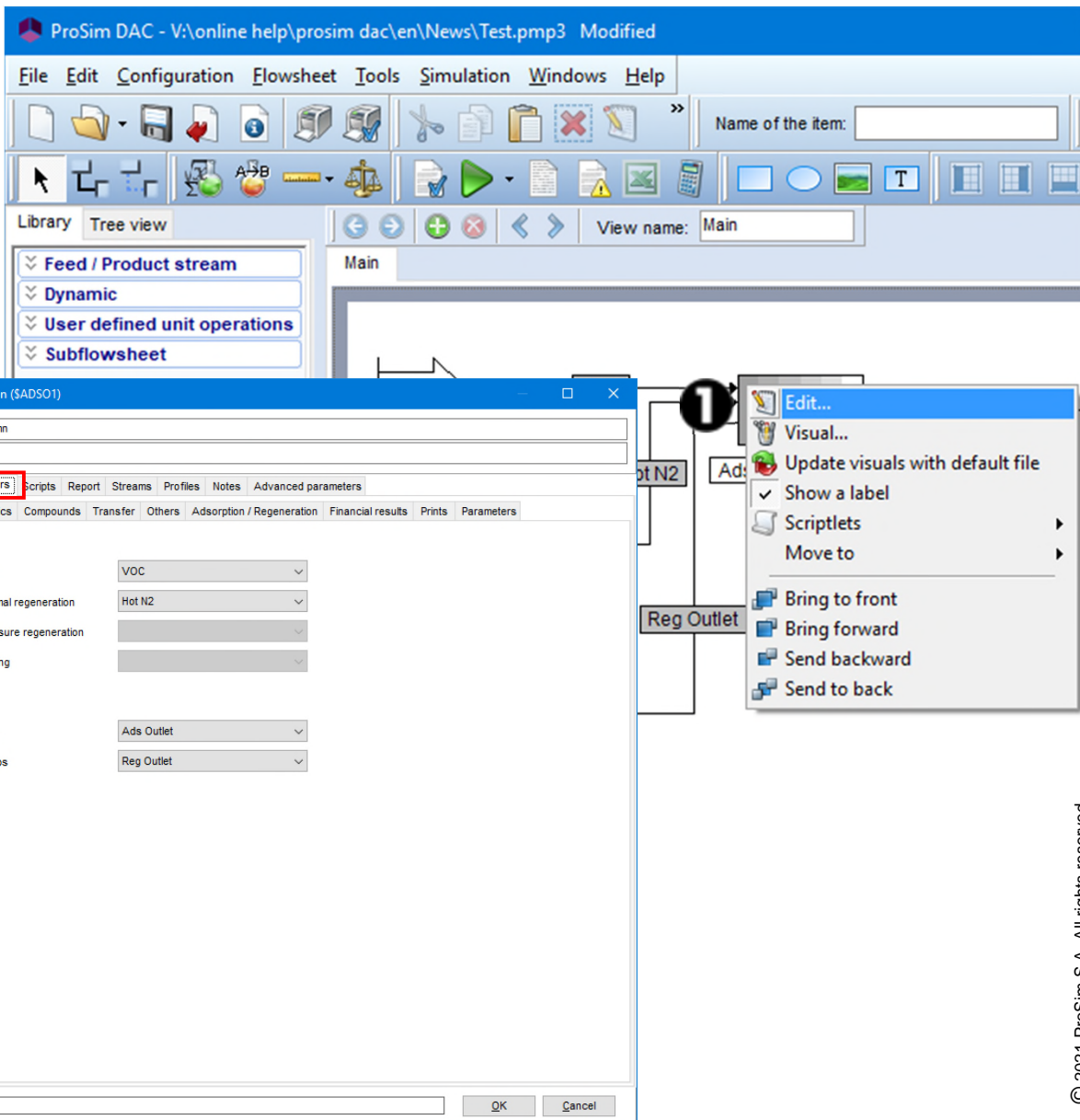
OK Cancel

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

Adsorption column (\$ADSO1)

Name: Adsorption column

Desc:

Identification Parameters Scripts Report Streams Profiles Notes Advanced parameters

Streams Characteristics Compounds Transfer Others Adsorption / Regeneration Financial results Prints Parameters

Feeds

☒ Adsorbates flow VOC

☒ Flow for the thermal regeneration Hot N2

☐ Flow for the pressure regeneration

☐ Flow for the cooling

Outlets

☒ Adsorption steps Ads Outlet

☒ Regeneration steps Reg Outlet

OK Cancel

Step 3: Create the flowsheet

D- Adsorption column

- “Characteristics” tab
 - Fill in the main characteristics of the column

Size of the bed

The screenshot shows the 'Adsorption column (SADSO1)' window with the 'Characteristics' tab selected. The 'Column' section has 'Lengthwise flow column' selected. The 'Initialization' section shows 'Supplied by user' for initialization type, with initial pressure of 1 atm and initial temperature of 20 °C. The 'Adsorbent' section has a 'Load...' button and various parameters: Bed void ratio (0.37 m³/m³), Particles diameter (4 mm), Particles density (750 kg/m³), Specific heat of the solid (1050 J/kg/K), and Particle surface/volume ratio (1500 m²/m³). The 'Measures conditions (T,P)' section has 'Normal' selected. A red dashed line connects the 'Edit...' button to a 'Lengthwise flow column' dialog box, which shows 'Column diameter (D)' as 5 cm and 'Column length (L)' as 27.5 cm. The dialog box also includes a diagram of the column with a red arrow indicating flow direction and a blue arrow indicating the bed length L.

Step 3: Create the flowsheet

D- Adsorption column

- “Characteristics” tab
 - Fill in the main characteristics of the column

Adsorption column (SADSO1)

Name: Adsorption column

Desc:

Identification Parameters Scripts Report Streams Profiles Notes Advanced parameters

Streams **Characteristics** Compounds Transfer Others Adsorption / Regeneration Financial results Prints Parameters

Column

Column type: Lengthwise flow column

Edit...

Heat transfer: Given heat duty and wall transfer

Wall temperature: 22 °C

Adsorbent

Load...

