

## PROSIM DAC APPLICATION EXAMPLE

# VTSA PROCESS FOR DIRECT ADSORPTION OF CO<sub>2</sub> FROM AIR

### EXAMPLE PURPOSE

This example deals with a VTSA (Vacuum Thermal Swing Adsorption) process for the direct adsorption of CO<sub>2</sub> from the air. A thermodynamic adsorption model is used to take into account the effect of air humidity on CO<sub>2</sub> adsorption. This process is modeled in *ProSim DAC*, Fives ProSim's dynamic simulation software dedicated to gas-solid adsorption columns.

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<b>CORRESPONDING PROSIM DAC FILES</b>	<i>PSPDYN_EN_FR-DAC.pmp3</i>
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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.*

### Energy

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# CONTENTS

<b>1.</b>	<b>PROCESS MODELING .....</b>	<b>3</b>
1.1.	Process description .....	3
1.2.	Simulation 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 duration.....	6
1.5.3.	Adsorption column.....	6
<b>2.</b>	<b>RESULTS .....</b>	<b>19</b>
2.1.	Adsorption column simulation report.....	19
2.2.	Adsorption column profiles .....	20
2.3.	Outlet streams profiles .....	23
<b>3.</b>	<b>BIBLIOGRAPHY .....</b>	<b>24</b>

# 1. PROCESS MODELING

## 1.1. Process description

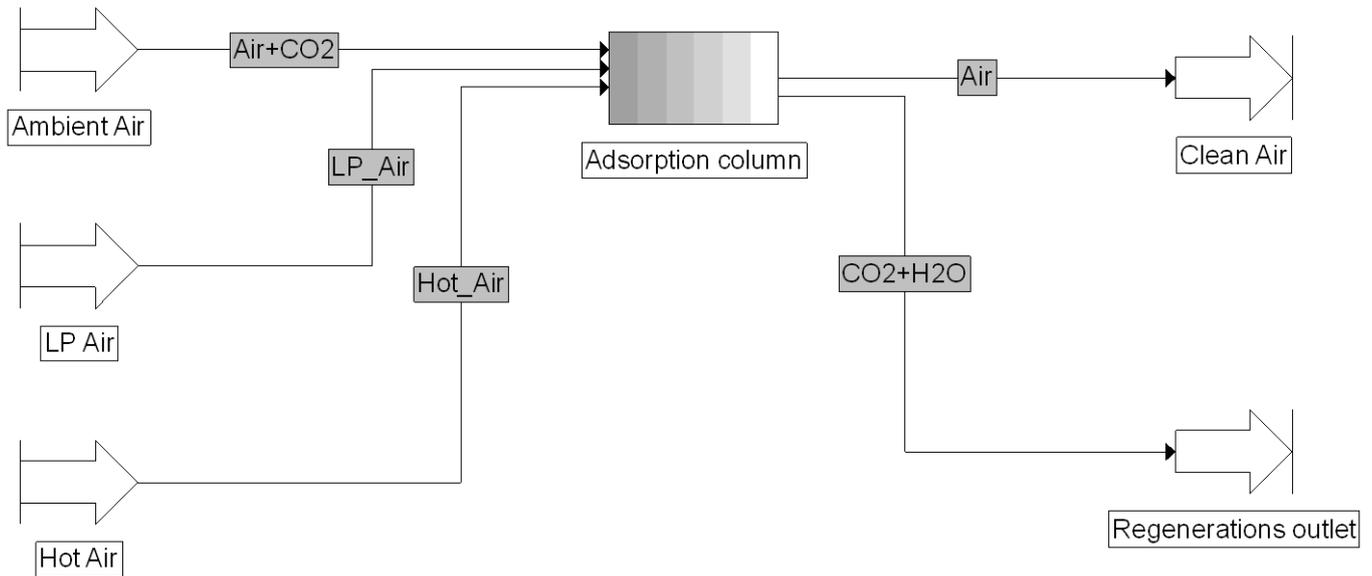
Carbon dioxide (CO<sub>2</sub>) is a common compound in the air and also the most important component of greenhouse gases [HAJ18b]. At present, about 44% of carbon dioxide comes from the combustion of fossil fuels such as oil, coal, and compressed natural gas [ZHA13]. In 1958, the concentration of carbon dioxide in the environment was about 315 ppm. In 1986, it had reached 350 ppm and in 2013, it exceeded 400 ppm. In addition, carbon dioxide emissions in 2040 are expected to increase by more than 40% compared to 2010 emissions.

