

**PROSIM DAC APPLICATION EXAMPLE**

**TSA PROCESS  
PROPANE ADSORPTION ON ACTIVATED  
CARBON**

**EXAMPLE PURPOSE**

This example deals with a TSA process (Thermal Swing Adsorption) in which propane is adsorbed on an activated carbon. The thermal regeneration of the activated carbon is done by a hot nitrogen stream. This process is modeled within ProSim DAC, ProSim's dynamic simulation software dedicated to gas adsorption columns.

|               |  |   |  |  |
|---------------|--|---|--|--|
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*Reader is reminded that this use case is only an example and should not be used for other purposes. Although this example is based on actual case it may not be considered as typical nor are the data used always the most accurate available. Fives ProSim shall have no responsibility or liability for damages arising out of or related to the use of the results of calculations based on this example.*

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## TABLE OF CONTENTS

|           |  |           |
|-----------|--|-----------|
| <b>1.</b> | <b>PROCESS MODELING</b> .....                    | <b>3</b>  |
| 1.1.      | Process description .....                        | 3         |
| 1.2.      | Process flowsheet .....                          | 4         |
| 1.3.      | Compounds .....                                  | 4         |
| 1.4.      | Thermodynamic model.....                         | 4         |
| 1.5.      | Operating parameters .....                       | 5         |
| 1.5.1.    | Process feeds .....                              | 5         |
| 1.5.2.    | Simulation time .....                            | 5         |
| 1.5.3.    | Adsorption column.....                           | 5         |
| <b>2.</b> | <b>RESULTS</b> .....                             | <b>18</b> |
| 2.1.      | Simulation report of the adsorption column ..... | 18        |
| 2.2.      | Profiles of the adsorption column.....           | 19        |
| 2.3.      | Profiles of the outlet stream .....              | 20        |
| <b>3.</b> | <b>REFERENCES</b> .....                          | <b>22</b> |

# 1. PROCESS MODELING

## 1.1. Process description

ProSim DAC is a dynamic simulation software based on mass and enthalpy balances dedicated to gas-solid adsorption columns. The adsorption and the regeneration steps can be modeled. The available types of regeneration are: thermal regeneration (co- or counter-current), steam regeneration (co- or counter-current) and pressure regeneration. The TSA (Thermal Swing Adsorption), PSA (Pressure Swing Adsorption) or VTSA (Vacuum Thermal Swing Adsorption) processes can be represented. A management system of events allows going from one step to another depending on criterions specified by the user (duration, breakthrough ratio, concentration...). An end simulation time or a number of cycles can be defined. The characteristics (temperature, pressure, flow rate, compositions) of the feeds (flow to be purified, regenerating flows...) can be constant or time dependent. The main models of adsorption isotherm (Langmuir, Toth, Dubinin-Radushkevich, Langmuir extended, Sips...) are available. The mass and heat transfer coefficients can be specified by the user or calculated by ProSim DAC. A data base of activated carbons and of adsorption isotherms of VOCs on activated carbons is available. An economical balance of the regeneration steps can be performed to compare different solutions.

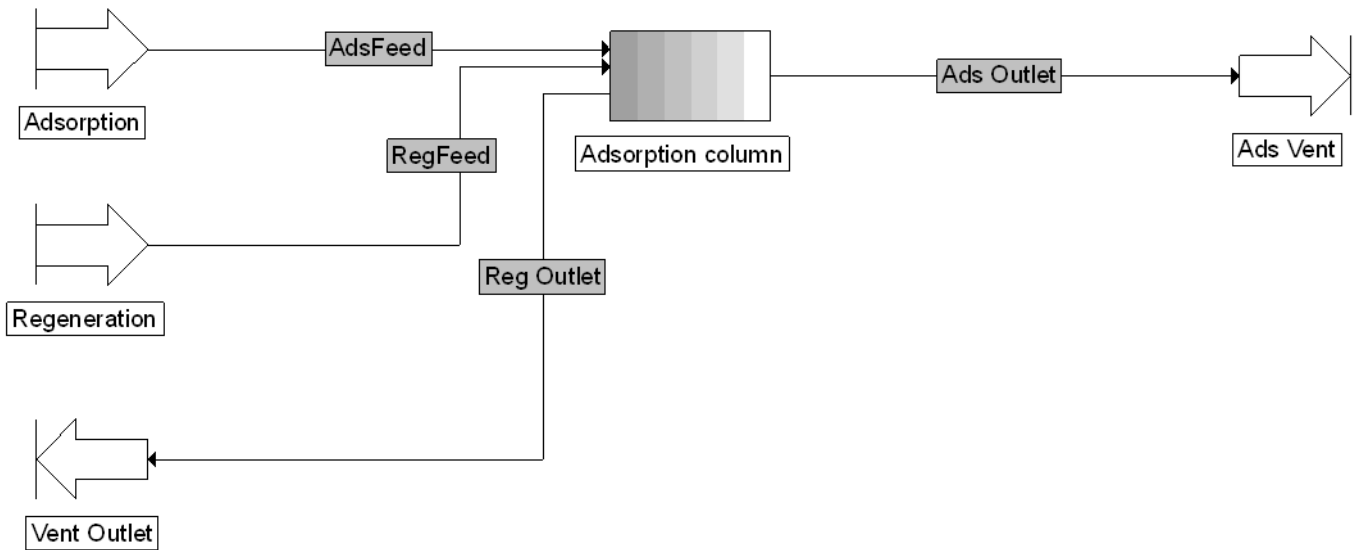
In this example, propane is adsorbed on a Witco JCX activated carbon. The regeneration of the adsorbent is done by a hot pure nitrogen stream (TSA process). The regeneration flow is counter-current compared to the adsorption flow.

Two inlet streams are used in this example: the "AdsFeed" stream and the "RegFeed" stream. During the adsorption step only the "AdsFeed" stream is used. This stream is the gas stream to be purified (i.e. in which the propane has to be removed). During the regeneration step only the "RegFeed" stream is used. This stream is the hot nitrogen stream used to regenerate the bed of adsorbent. The sequence of the steps is done automatically thanks to the definition of events ending the different steps.