Bed void ratio: 0.37 m³/m³

Particles diameter: 4 mm

Particles density: 750 kg/m³

Specific heat of the solid: 1050 J/kg/K

Particle surface/volume ratio: 1500 m²/m³

Measures conditions (T,P)

Conditions: Normal

Initialization

Initialization type: Supplied by user

Initial pressure: 1 atm

Initial temperature: 20 °C

Initial molar fractions

1	DICHLOROMETHANE	0
2	NITROGEN	1

Summation: 1.0000

OK Cancel

State of the column before the first adsorption

Adsorbent data base

T, P reference for the concentrations

Step 3: Create the flowsheet

D- Adsorption column

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

Adsorption column (SADSO1)

Name: Adsorption column

Desc:

Identification Parameters **Compounds** Scripts Report Streams Profiles Notes Advanced parameters

Streams Characteristics **Compounds** Transfer Others Adsorption / Regeneration Financial results Prints Parameters

Characteristics

DICHLOROMETHANE
NITROGEN

Adsorption enthalpy

Enthalpy of adsorption: Given

Adsorption heat: -51 kJ/mol **Load...**

Adsorption isotherm

Correlation: Langmuir

$$q_i = \frac{\left[q_{m0} \exp\left(\frac{q_{m1}}{T}\right) \right] \left[K_0 \exp\left(\frac{K_1}{T}\right) \right] P_i}{1 + \left[K_0 \exp\left(\frac{K_1}{T}\right) \right] P_i}$$

qm0: 1.094644264 mol/kg **Load...**

K0: 0.045997002 atm⁻¹

qm1: 628.3009558 K

K1: 2427.456107 K

OK Cancel

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

Adsorption column (\$ADS01)

Name: Adsorption column

Desc:

Identification Parameters **Scripts** Report Streams Profiles Notes Advanced parameters

Streams Characteristics **Compounds** Transfer Others Adsorption / Regeneration Financial results Prints Parameters

Characteristics

DICHLOROMETHANE
NITROGEN

Adsorption enthalpy

Enthalpy of adsorption Given

Adsorption heat 0 cal/mol Load...

Adsorption isotherm

Correlation Langmuir

$$q_i = \frac{q_{m0} \exp\left(-\frac{q_{m1}}{T}\right) \left[K_0 \exp\left(\frac{K_1}{T}\right) P_i \right]}{1 + \left[K_0 \exp\left(\frac{K_1}{T}\right) P_i \right]}$$

q_{m0} 0 mol/kg Load...

K₀ 0 atm⁻¹

q_{m1} 0 K

K₁ 0 K

OK Cancel

The nitrogen is assumed 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

Adsorption column (\$ADS01)

Name: Adsorption column
Desc:

Identification Parameters Scripts Report Streams Profiles Notes Advanced parameters

Streams Characteristics Compounds **Transfer** Others Adsorption / Regeneration Financial results Prints Parameters

Material transfer

Transfer type: Gas and solid transfer

Gas material transfer

Gas transfer type: kf calculated, Petrovic-Thodos

Solid material transfer

Solid transfer type: kf supplied

Material transfer coefficients of solid phase (s⁻¹)

1	DICHLOROMETHANE	0.1
2	NITROGEN	0

Thermal transfer

Enthalpy balances ? ☒

Gas-adsorbent: Calculated (Satterfield)

Gas-wall: Calculated (Leva)

Wall thermal inertia

☐ Take into account thermal inertia of the column wall

Mass (wall): 0 kg

Specific heat (wall): 0 cal/g/K

Thickness (wall): 0 m

Thermal conductivity: 0 W/m/K

Wall-outside transfer coefficient: Given

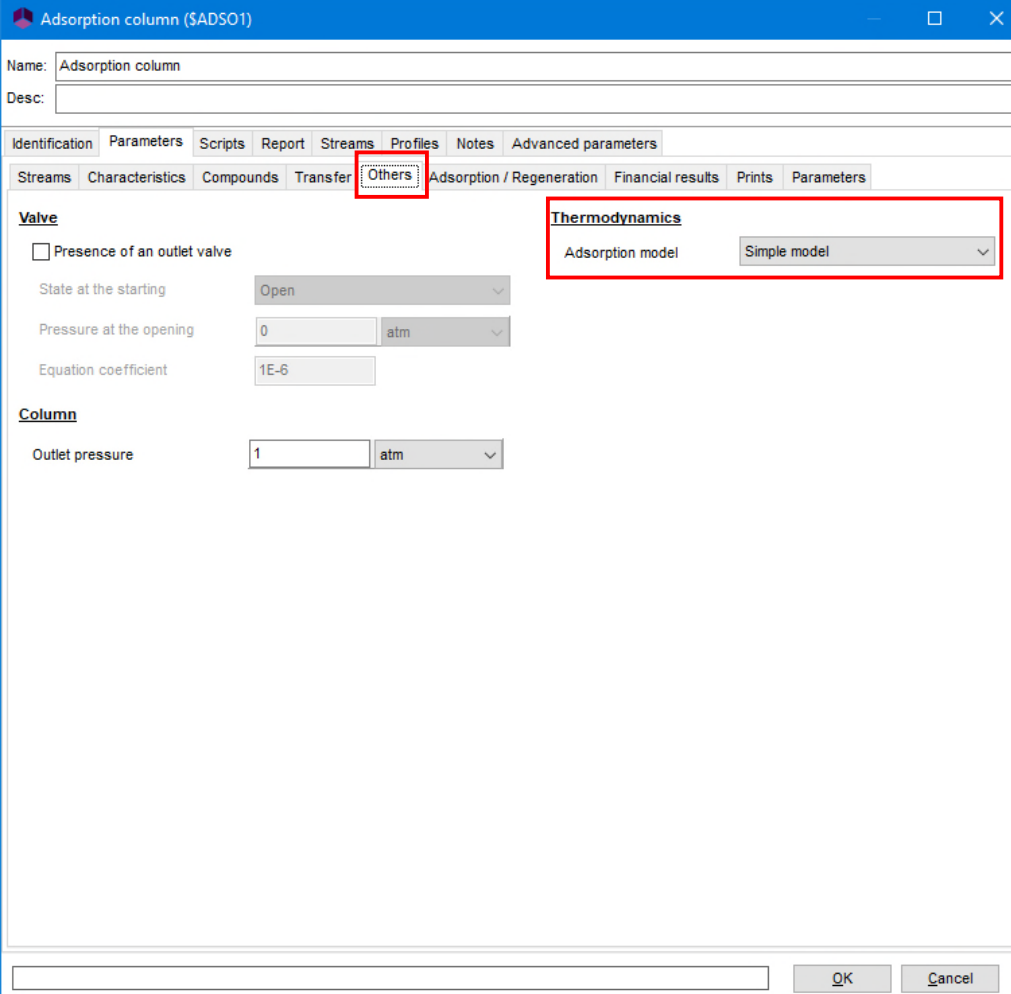
Coefficient: 4.000000956022 kcal/h/m²/K

OK Cancel

Step 3: Create the flowsheet

D- Adsorption column

- “Others” tab
 - Select the thermodynamic adsorption model



Adsorption column (\$ADS01)

Name: Adsorption column

Desc:

Identification Parameters Scripts Report Streams Profiles Notes Advanced parameters