Many techniques for capturing CO<sub>2</sub> from the atmosphere, such as membrane separation, chemical absorption by various solvents (ionic liquids [RAZ16], nano-fluids [HAJ18a], amino acid salt solutions [SOR19], etc.), electrochemical separation, low-temperature separation, solid adsorption, and other carbon capture technologies, have been investigated. Solid adsorption technology has become one of the most commonly used methods for CO<sub>2</sub> capture due to the low cost of solid adsorbents and low energy consumption in the adsorption process [WAL08]. The TSA (Temperature Swing Adsorption), PTSA (Pressure Temperature Swing Adsorption) and VTSA (Vacuum Temperature Swing Adsorption) processes are the most commonly encountered in the literature for the direct adsorption of CO<sub>2</sub> [JIA23].

This example is based on the publication [BAL24]. This publication describes the adsorption in a laboratory column of wet air containing CO<sub>2</sub> on a bed of APDES-NFC-FD-S which is a chemisorbent functionalized by amines (3-aminopropylmethyldiethoxysilane). *ProSim DAC* automatically calculates the amount of water to be added to air to meet the specified relative humidity. The process is a VTSA (Vacuum Thermal Swing Adsorption) process. Adsorption takes place at atmospheric pressure. The short pressure regeneration (80 s) corresponds to the vacuum step. The bed is regenerated mainly during the temperature regeneration step. This step is co-current with respect to adsorption. The air flow to be decarbonized enters the "Adsorption column" via the "Air+CO2" stream. The hot air for temperature regeneration enters the column via the "Hot\_Air" stream. The "LP\_Air" stream represents the low-pressure air sweep after the depressurization step. But this flow is not used in this simulation. The carbon-free air leaves the column via the "Air" stream. The flow of CO<sub>2</sub> and water leaving the column during regeneration constitutes the "CO2+H2O" stream.

## 1.2. Simulation flowsheet

The simulation flowsheet is shown in the following figure.



## 1.3. Compounds

The compounds considered in the simulation, their chemical formulae and CAS® numbers<sup>1</sup> are presented in the table below. Their pure compound properties are extracted from the standard database provided with *ProSim DAC* [ROW24].

Compound	Chemical formula	CAS number
Air		
Carbon dioxide	CO <sub>2</sub>	124-38-9
Water	H <sub>2</sub> O	7732-18-5

## 1.4. Thermodynamic model

Adsorption and regenerations are carried out at pressures equal to or lower than atmospheric pressure and at temperatures below 102°C. Thus, the "Ideal" thermodynamic profile is selected in the Simulis Thermodynamics calculator.

<sup>1</sup> CAS Registry Numbers® 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® have not been verified by ACS and may be inaccurate.