The parameters of the column (size, thermal behavior...), the adsorption isotherms, the type of the cycle (TSA, VTSA, PSA), the step events (breakthrough level, temperature, concentration...) are defined within the "Adsorption column" unit operation module.

This example is adapted from [SCH88].

## 1.2. Process flowsheet



## 1.3. Compounds

The compounds used in the simulation, their chemical formula, and CAS Registry Numbers<sup>® 1</sup> are shown in the following table. Their pure component properties are extracted from the standard data base provided with ProSim DAC [ROW11].

| Compound | Chemical formula              | CAS number <sup>®</sup> |
|----------|-------------------------------|-------------------------|
| Propane  | C <sub>3</sub> H <sub>8</sub> | 74-98-6                 |
| Nitrogen | N <sub>2</sub>                | 7727-37-9               |

## 1.4. Thermodynamic model

The adsorption and the regeneration are done at a moderate pressure level (around 2,5 atm) and at temperature below 100°C. Thus the “Ideal” thermodynamic profile is selected in the Simulis Thermodynamics calculator.

<sup>1</sup> CAS Registry Numbers<sup>®</sup> are the intellectual property of the American Chemical Society and are used by Fives ProSim SAS with the express permission of ACS. CAS Registry Numbers<sup>®</sup> have not been verified by ACS and may be inaccurate.

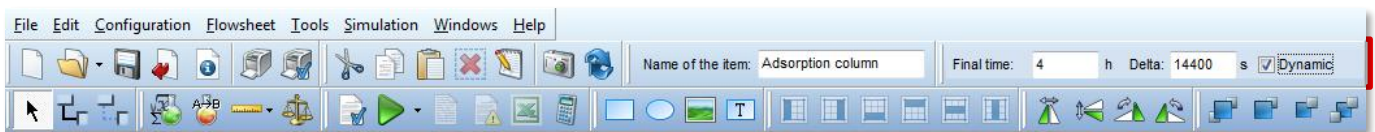
## 1.5. Operating parameters

### 1.5.1. Process feeds

|                          | Propane stream | Hot nitrogen stream |
|--------------------------|----------------|---------------------|
| Temperature (°C)         | 23             | 100                 |
| Pressure (mmHg)          | 1 882          | 1 849               |
| Total flow rate (kmol/h) | 0,09396        | 0,10332             |
| <b>Mole fractions</b>    |                |                     |
| Dichloromethane          | 0,0106         | 0                   |
| Nitrogen                 | 0,9894         | 1                   |

### 1.5.2. Simulation time

The “Final time” is the real working duration of the process (adsorption + thermal regeneration in this example). The “Delta” is the duration during which the “Adsorption column” module is working. As only one module is present, the “Final time” and the “Delta” should be identical. These two values are specified in the icon bar of ProSim DAC:



| Simulation time | Value    |
|-----------------|----------|
| Final           | 4 h      |
| Delta           | 14 400 s |

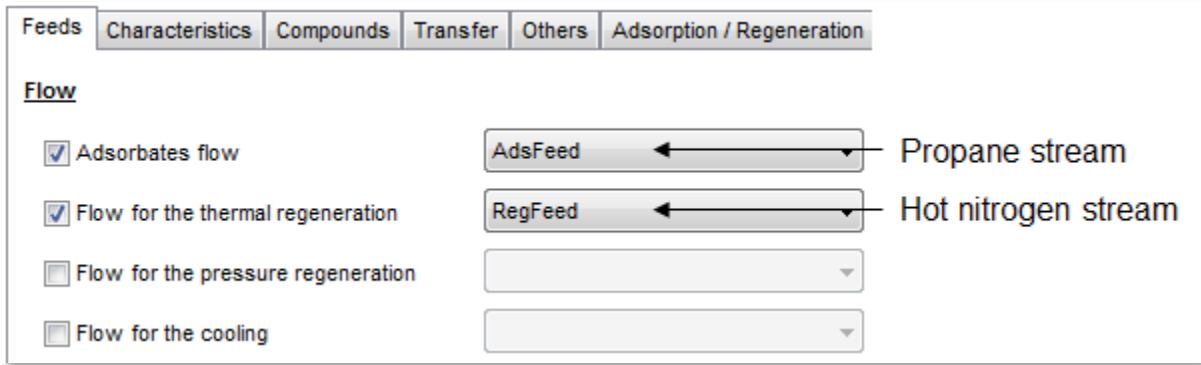
### 1.5.3. Adsorption column

#### 1.5.3.1. Feeds

Four feeds can be used in ProSim DAC:

- ✓ Adsorbates flow: Flow to be purified during the adsorption step.
- ✓ Flow for the thermal regeneration: Flow used during the thermal regeneration (hot nitrogen, steam...).
- ✓ Flow for the pressure regeneration: Flow used during the pressure regeneration (low pressure nitrogen...).
- ✓ Flow for the cooling: Flow used to cool the column at the end of the thermal regeneration step.

Only the two first feeds are used in this example as shown on the screenshot below.

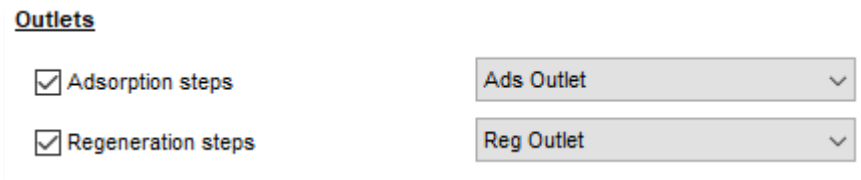


### 1.5.3.2. Outlets

Two outlets can be used in ProSim DAC:

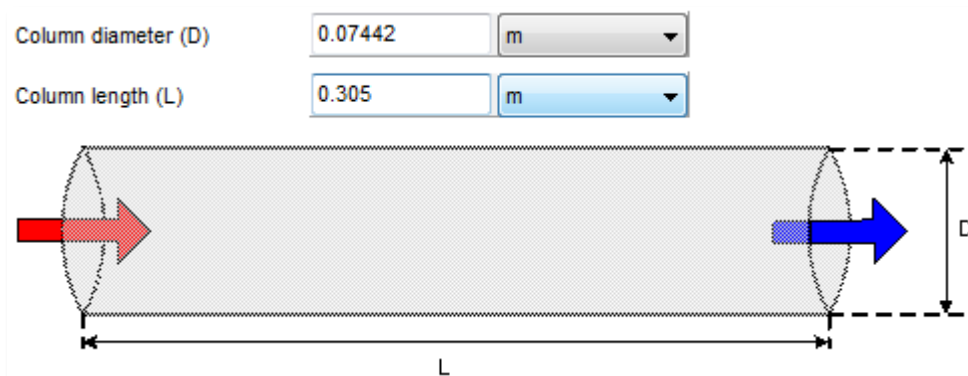
- ✓ Adsorption steps: Output stream during the adsorption steps.
- ✓ Regeneration steps: Output stream during the regeneration steps.