Streams Characteristics Compounds Transfer **Others** Adsorption / Regeneration Financial results Prints Parameters

Valve

☐ Presence of an outlet valve

State at the starting: Open

Pressure at the opening: 0 atm

Equation coefficient: 1E-6

Column

Outlet pressure: 1 atm

Thermodynamics

Adsorption model: Simple model

OK Cancel

Step 3: Create the flowsheet

D- Adsorption column

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

Adsorption column (\$ADS01)

Name: Adsorption column

Desc:

Identification Parameters Scripts Report Streams Profiles Notes **Advanced parameters**

Streams Characteristics Compounds Transfer Others **Adsorption / Regeneration** Financial results Prints Parameters

Adsorption and regeneration

Sequence type

Adsorption + thermal regeneration

Adsorption only

Adsorption + thermal regeneration

Adsorption + pressure regeneration

Adsorption + pressure regeneration + thermal regeneration

Adsorption + thermal regeneration + pressure regeneration

Adsorption

Parameters...

Events...

Thermal regeneration

Parameters...

Events...

End of simulation

Events...

A: Adsorption

EVA: Stop adsorption events

RT: Thermal regeneration

EVT: Stop thermal regeneration events

OK Cancel

Step 3: Create the flowsheet

D- Adsorption column

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

Adsorption column (\$ADS01)

Name: Adsorption column
Desc:

Identification Parameters Scripts Report Streams Profiles Notes Advanced parameters

Streams Characteristics Compounds Transfer Others **Adsorption / Regeneration** Financial results Prints Parameters

Adsorption and regeneration

Sequence type: Adsorption + thermal regeneration

Adsorption

Parameters... Events...

Thermal regeneration

Parameters... Events...

End of simulation

Events...

Flowchart:

```

graph TD
    A[A: Adsorption] --> EVA((EVA: Stop adsorption events))
    EVA --> RT[RT: Thermal regeneration]
    RT --> EVT((EVT: Stop thermal regeneration events))
    EVT --> A
  
```

OK Cancel

Adsorption parameters

Parameters

☐ Column cooling through the wall

Wall temperature: 0 K

Exchanged heat duty in the bed: 0 kcal/h

Positive value for an heating, negative for a cooling.

OK Cancel

Step 3: Create the flowsheet

D- Adsorption column

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

The screenshot shows the configuration window for an Adsorption column (\$ADS01). The "Adsorption / Regeneration" tab is selected, and the "Adsorption and regeneration" section is visible. The sequence type is set to "Adsorption + thermal regeneration". The process flow diagram shows the following steps: Adsorption (A) → EVA → Thermal regeneration (RT) → EVT. The "Events..." button for the Adsorption step is highlighted with a red box, and a red dashed line connects it to the "Adsorption events" dialog.

The "Adsorption events" dialog is open, showing the following settings:

Event	Value	Unit	Position	Unit
<input checked="" type="checkbox"/> Duration	12600	s	0	m
<input type="checkbox"/> Break through	0		0	m
<input type="checkbox"/> Gas phase concentration	0	mol/l	0	m
<input type="checkbox"/> Solid phase concentration	0	mol/kg	0	m
<input type="checkbox"/> Maximum temperature	0	K	0	m
<input type="checkbox"/> Maximum pressure	0	atm	0	m
Compound to follow				

The dialog also includes "OK" and "Cancel" buttons at the bottom right.

Step 3: Create the flowsheet

D- Adsorption column

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

Adsorption column (\$ADS01)

Name: Adsorption column
Desc:

Identification Parameters Scripts Report Streams Profiles Notes Advanced parameters

Streams Characteristics Compounds Transfer Others **Adsorption / Regeneration** Financial results Prints Parameters

Adsorption and regeneration

Sequence type: Adsorption + thermal regeneration

Adsorption

Parameters... Events...

Thermal regeneration

Parameters... Events...

End of simulation

Events...

Flowchart:

```

graph TD
    A[A: Adsorption] --> EVA((EVA: Stop adsorption events))
    EVA --> RT[RT: Thermal regeneration]
    RT --> EVT((EVT: Stop thermal regeneration events))
    EVT --> A
  
```

OK Cancel

Thermal regeneration parameters

Parameters

Regeneration type: Counter-current

☐ Column preheating

Heating type: Bed heating

Preheating power: 0 kcal/h

Preheating duration: 0 h

☐ Column cooling

Cooling duration: 0 h

☐ Column temporisation

Temporisation duration: 0 h

Exchanged heat duty in the bed: 0 kcal/h

Positive value for an heating, negative for a cooling.

OK Cancel

Step 3: Create the flowsheet

D- Adsorption column

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

The screenshot shows the configuration window for an Adsorption column (\$ADS01). The "Adsorption / Regeneration" tab is selected, and the "Sequence type" is set to "Adsorption + thermal regeneration". The process flow diagram shows a sequence of steps: Adsorption (A), Thermal regeneration (RT), and End of simulation (EVT). The "Events..." button for the Thermal regeneration step is highlighted with a red box. A red dashed line connects this button to the "Thermal regeneration events" dialog box.

The "Thermal regeneration events" dialog box shows the following settings:

Events		
<input checked="" type="checkbox"/> Duration	4845	s
<input type="checkbox"/> Gas phase concentration	0	mol/l
<input type="checkbox"/> Solid phase concentration	0	mol/kg
<input type="checkbox"/> Maximum temperature	0	K
<input type="checkbox"/> Maximum pressure	0	atm
<input type="checkbox"/> Amount produced	0	kmol
Compound to follow		
Position 0 m		

The dialog box also includes "OK" and "Cancel" buttons at the bottom right.

Step 3: Create the flowsheet

D- Adsorption column

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

The screenshot shows the configuration window for an Adsorption column (\$ADS01). The "Adsorption / Regeneration" tab is selected, and the "End simulation events" dialog is open.

Adsorption column (\$ADS01) Configuration:

- Name: Adsorption column
- Desc:
- Sequence type: Adsorption + thermal regeneration
- Flowchart: A process flow diagram showing the sequence of operations: Adsorption (A) → Thermal regeneration (RT) → End of simulation (EVT). The flowchart is divided into three sections: Adsorption, Thermal regeneration, and End of simulation. Each section has a "Parameters..." button and an "Events..." button. The "Events..." button under "End of simulation" is highlighted with a red box.