## 1.5. Operating parameters

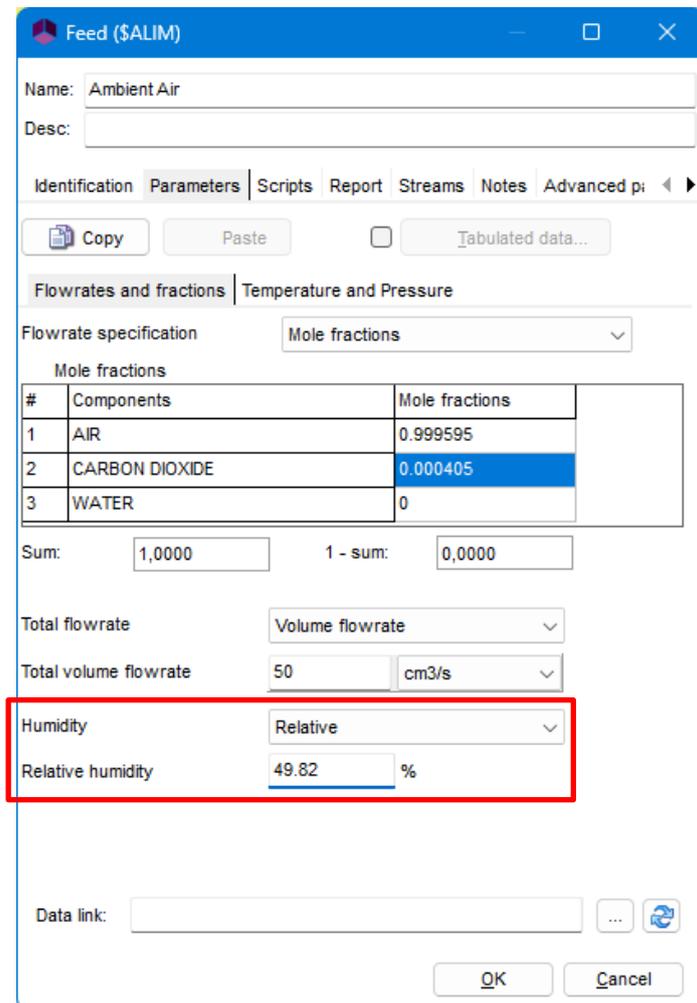
### 1.5.1. Process feeds

The characteristics of the three process feeds are described in the table below.

	Ambient Air	LP Air	Hot Air
Temperature (°C)	20	20	120
Pressure (bar)	1.01325	0.050	0.050
Total flow rate (cm <sup>3</sup> /s)	50	25	25
Relative humidity (%)	49.82	0	0
<b>Molar fractions</b>			
Air	0.999595	1	1
Carbon dioxide	0.000405	0	0
Water	0*	0	0

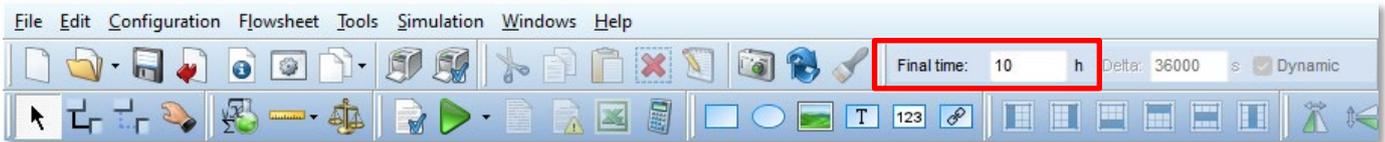
\* The water content required to achieve the specified relative humidity will be automatically calculated by the corresponding "Feed" module.

The following screenshot shows the configuration of the "Ambient Air" feed.



## 1.5.2. Simulation duration

The "Final time" is the actual operating time of the operation (adsorption + vacuum regeneration + temperature regeneration in this example). The "Final time" is entered in the *ProSim DAC* icon bars:



Simulation duration	Value
Final time	10 h

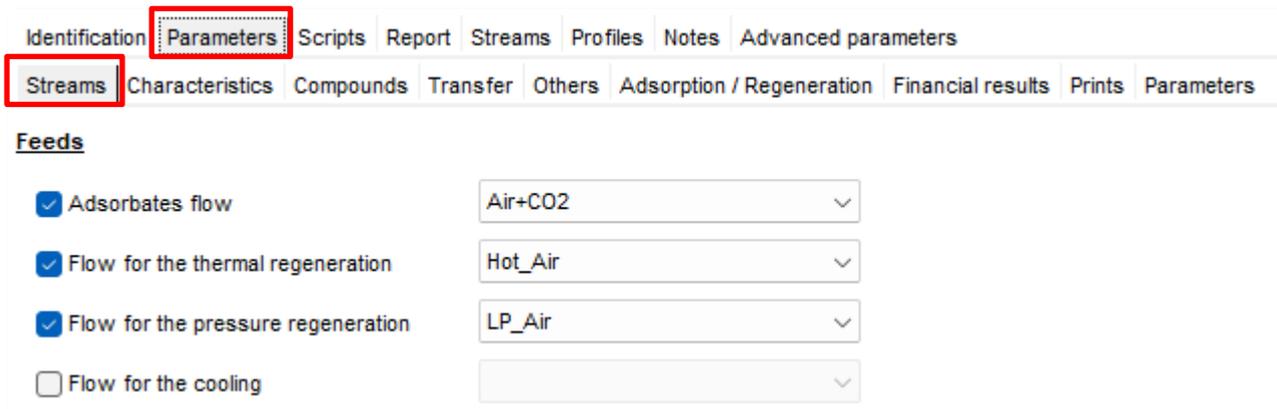
## 1.5.3. Adsorption column

### 1.5.3.1. Feeds

Four feeds can be used in *ProSim DAC*:

- ✓ Adsorbates flow: Flux to be purified during the adsorption step
- ✓ Flow for the thermal regeneration: Flow used during the temperature regeneration (hot inert, water vapor, etc.)
- ✓ Flow for the pressure regeneration: Flow used during the pressure regeneration (inert at pressure lower than the one of adsorption, etc.)
- ✓ Flow for the cooling: Flow used to cool the column at the end of the temperature regeneration step

The first three feeds are used in this example as shown in the screenshot below.

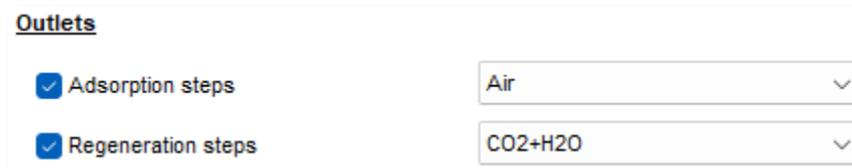


### 1.5.3.2. Outlets

Two outlets can be used in *ProSim DAC*:

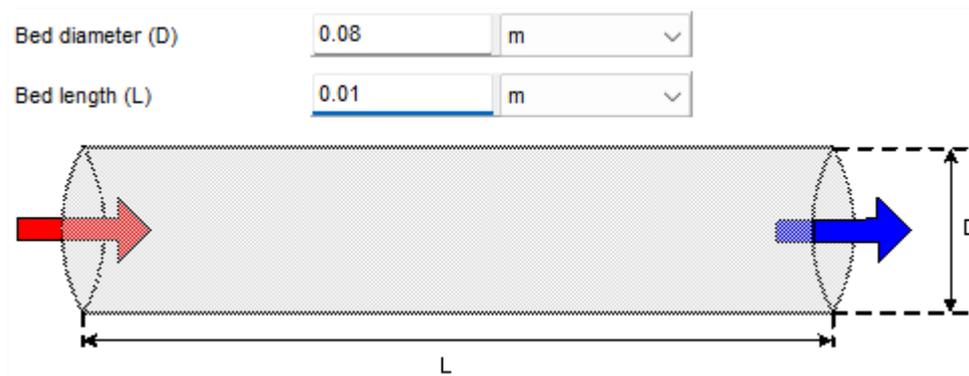
- ✓ Adsorption steps: Outlet during the adsorption steps
- ✓ Regeneration steps: Outlet during the regeneration steps

The screenshot below shows the outlets used.



### 1.5.3.3. Column characteristics

The column used is a lengthwise flow column. Its characteristics are shown in the screenshot below. The dimensions to be provided are those of the adsorbent bed. It should be noted that *ProSim DAC* also allows to model a transverse flow column.



### 1.5.3.4. Thermal behavior

*ProSim DAC* allows you to model the following heat exchange modes:

- ✓ Heat exchange in the bed: "Given heat duty without wall transfer"  
This possibility allows to model an adiabatic operation or an operation at given amount of heat duty for each step (exchanger within the adsorbent bed).
- ✓ Transfer through the wall + heat exchange in the bed: "Given heat duty and wall transfer "  
Heat exchange takes place through the column wall. The wall temperature is by default constant over time and along the column. To overcome this hypothesis, it is necessary to activate the "Take into account thermal inertia of the column wall" option. It is possible to add to this transfer mode a given amount of heat in the adsorption bed for each step (by default zero).

In this example, the heat transfer takes place through the column wall and without direct heat input into the adsorbent bed. The wall temperature specified in the "Characteristics" tab is the temperature of the wall during the regeneration steps. The wall temperature during the adsorption step is specified later.

Thermal behavior	
Thermal transfer	Given heat duty and wall transfer
Wall temperature	120°C

#### 1.5.3.5. Bed adsorbent characteristic

Bed adsorbent characteristic	
Bed void ratio	0.092 m <sup>3</sup> /m <sup>3</sup>

#### 1.5.3.6. Adsorbent characteristics

The density of the particles takes into account the intra-particle porosity. The surface-to-volume ratio is the ratio between the geometric surface and the geometric volume of one of the particles.