The output stream during the adsorption steps corresponds to “Ads Outlet” and the output stream during the regeneration steps corresponds to “Reg Outlet”, as shown on the screen shot below.



### 1.5.3.3. Column characteristics

The column used is a lengthwise flow column which characteristics are shown on the following screen shot. The dimensions to be specified are the ones of the adsorbent bed.



Transvers flow columns can also be modeled in ProSim DAC.

#### 1.5.3.4. Thermal behavior

The following thermal heat exchanges can be modeled in ProSim DAC:

- ✓ Heat exchange in the bed: “Given heat duty without wall transfer”.  
This possibility allows to model an adiabatic working or a given heat duty for each step working (heat exchanger in the adsorbent bed).
- ✓ Wall heat transfer + thermal heat exchange in the bed: “Given heat duty and wall transfer”.  
The heat exchange is done by the wall of the column. By default, the wall temperature is constant during the time and along the length of the column. To go beyond this assumption, the option “take into account thermal inertia of the column wall” has to be activated. It is possible to add a given heat duty (by default zero) in the adsorbent bed for each step.

In this example, the thermal transfer is done by the wall without any direct heating/cooling in the bed of adsorbent:

| Thermal behavior |                                   |
|------------------|-----------------------------------|
| Heat transfer    | Given heat duty and wall transfer |
| Wall temperature | 23°C                              |

#### 1.5.3.5. Adsorbent bed characteristics

| Bed characteristics |      |
|---------------------|------|
| Void ratio          | 0,44 |

#### 1.5.3.6. Adsorbent characteristics

The density of the particles takes into account of the intra-particulate porosity.

| Particles characteristics |                                      |
|---------------------------|--------------------------------------|
| Diameter                  | 3,2 mm                               |
| Density                   | 827 kg/m <sup>3</sup>                |
| Specific heat             | 0,2 cal/g/K                          |
| Surface/Volume ratio      | 1 320 m <sup>2</sup> /m <sup>3</sup> |

#### 1.5.3.7. Measures conditions for concentration results

The user can specify the temperature and pressure conditions he wants to calculate the volumetric concentrations in the gas phase. Indeed, the density is then necessary and this one, particularly in the case of a gas, is sensitive to the temperature and the pressure. In this example, the volumetric concentrations in the gas phase are evaluated at the temperature and pressure conditions of the column outlet.

| Measures conditions | Value  |
|---------------------|--------|
| Conditions          | Column |

### 1.5.3.8. Initialization

It's necessary to define the state of the column before its first use. In this example, it's assumed that the column is inerted with nitrogen at temperature and pressure levels corresponding to the flow to be purified.

| Initialization  | Value                |
|-----------------|----------------------|
| Type            | Supplied by the user |
| Pressure        | 1 882 mmHg           |
| Temperature     | 23°C                 |
| Molar fractions |                      |
| Propane         | 0                    |
| Nitrogen        | 1                    |

The screen shot below shows the information of the previous paragraphs (from paragraph 1.5.3.3 to paragraph 1.5.3.8 included) specified in the module interface: "Parameters" tab, "Characteristics" sub-tab.

### 1.5.3.9. Adsorption isotherms and enthalpies

The Langmuir model is selected for the adsorption isotherm of propane:

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

The linear model is selected for the adsorption isotherm of nitrogen:

$$q_i = \left[ K_0 \exp\left(\frac{K_1}{T}\right) \right] P_i$$

The values of the parameters with the corresponding units are displayed in the table below.

| Propane                                 |            | Nitrogen                          |          |
|---|------------|-----------------------------------|----------|
| <b>Isotherm</b>                         | Langmuir   | <b>Isotherm</b>                   | Linear   |
| <b>q<sub>m0</sub> (mol/kg)</b>          | 0,93589302 | <b>K<sub>0</sub> (mol/kg/atm)</b> | 0,000988 |
| <b>K<sub>0</sub> (atm<sup>-1</sup>)</b> | 0,50456976 | <b>K<sub>1</sub> (K)</b>          | 1752     |
| <b>q<sub>m1</sub> (K)</b>               | 425,905386 |                                   |          |
| <b>K<sub>1</sub> (K)</b>                | 1299,44563 |                                   |          |

The adsorption phenomenon being exothermic, the values of the enthalpies of adsorption are negatives.

| Adsorption enthalpy               | Propane | Nitrogen |
|-----------------------------------|---------|----------|
| <b>Type</b>                       | Given   |          |
| <b>ΔH<sub>ads</sub> (cal/mol)</b> | -9 500  | -3 840   |

This information has to be specified in the “Parameters” tab, “Compounds” sub-tab:

### 1.5.3.10. Mass transfer

The following options are available for the mass transfer:

- ✓ Transfer coupled in gas and solid phase.
- ✓ Mass transfer resistance (“linear driving force” model in gas phase and/or in solid phase, the mass transfer coefficient needed could be specified by the user or calculated by ProSim DAC. It’s also possible to neglect the mass transfer resistance.

In this example, the mass transfer resistance has been taken into account in the two phases and the necessary coefficients are calculated by ProSim DAC.