End simulation events Dialog:

- Events:**
 - ☒ End simulation time
 - ☐ Number of cycles: 0
 - ☐ Total amount produced: 0 kmol
 - ☐ Maximum temperature: 0 K
 - ☐ Maximum pressure: 0 atm
 - ☐ Total amount used: 0 kmol
 - Compound to follow: (empty dropdown)
- Position: 0 m (for all three conditions)
- Buttons: OK, Cancel

Step 3: Create the flowsheet

D- Adsorption column

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

The screenshot shows the 'Adsorption column (\$ADSO1)' window. The 'Advanced parameters' tab is selected, and the 'Financial results' sub-tab is highlighted with a red box. The window contains the following fields:

Name: Adsorption column
 Desc:

Identification Parameters Scripts Report Streams Profiles Notes Advanced parameters

Streams Characteristics Compounds Transfer Others Adsorption / Regeneration **Financial results** Prints Parameters

Thermal regeneration costs

Cost of regeneration flow: 0.2 €/Nm³
 Cost of regeneration flow heating: 100 €/MWh
 Cost of bed preheating: 120 €/MWh

Pressure regeneration costs

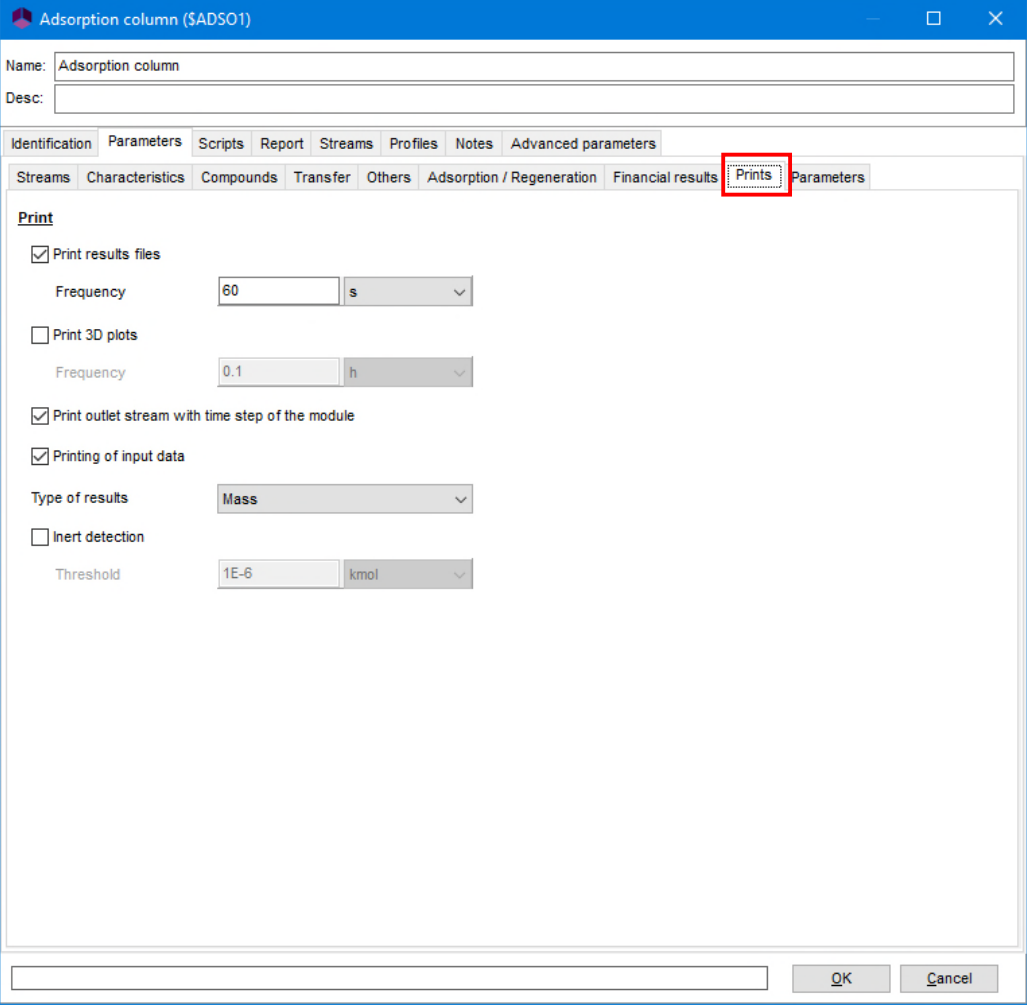
Cost of electricity: 100 €/MWh
 Power of vacuum pump: 0 kcal/h

OK Cancel

Step 3: Create the flowsheet

D- Adsorption column

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



Adsorption column (\$ADSO1)

Name: Adsorption column

Desc:

Identification Parameters Scripts Report Streams Profiles Notes Advanced parameters

Streams Characteristics Compounds Transfer Others Adsorption / Regeneration Financial results **Prints** Parameters

Print

☒ Print results files

Frequency 60 s

☐ Print 3D plots

Frequency 0.1 h

☒ Print outlet stream with time step of the module

☒ Printing of input data

Type of results Mass

☐ Inert detection

Threshold 1E-6 kmol

OK Cancel

Step 3: Create the flowsheet

D- Adsorption column

- “Parameters” tab
 - Fill in the numerical parameters and the model parameters

Adsorption column (\$ADSO1)

Name: Adsorption column

Desc:

Identification Parameters Scripts Report Streams Profiles Notes Advanced parameters

Streams Characteristics Compounds Transfer Others Adsorption / Regeneration Financial results Prints **Parameters**

Integration

Max. integration step: 60 s

Initial integration step: 0.005 s

Integration method: Hollow matrix, analytical evaluation

Step count: 2

Derivatives: calculated analytically

Tolerances

	Relative	Absolute
Partial concentrations	1E-5	1E-5
Concentrations	0.0001	0.0001
Temperatures	0.001	0.001
Pressures	0.001	0.001
Enthalpies	0.1	0.1
Speed	0.1	0.1

Model parameters

Number of discretization cells: 7

Axial dispersion coefficient: 0 m²/s

$\Delta H_{\text{Regeneration}} / \Delta H_{\text{Adsorption}}$ (ratio): 1

☒ Thermal accumulation in the solid taken into account

Heat duty applied to: Gas enthalpy balance

Duration of the cubic spline: 0 h

Solid transfer: Given

Material transfer coefficients of solid phase (s⁻¹)