Particles characteristics	
Diameter	7,5 mm
Density	61 kg/m <sup>3</sup>
Specific heat	2 070 J/kg/K
Surface/volume ratio	800 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 that he wants to use to calculate the volume concentrations in the gas phase. Indeed, density is then necessary and, particularly in the case of a gas, is sensitive to temperature and pressure. In this example, the volume concentrations in the gas phase are evaluated under normal temperature and pressure conditions.

Measures conditions	Value
Conditions	Normal

### 1.5.3.8. Initialization

It is necessary to set the state of the column at startup. In this example, it is assumed that the column is at the temperature at the end of the temperature regeneration and at the composition of the air to be purified.

Initialization	Value
Type	Supplied by user
Pressure	1 atm
Temperature	120°C
Molar fractions	
Air	0.9881
Carbon dioxide	0.0004
Water	0.0115

The screenshot below shows the information from the previous paragraphs (from paragraph 1.5.3.3. to paragraph 1.5.3.8. included) entered into the module interface: "Parameters" tab, "Characteristics" sub-tab.

The screenshot displays the software interface for the 'Parameters' tab, specifically the 'Characteristics' sub-tab. The 'Initialization' section is active, showing the following settings:

- Column type:** Lengthwise flow column
- Heat transfer:** Given heat duty and wall transfer
- Wall temperature:** 120 °C
- Adsorbent:** Load... (button)
- Bed void ratio:** 0.092 m<sup>3</sup>/m<sup>3</sup>
- Particles diameter:** 0.0075 m
- Particles density:** 61 kg/m<sup>3</sup>
- Specific heat of the solid:** 2070 J/kg/K
- Particle surface/volume ratio:** 800 m<sup>2</sup>/m<sup>3</sup>
- Measures conditions (T,P):** Normal
- Initialization type:** Supplied by user
- Initial pressure:** 1 atm
- Initial temperature:** 120 °C
- Initial molar fractions table:**

1	AIR	0.9881
2	CARBON DIOXIDE	0.0004
3	WATER	0.0115
- Summation:** 1,0000

### 1.5.3.9. Adsorption isotherm

It is assumed that air does not adsorb. It is represented by a linear isotherm with the parameters of the table below.

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

<b>K<sub>0</sub> (mol/kg/atm)</b>	0
<b>K<sub>1</sub> (K)</b>	0
<b>ΔH<sub>ads</sub> (J/mol)</b>	0

The generalized Toth isotherm was chosen for carbon dioxide:

$$q_i = \frac{q_s b P_i}{[K + (b P_i)^\omega]^{1/\omega}}$$

$$q_s = q_{s,0} \exp\left[\chi \left(1 - \frac{T}{T_0}\right)\right] \quad b = b_0 \exp\left[-\frac{\Delta H_a}{RT_0} \left(\frac{T_0}{T} - 1\right)\right] \quad \omega = \omega_0 + \alpha \left(1 - \frac{T}{T_0}\right)$$

<b>q<sub>s0</sub> (mol/kg)</b>	2.2
<b>b<sub>0</sub> (atm<sup>-1</sup>)</b>	37 794.225
<b>ω<sub>0</sub> (-)</b>	0.4247
<b>χ (-)</b>	0
<b>ΔH<sub>a</sub> (J/mol)</b>	-60 000
<b>α (-)</b>	-0.4921
<b>T<sub>0</sub> (K)</b>	296
<b>K (-)</b>	1
<b>ΔH<sub>ads</sub> (J/mol)</b>	-60 000

The GAB isotherm (Guggenheim - Anderson - de Boer) was chosen for water:

$$q_i = \frac{C_m C_G K_{ads} \frac{P_i}{P_i^{sat}}}{\left(1 - K_{ads} \frac{P_i}{P_i^{sat}}\right) \left(1 + (C_G - 1) K_{ads} \frac{P_i}{P_i^{sat}}\right)}$$

$$C_m = C_{m0} \exp\left(\frac{\beta}{T}\right) \quad C_G = C_{G0} \exp\left(\frac{\Delta H_C}{RT}\right) \quad K_{ads} = K_{ads0} \exp\left(\frac{\Delta H_K}{RT}\right)$$