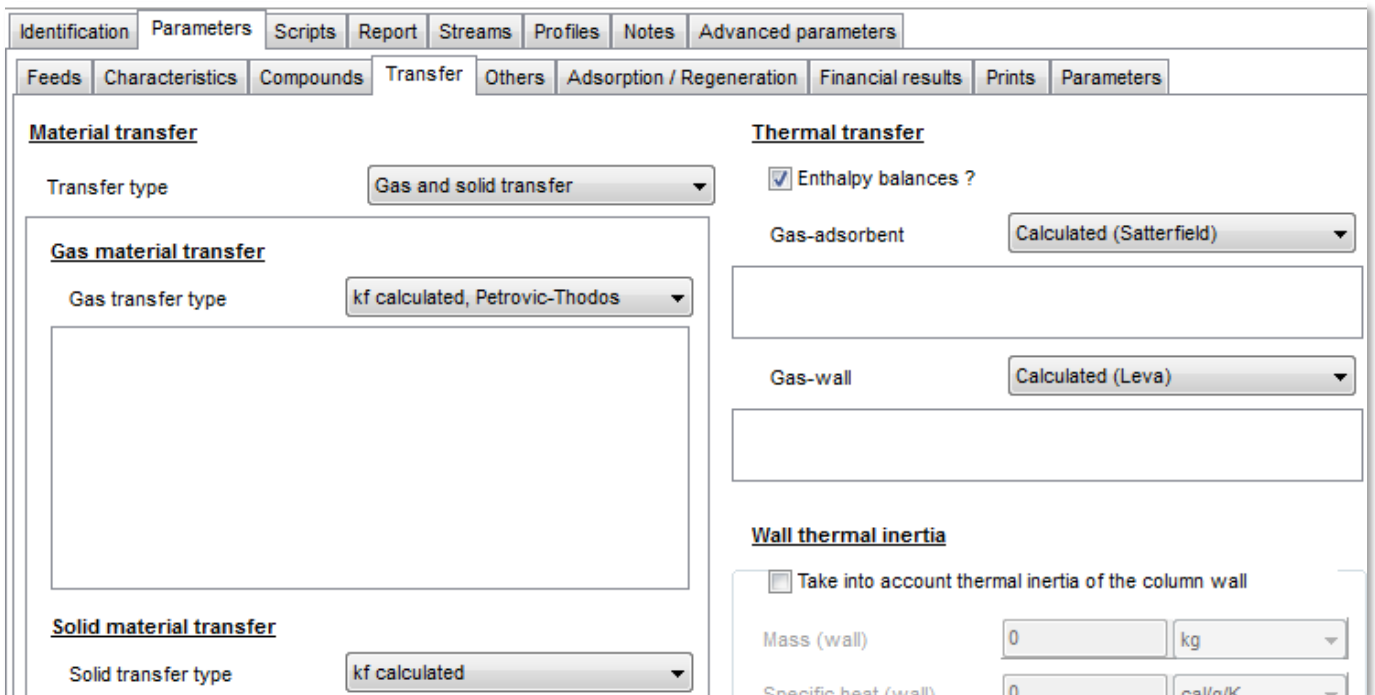
|                            | <b>Value</b>                   |
|----------------------------|--------------------------------|
| <b>Mass transfer</b>       |                                |
| Type                       | Gas and solid transfer         |
| <b>Gas mass transfer</b>   |                                |
| Type                       | kf calculated, Petrovic-Thodos |
| <b>Solid mass transfer</b> |                                |
| Type                       | kf calculated                  |

### 1.5.3.11. Thermal transfer

It’s possible to take into account the enthalpy balance in ProSim DAC or to ignore it. An isothermal working can be modeled if the enthalpy balance is not taken into account. If the enthalpy balance is taken into account, the gas-adsorbent and the gas-wall heat transfer coefficients are necessary. They can be calculated, as in this example, or specified.

| <b>Thermal transfer</b> | <b>Value</b>             |
|-------------------------|--------------------------|
| Enthalpy balances       | Taken into account       |
| Gas – Adsorbent         | Calculated (Satterfield) |
| Gas – Wall              | Calculated (Leva)        |

The screen shot below shows the information of the previous paragraphs 1.5.3.10 and 1.5.3.11 specified in the module interface: “Parameters” tab, “Transfer” sub-tab.



### 1.5.3.12. Adsorption thermodynamics

The adsorption thermodynamic models available are:

- ✓ Simple model: This model doesn't take into account the influence of the compounds on each other's. The adsorbed quantity of a given compound is directly given by its adsorption isotherm specified by the user.
- ✓ IAS or RAS: This model takes into account the influence of the compounds on each other's. The IAS model assumes an ideal adsorbed phase. The RAS model is used if an activity coefficient model is selected in the thermodynamic profile of the Simulis Thermodynamics calculator.
- ✓ Langmuir extended: This model takes into account the influence of the compounds on each other's. It has to be used with pure compound adsorption isotherms of the type "Langmuir extended".

In this example, the simple model is selected.

| Adsorption thermodynamics | Value        |
|---------------------------|--------------|
| Adsorption model          | Simple model |

The adsorption thermodynamic model is specified in the "Parameters" tab, "Others" sub-tab. The left part of this sub-tab is used to specify an optional valve at the column outlet during the adsorption step.

|   |                 |           |          |  |                           |                   |                     |            |
|---|-----------------|-----------|----------|--|---------------------------|-------------------|---------------------|------------|
| Identification  | Parameters      | Scripts   | Report   | Streams                                    | Profiles                  | Notes             | Advanced parameters |            |
| Feeds   | Characteristics | Compounds | Transfer | Others                                     | Adsorption / Regeneration | Financial results | Prints              | Parameters |
| <b>Valve</b>  |                 |           |          | <b>Thermodynamics</b>                      |                           |                   |                     |            |
| <input type="checkbox"/> Presence of an outlet valve    |                 |           |          | Adsorption model <span>Simple model</span> |                           |                   |                     |            |
| State at the starting <span>Open</span>                 |                 |           |          |  |                           |                   |                     |            |
| Pressure at the opening <span>0</span> <span>atm</span> |                 |           |          |  |                           |                   |                     |            |
| Equation coefficient <span>1E-6</span>                  |                 |           |          |  |                           |                   |                     |            |
| <b>Column</b>   |                 |           |          |  |                           |                   |                     |            |
| Outlet pressure <span>1</span> <span>atm</span>         |                 |           |          |  |                           |                   |                     |            |

### 1.5.3.13. Sequence

The “Adsorption/Regeneration” sub-tab of the “Parameters” tab allows to select the type of the cycle to simulate between the five available:

1. Adsorption only
2. Adsorption + thermal regeneration
3. Adsorption + pressure regeneration
4. Adsorption + pressure regeneration + thermal regeneration
5. Adsorption + thermal regeneration + pressure regeneration

The cycle “Adsorption + thermal regeneration” is used in this example to model a TSA (Thermal Swing Adsorption) process as shown in the following figure.