1	DICHLOROMETHANE	0.006
2	NITROGEN	0

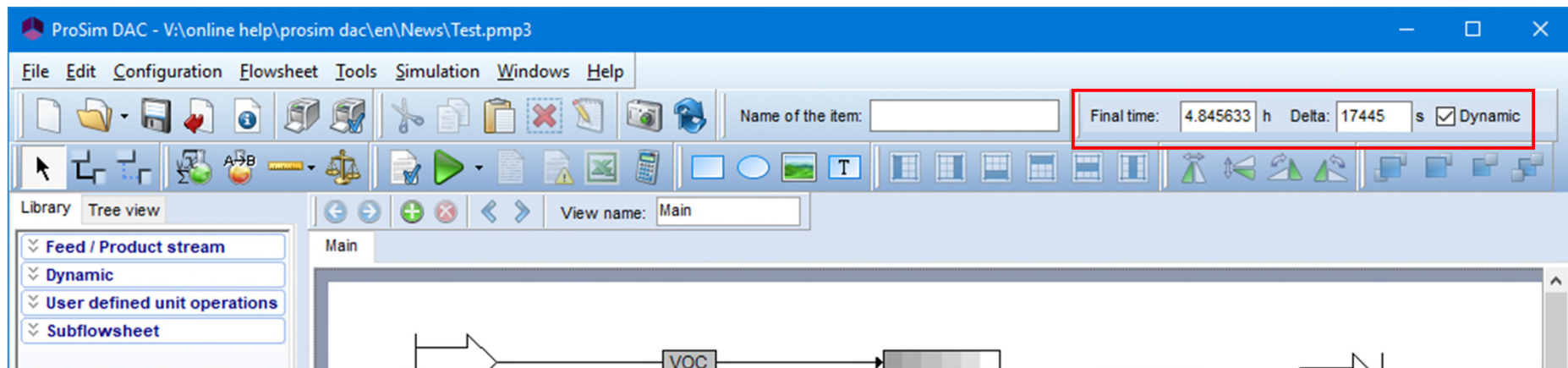
OK Cancel

Number of longitudinal
discretization cells

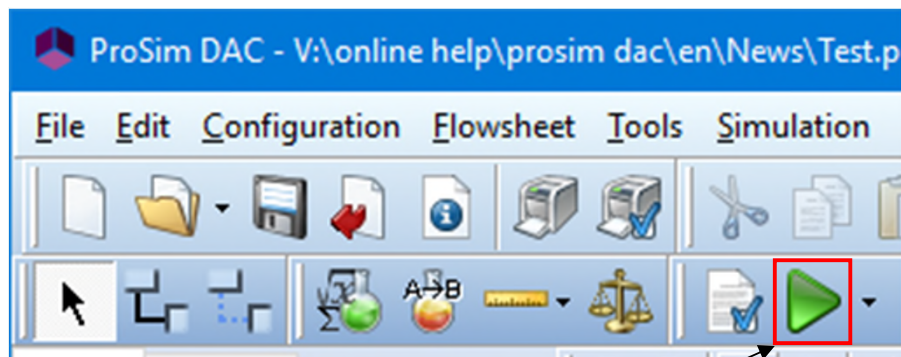
Step 3: Create the flowsheet

D- Operating time

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

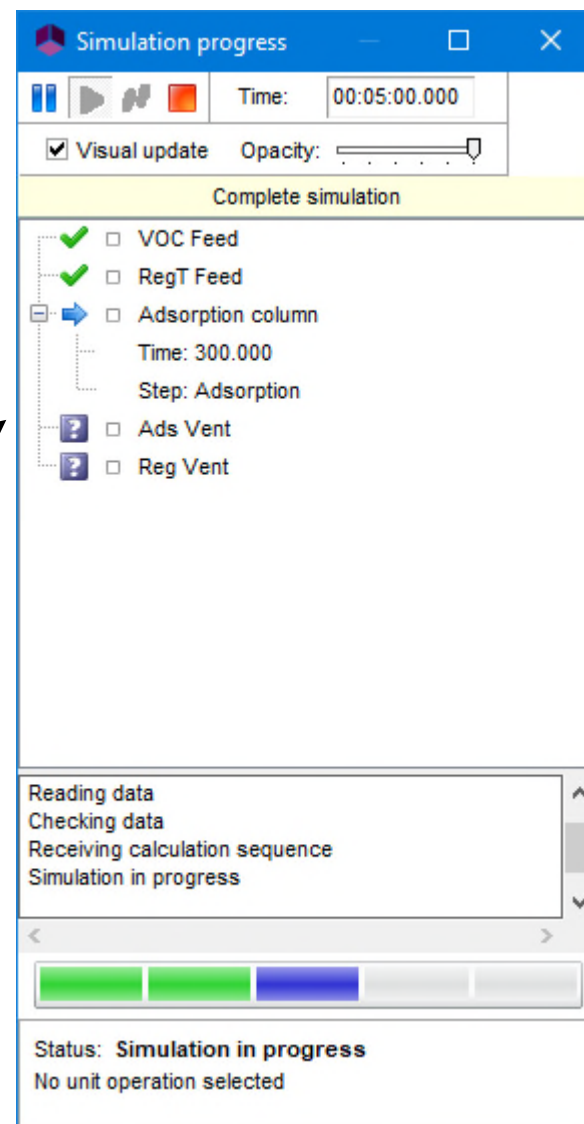


Step 4: Running the simulation







Click on the green arrow to start the simulation

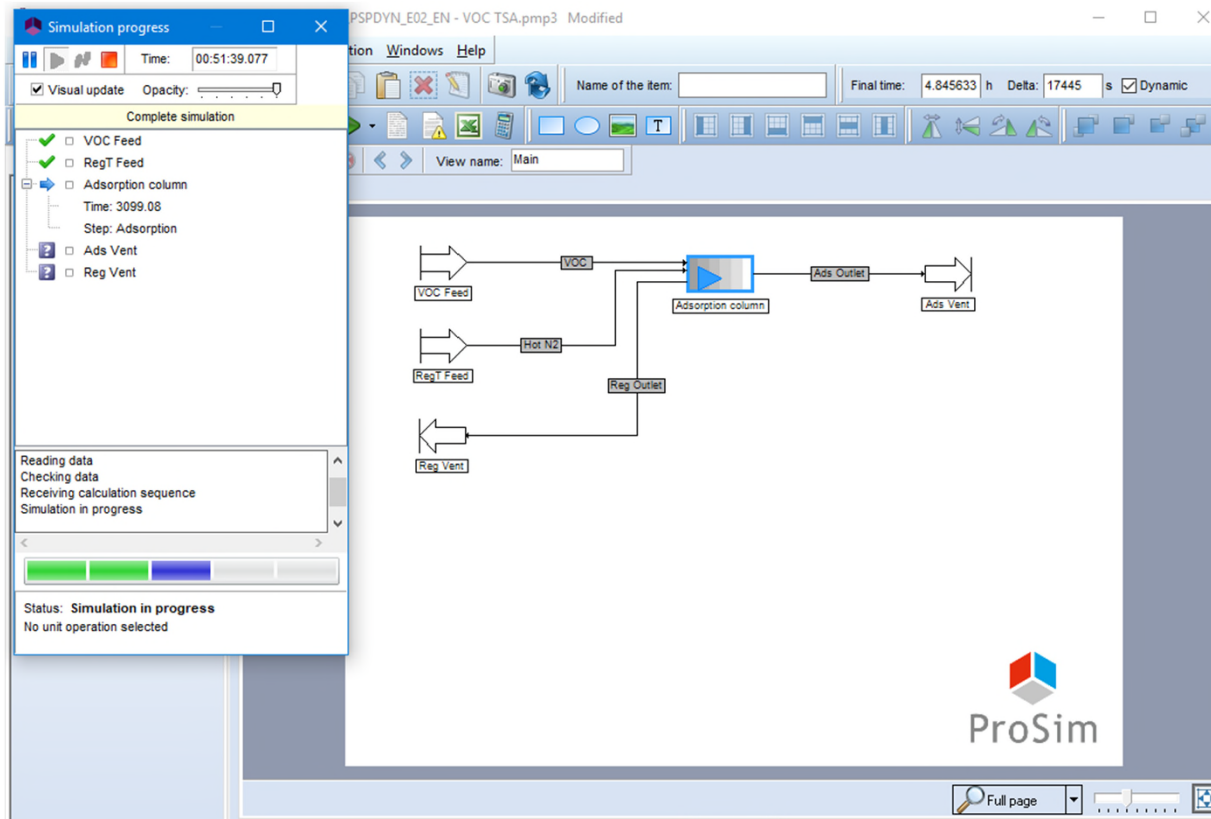
When the simulation starts,
the "Simulation progress" window
opens.