Identification Parameters Scripts Report Streams Profiles Notes Advanced parameters

Feeds 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...

```

graph TD
    A[A] --> EVA((EVA))
    EVA --> RT[RT]
    RT --> EVT((EVT))
    EVT --> A
  
```

A: Adsorption  
EVA: Stop adsorption events  
RT: Thermal regeneration  
EVT: Stop thermal regeneration events

Optional parameters can be defined for each step (“Parameters...” buttons):

- ✓ Adsorption:
  - Wall temperature specific to this step.
  - Heat duty exchanged in the bed.
- ✓ Thermal regeneration:
  - Co- or counter-current regeneration
  - Bed and/or wall preheating of the column.
  - Cooling of the column at the end of the step.
  - Temporization of the column at the end of the step.
  - Heat duty exchanged in the bed.

Each step is ended by an event. The first event reached starts the next step. The available events are the following ones (“Events...” buttons):

- ✓ Adsorption
  - Step duration.
  - Breakthrough rate of a compound at a given position in the column.
  - Gas phase concentration of a compound at a given position in the column.
  - Solid phase concentration of a compound at a given position in the column.
  - Maximal temperature reached at a given position in the column.
  - Maximal pressure reached at a given position in the column.
- ✓ Thermal or pressure regeneration
  - Step duration.
  - Gas phase concentration of a compound at a given position in the column.
  - Solid phase concentration of a compound at a given position in the column.
  - Maximal temperature reached at a given position in the column.
  - Maximal pressure reached at a given position in the column.
  - Amount produced of a compound at a given position in the column.
- ✓ Simulation end
  - End simulation time (§ 1.5.2 or number of cycles.
  - Total amount produced of a compound at a given position in the column.
  - Maximal temperature reached at a given position in the column.
  - Maximal pressure reached at a given position in the column.
  - Total amount treated of a compound.

In this example, the regeneration of the bed of adsorbent is a thermal regeneration done by a hot nitrogen stream. This stream flows counter-currently compared to the adsorption flow. The default parameters are kept for the two steps (adsorption and thermal regeneration). These two steps and the simulation are stopped by a duration.

|                             | Value                             |
|-----------------------------|-----------------------------------|
| <b>Sequence</b>             |                                   |
| Type                        | Adsorption + Thermal regeneration |
| <b>Adsorption</b>           |                                   |
| Parameters                  | Default values                    |
| Events                      | Duration = 7 200 s                |
| <b>Thermal regeneration</b> |                                   |
| Parameters                  | Default values                    |
| Events                      | Duration = 7 200 s                |
| <b>End of simulation</b>    |                                   |
| Events                      | End simulation time               |

### 1.5.3.14. Financial balance

ProSim DAC performs a financial balance on the regeneration steps. If the user is interested, it's possible to modify the parameters default values in the "Financial results" sub-tab of the "Parameters" tab.

| Identification                     | Parameters                       | Scripts           | Report   | Streams | Profiles                  | Notes             | Advanced parameters |            |
|------------------------------------|----------------------------------|-------------------|----------|---------|---------------------------|-------------------|---------------------|------------|
| Feeds                              | Characteristics                  | Compounds         | Transfer | Others  | Adsorption / Regeneration | Financial results | Prints              | Parameters |
| <b>Thermal regeneration costs</b>  |                                  |                   |          |         |                           |                   |                     |            |
| Cost of regeneration flow          | <input type="text" value="0.2"/> | €/Nm <sup>3</sup> |          |         |                           |                   |                     |            |
| Cost of regeneration flow heating  | <input type="text" value="100"/> | €/MWh             |          |         |                           |                   |                     |            |
| Cost of bed preheating             | <input type="text" value="120"/> | €/MWh             |          |         |                           |                   |                     |            |
| <b>Pressure regeneration costs</b> |                                  |                   |          |         |                           |                   |                     |            |
| Cost of electricity                | <input type="text" value="100"/> | €/MWh             |          |         |                           |                   |                     |            |
| Power of vacuum pump               | <input type="text" value="0"/>   | kcal/h            |          |         |                           |                   |                     |            |

### 1.5.3.15. Prints

ProSim DAC offers different options for the printing of the calculation results. The parameters specified for this example are listed in the table below.

| Parameters                                   | Value            |
|--|------------------|
| Print results files                          | Frequency = 60 s |
| Print 3D plots                               | Not activated    |
| Print output stream with time step of module | Activated        |
| Printing of inlet data                       | Activated        |
| Type of results                              | Molar            |
| Inert detection                              | Not activated    |

The following screen shot shows this information specified in the "Prints" sub-tab of the "Parameters" tab.

**Print**

Print results files  
 Frequency: 60 s

Print 3D plots  
 Frequency: 0,1 h

Print output stream with time step of module

Printing of inlet data

Type of results: Molar

Inert detection  
 Threshold: 1E-6 kmol

### 1.5.3.16. Integration, tolerances and model parameters

In ProSim DAC, the user has access to a set of integration, tolerances and model parameters. Only the parameters shown in the table below are modified compared to the default values. The use of the analytical calculation of the derivatives speeds up the solving of the problem. The model consists in a numerical time integration and on a spatial discretization. In this example, the column is discretized in 30 cells to obtain a precise solving of the problem. The thermal accumulation of the solid has a weak influence in this example. Thus, this option is deactivated to decrease the computational time required.

| Parameters                        | Value                   |
|-----------------------------------|-------------------------|
| Derivatives                       | Calculated analytically |
| Number of discretization cells    | 30                      |
| Thermal accumulation in the solid | Not taken into account  |
| Other parameters                  | Default values          |

The following screen shot shows this information specified in the “Parameters” sub-tab of the “Parameters” tab.