Step 4: Running the simulation

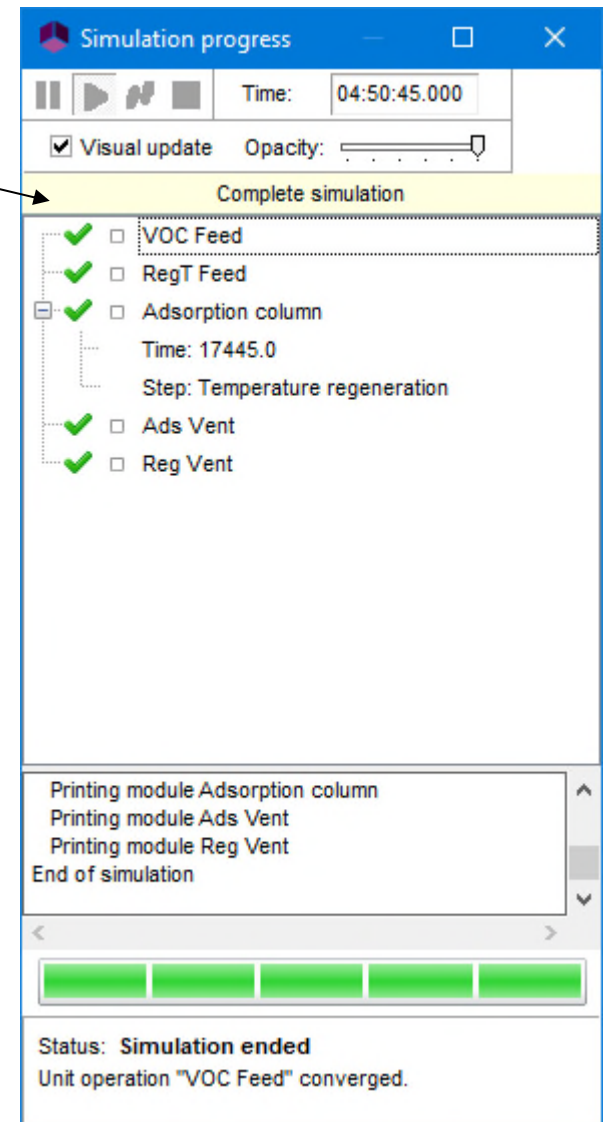
During the calculation, different symbols and indications will appear and disappear in the “Simulation progress” window and in the drawing area.

-  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 can 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.

ProSimPlus Simulation Report (V:\online help\prosim dac\en\News\PSPDYN_E02_EN - VOC TSA.htm)

Enthalpic flow 0 kW - 0 kcal/h

EQUIPMENT : Adsorption column
TYPE : Adsorption column
DESCRIPTION :

INLET STREAMS:
[VOC](#)
[Hot N2](#)

OUTLET STREAMS:
[Ads Outlet](#)
[Reg Outlet](#)

THERMODYNAMIC CALCULATOR : [\[New calculator\]](#)

SIMULATION INLET DATA

FEED(S)

Adsorbat feed : VOC
Thermal regeneration feed: Hot N2
Pressure regeneration : Not used
Cooling feed : Not used

COLUMN GENERAL CHARACTERISTICS

Lenghtwise flow column
Diameter: 5.000000E-02 (M)
Lenght : 0.275000 (M)
Thermal operting condition
Wall transfer and given heat duties
Wall temperature: 22.00 (C)
Outlet pressure: 1.00 (ATH)