| Identification  |                                      | Parameters        | Scripts                          | Report   | Streams | Notes                     | Advanced parameters |        |            |          |
|---|--------------------------------------|-------------------|----------------------------------|----------|---------|---------------------------|---------------------|--------|------------|----------|
| Streams   |                                      | Characteristics   | Compounds                        | Transfer | Others  | Adsorption / Regeneration | Financial results   | Prints | Parameters |          |
| <b>Integration</b>  |                                      |                   | <b>Tolerances (adsorption)</b>   |          |         |                           |                     |        | Relative   | Absolute |
| Max. integration step   | 500                                  | s                 | Partial concentrations           | 1E-5     | 1E-5    | mol/m <sup>3</sup>        |                     |        |            |          |
| Initial integration step  | 0,005                                | s                 | Concentrations                   | 0,0001   | 0,0001  | mol/m <sup>3</sup>        |                     |        |            |          |
| Integration method  | Sparse matrix, analytical evaluation |                   | Temperatures                     | 0,001    | 0,001   | K                         |                     |        |            |          |
| Step count  | 2                                    |                   | Pressures                        | 0,001    | 0,001   | atm                       |                     |        |            |          |
| Derivatives   | calculated analytically              |                   | Enthalpies                       | 0,1      | 0,1     | J/kg                      |                     |        |            |          |
| <b>Model parameters</b>   |                                      |                   | Speed                            | 0,1      | 0,1     | m/s                       |                     |        |            |          |
| Number of discretization cells  | 30                                   |                   | Production                       | 0,0001   | 0,0001  |                           |                     |        |            |          |
| Axial dispersion coefficient  | 0                                    | m <sup>2</sup> /s | <b>Tolerances (regeneration)</b> |          |         |                           |                     |        |            |          |
| $\Delta H_{\text{Regeneration}} / \Delta H_{\text{Adsorption}}$ (ratio)       | 1                                    |                   | Partial concentrations           | 1E-5     | 1E-5    | mol/m <sup>3</sup>        |                     |        |            |          |
| <input type="checkbox"/> Thermal accumulation in the solid taken into account |                                      |                   | Concentrations                   | 0,0001   | 0,0001  | mol/m <sup>3</sup>        |                     |        |            |          |
| Heat duty applied to  | Gas enthalpy balance                 |                   | Temperatures                     | 0,001    | 0,001   | K                         |                     |        |            |          |
| Duration of the cubic spline  | 0                                    | h                 | Pressures                        | 0,001    | 0,001   | atm                       |                     |        |            |          |
| Solid transfer (regeneration)   | Same as the adsorption               |                   | Enthalpies                       | 0,1      | 0,1     | J/kg                      |                     |        |            |          |
|   |                                      |                   | Speed                            | 0,1      | 0,1     | m/s                       |                     |        |            |          |
|   |                                      |                   | Production                       | 0,0001   | 0,0001  |                           |                     |        |            |          |

## 2. RESULTS

### 2.1. Simulation report of the adsorption column

The simulation report of the adsorption column ("Report") presents global results (integrated during the time): initial characteristics of the column, adsorbed quantities, quantities recovered during the regeneration...

The mass of adsorbent is not directly specified in the input data. This value is calculated by ProSim DAC depending on the geometrical characteristics of the bed and the adsorbent characteristics. It's then interesting to verify in the simulation report the mass of adsorbent calculated corresponds to the end wished. For this example, the mass of adsorbent is about 615 g.

| COLUMN GENERAL CHARACTERISTICS |            |     |
|--------------------------------|------------|-----|
| Adsorbent mass in the column:  | 614.416    | (G) |
| Column volume                  | : 1.32669  | (L) |
| Solid volume                   | : 0.742946 | (L) |
| Void volume                    | : 0.583743 | (L) |

With the operating parameters specified (see 1.5.3.13 among others), the bed of adsorbent is nearly completely regenerated (number of moles of propane adsorbed close to the number of moles of propane regenerated).