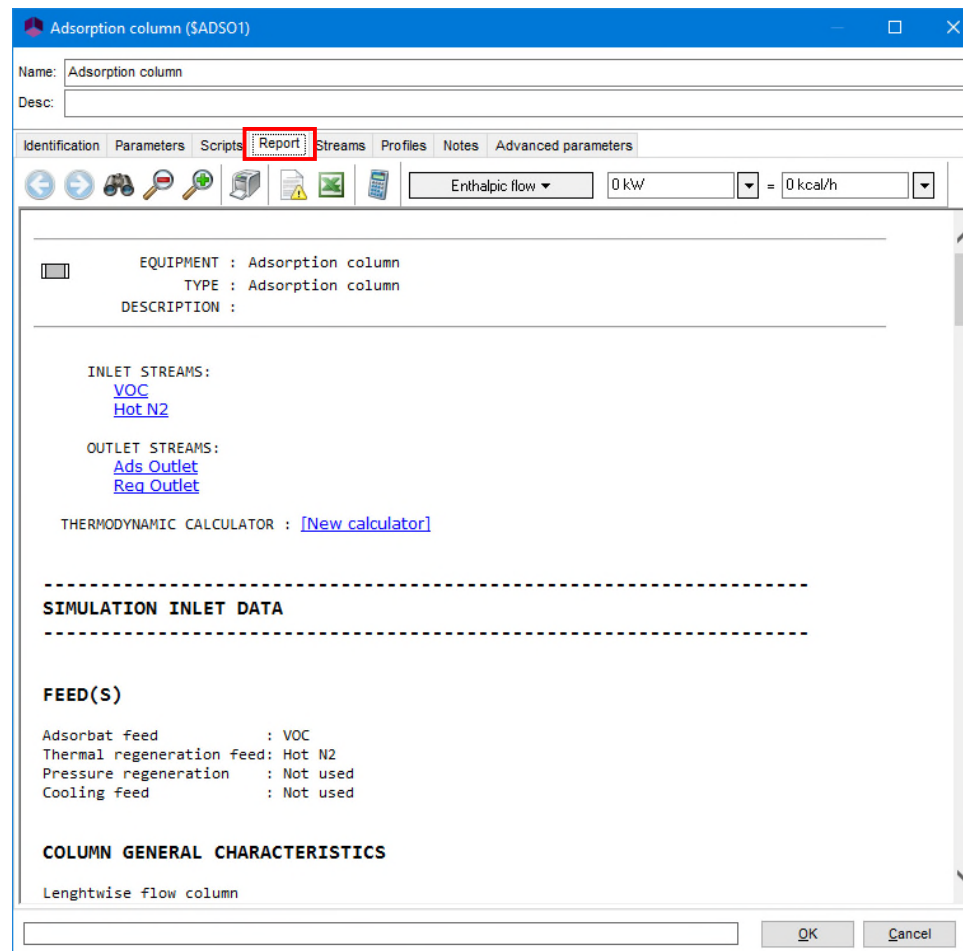
ADSORBENT CHARACTERISTICS

Bed vacuum ratio : 0.370000
Particles diameter : 4.000000E-03 (M)
Particles density : 750.00 (KG/M3)
Solide specific heat: 0.25 (CAL/G/K)

Step 5: Simulation reports

B- Adsorption column report and profiles

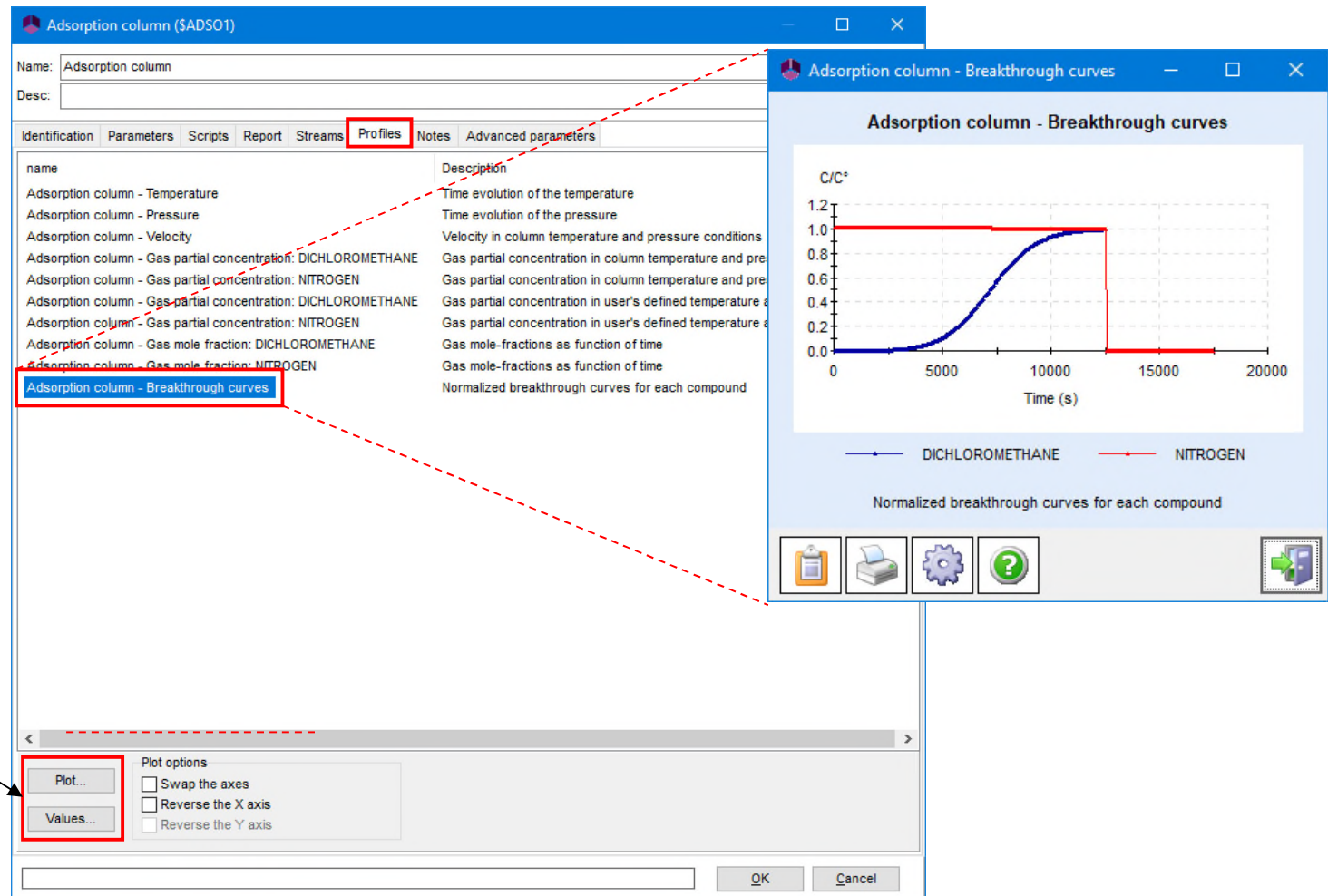
- Tabulated results are also available in the “Report” tab of the adsorption column module
 - Adsorbed quantities, regenerated quantities, etc.



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

Material Stream (\$MSTR1)

Name: Ads Outlet

Desc:

Parameters Report Notes Advanced parameters

Copy Paste Tabulated results...