#### AMOUNT ADSORBED (MOL)

| COMPONENT | Cycle N° 1    |
|-----------|---------------|
| PROPANE   | 1.24936       |
| NITROGEN  | -6.550613E-03 |

#### AMOUNT RECOVERED DURING THERMAL REGENERATION (MOL)

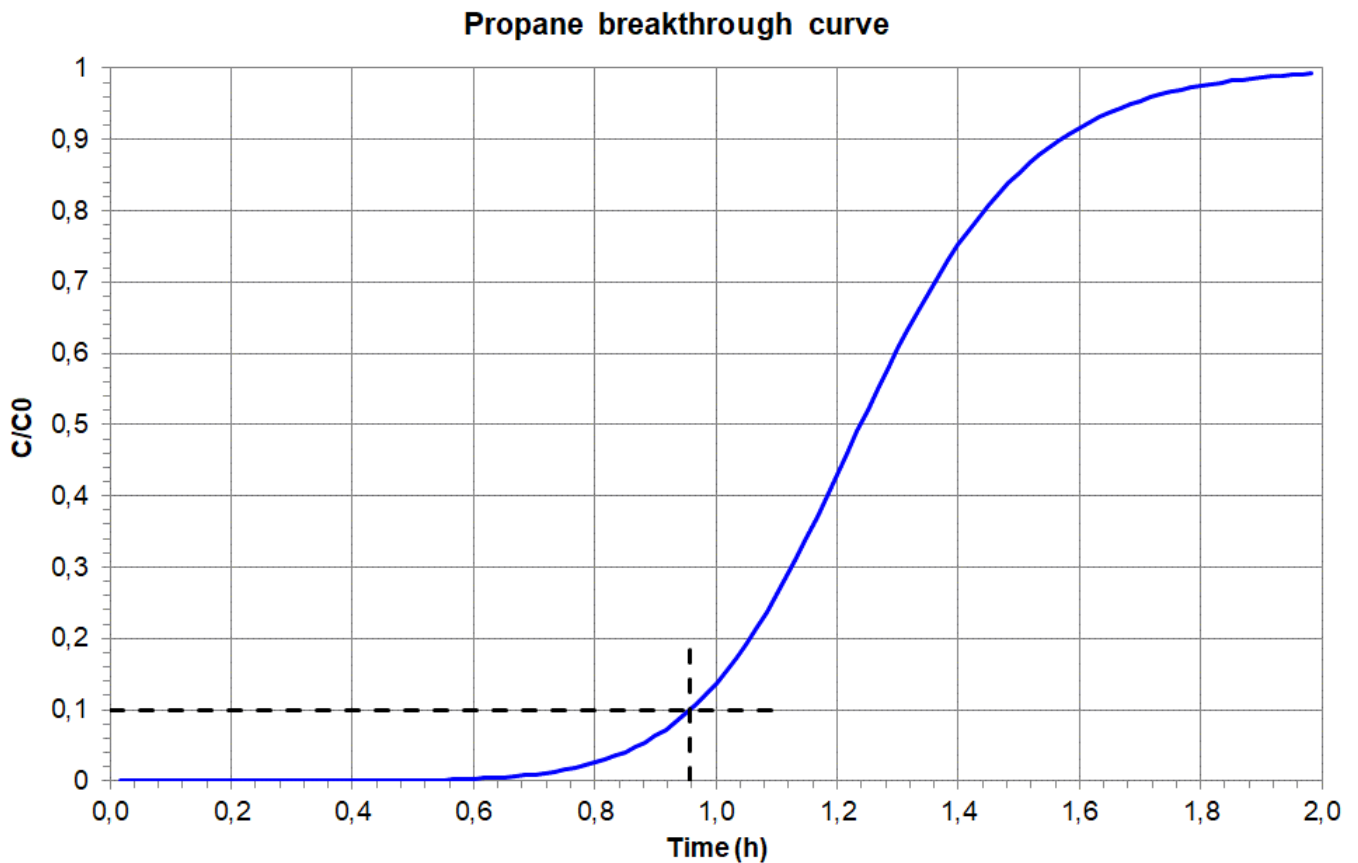
| COMPONENT | Cycle N° 1 |
|-----------|------------|
| PROPANE   | 1.24849    |
| NITROGEN  | 206.948    |

The negative value of the amount of nitrogen adsorbed corresponds to the mas balance deviation.

## 2.2. Profiles of the adsorption column

Several profiles (temperatures, pressures, velocities, concentrations, compositions, and breakthrough curves) in the adsorption column are available after the simulation from the module edition window ("Profiles" tab).

The following figure shows the breakthrough curve of propane. The breakthrough is assumed to be reached when the concentration at the column outlet is equal to 10% of the inlet concentration. The breakthrough is reached after 57 min (0.96 h). The bed of adsorbent is saturated when the outlet concentration is equal to the inlet one. This is the case after 2 h.



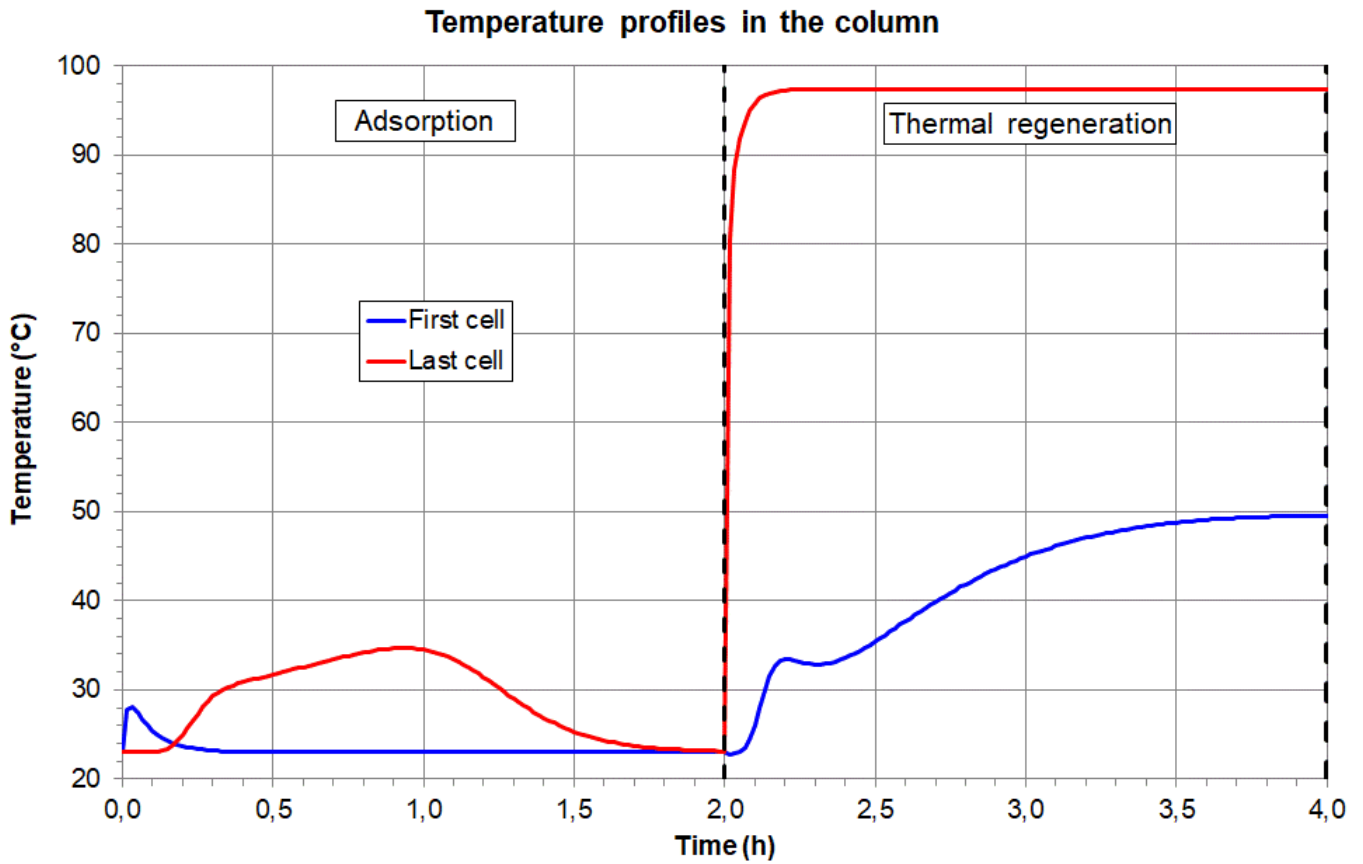
The figure below presents the temperature profile in the first and the last discretization cell. In the case of the adsorption:

- ✓ First cell: Inlet cell of the column
- ✓ Last cell: Outlet cell of the column

As the regeneration is done counter-currently:

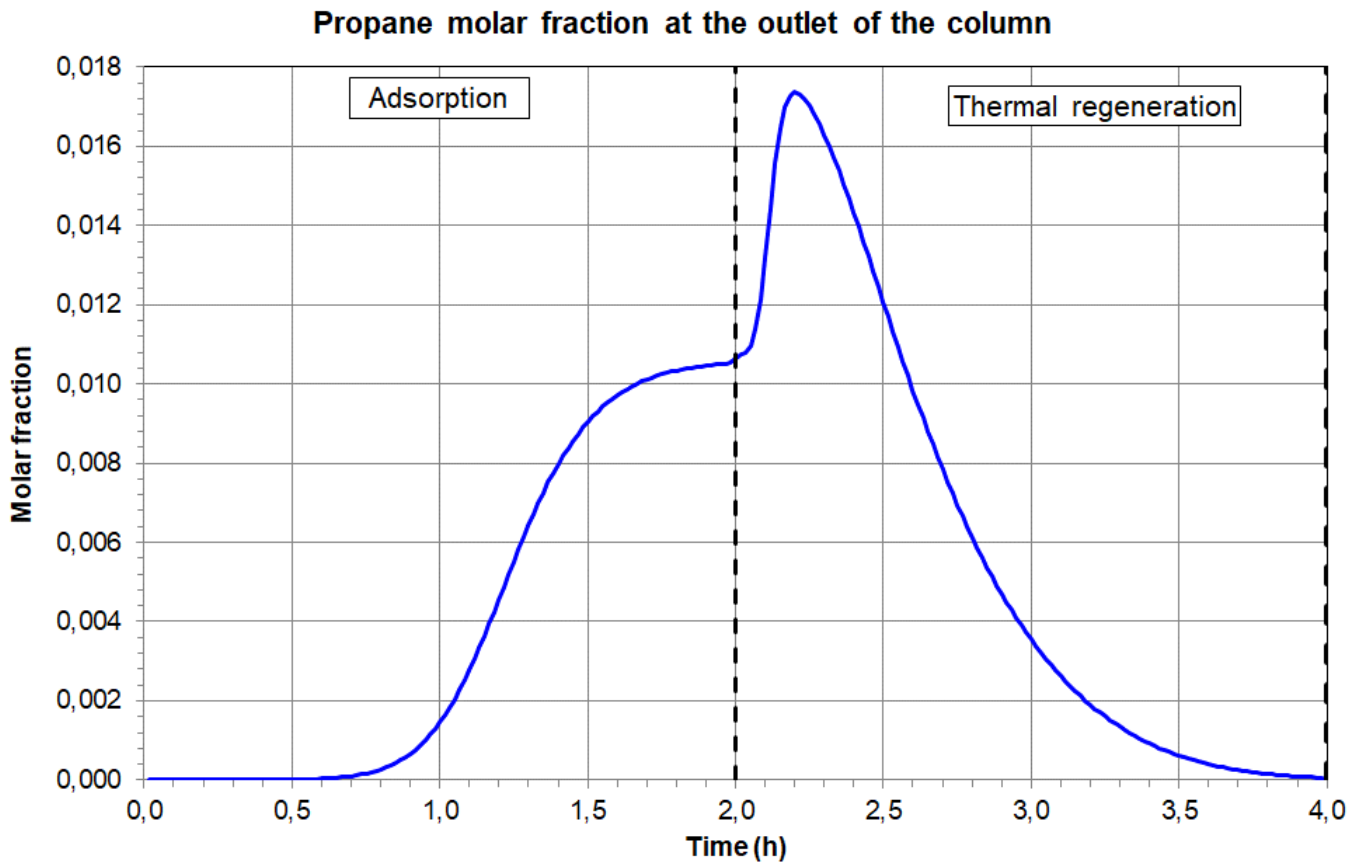
- ✓ First cell: Outlet cell of the column
- ✓ Last cell: Inlet cell of the column

The temperature profiles during the adsorption step show the corresponding temperature peak. During the thermal regeneration the temperature gradient is higher. Indeed, the extremity where the hot gas enters (last cell) is rapidly at the thermal equilibrium with the incoming flow (100°C). At the opposite extremity, the temperature increase is less and the equilibrium between the wall temperature (23°C) and the hot gas (100°C) has the time to be reached.



### 2.3. Profiles of the outlet stream

The following figure shows the evolution of the molar fraction of propane at the column outlet. Once the breakthrough is not reached, the adsorbent plays its role and the propane amount at the column outlet is null. When the breakthrough time is reached, the outlet stream is charged progressively in propane. In this example, the adsorption step is ended at the time corresponding to the saturation of the bed. The bed no more retained the propane, and its outlet concentration is equal to its inlet concentration. The counter-current thermal regeneration by a hot nitrogen stream allows to desorb the propane retained in the adsorbent. After a peak corresponding to the propane accumulated in the bed, the propane amount decreases because of the bed regeneration. This step is ended at the time corresponding to a complete regeneration of the bed.



The above profile and other ones (temperature, pressure, flow rate, enthalpy, and compositions) are available for the column outlet stream at the end of the simulation from the outlet stream edition window ("Tabulated results..." button in the "Parameters" tab).

### 3. REFERENCES

- [ROW11] ROWLEY R.L., WILDING W.V., OSCARSON J.L., GILES N.F., "DIPPR® Data Compilation of Pure Chemical Properties", Design Institute for Physical Properties, AIChE, New York, NY (2011)
- [SCH88] SCHORK J.M., FAIR J.R., "Parametric Analysis of Thermal Regeneration of Adsorption Beds", Ind. Eng. Chem. Res, 27, 457-469 (1988)