☐ Initialized stream

Flowrates and fractions Temperature and Pressure

Flowrate specification Partial mass flowrates

Partial mass flowrates

Unit kg/h

#	Components	Mass flow rates
1	DICHLOROMETHANE	0
2	NITROGEN	0

Data link:

OK Cancel

Test.pmp3

Name of the item: Final time: 4.845633 h Delta: 17445 s

View name: Main

Feed VOC Adsorption column Reg Outlet Ads Outlet Ads Vent

Hot N2

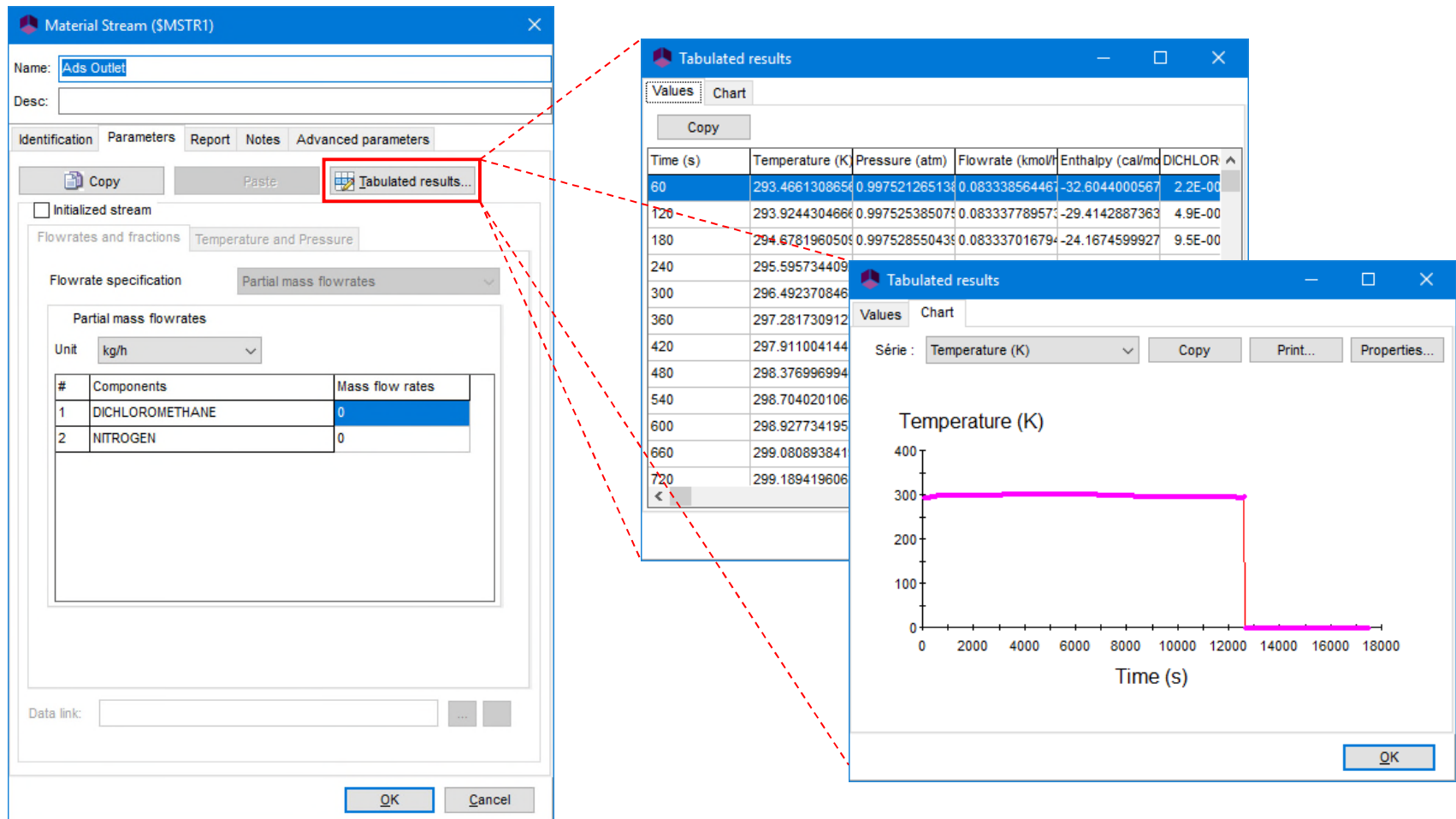
Feed

Vent

Step 5: Simulation reports

C- Outlet streams profiles

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

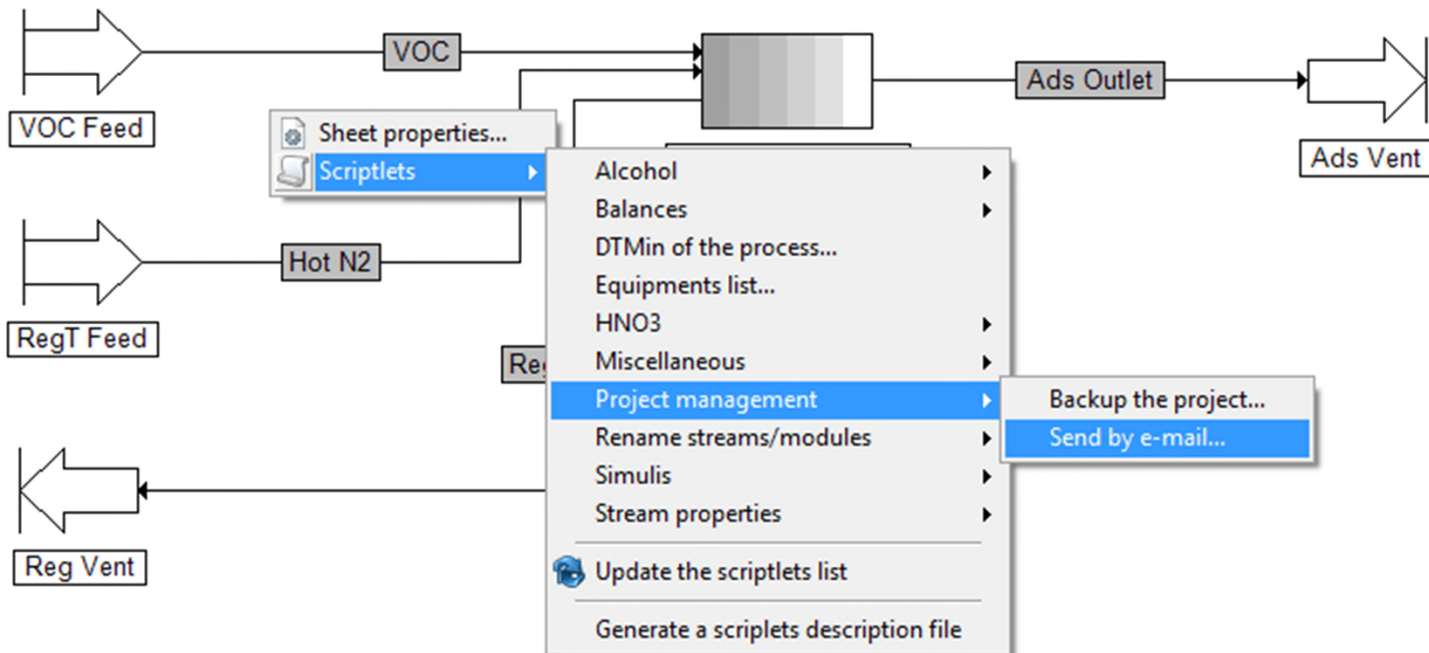


Step 6: Sharing the simulation

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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