<b>C<sub>m0</sub> (mol/kg)</b>	36.48
<b>C<sub>G0</sub> (-)</b>	0.1489
<b>K<sub>ads</sub> (-)</b>	0.5751
<b>β (K)</b>	0
<b>ΔH<sub>C</sub> (J/mol)</b>	0
<b>ΔH<sub>K</sub> (J/mol)</b>	0
<b>ΔH<sub>ads</sub> (J/mol)</b>	-43 800

This information must be provided in the "Parameters" tab, "Compounds" sub-tab:

Identification Parameters Scripts Report Streams Profiles Notes Advanced parameters

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

**Characteristics**

AIR  
CARBON DIOXIDE  
WATER

**Adsorption enthalpy**

Enthalpy of adsorption: Given

Adsorption heat: 0 cal/mol Load...

**Adsorption isotherm**

Correlation: Linear isotherm

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

K0: 0 mol/kg/atm  
K1: 0 K

AIR  
CARBON DIOXIDE  
WATER

**Adsorption enthalpy**

Enthalpy of adsorption: Given

Adsorption heat: -60000 J/mol Load...

**Adsorption isotherm**

Correlation: Generalized Toth

$$q_i = \frac{q_{s0} \exp\left[\chi \left(1 - \frac{T}{T_0}\right)\right] b_0 \exp\left[\frac{\Delta H_a}{RT_0} \left(\frac{T_0}{T} - 1\right)\right] P_i}{\left[ K + \left( b_0 \exp\left[\frac{\Delta H_a}{RT_0} \left(\frac{T_0}{T} - 1\right)\right] P_i \right)^{\omega_0 + \alpha} \left(1 - \frac{T}{T_0}\right) \right]^{\frac{1}{\omega_0 + \alpha} \left(1 - \frac{T}{T_0}\right)}}$$

qs0: 2,2 mol/kg    ΔHa: -60000 J/mol  
b0: 37794,225 atm<sup>χ</sup>    α: -0,4921  
w0: 0,4247    T0: 296 K  
X: 0    K: 1

AIR  
CARBON DIOXIDE  
WATER

**Adsorption enthalpy**

Enthalpy of adsorption: Given

Adsorption heat: -43800 J/mol Load...

**Adsorption isotherm**

Correlation: GAB (Guggenheim - Anderson - de Boer)

$$q_i = \frac{C_{m0} \exp\left(\frac{\beta}{T}\right) C_{G0} \exp\left(\frac{\Delta H_c}{RT}\right) K_{ads0} \exp\left(\frac{\Delta H_k}{RT}\right) \frac{P_i}{P_i^{sat}}}{\left(1 - K_{ads0} \exp\left(\frac{\Delta H_k}{RT}\right) \frac{P_i}{P_i^{sat}}\right) \left(1 + \left(C_{G0} \exp\left(\frac{\Delta H_c}{RT}\right) - 1\right) K_{ads0} \exp\left(\frac{\Delta H_k}{RT}\right) \frac{P_i}{P_i^{sat}}\right)}$$

Cm0: 36,48 mol/kg    ΔHc: 0 J/mol  
CG0: 0,1489    ΔHk: 0 J/mol  
Kads0: 0,5751  
β: 0 K

### 1.5.3.10. Mass transfer

The following options are available for mass transfer:

- ✓ Coupled gas and solid phase transfer
- ✓ Mass transfer resistance ("Linear Driving Force") in the gas and/or the solid phase, the necessary mass transfer coefficients can be provided by the user or calculated by *ProSim DAC*. It is also possible to neglect the transfer resistances.

In this example, the mass transfer resistance has been considered only in the solid phase. The mass transfer coefficients are specified.

	Value
<b>Mass transfer</b>	
Type	Gas and solid transfer
<b>Gas mass transfer</b>	
Type	No resistance
<b>Solid mass transfer</b>	
Type	kf supplied
Air	0 s <sup>-1</sup>
Carbon dioxide	0.0002 s <sup>-1</sup>
Water	0.001 s <sup>-1</sup>

### 1.5.3.11. Thermal transfer

It's possible to take into account or to ignore the enthalpy balance in *ProSim DAC*. Not taking into account the enthalpy balance makes possible to simulate isothermal operation. When enthalpy balances are taken into account, the calculations require the knowledge of the gas-adsorbent and gas-wall heat transfer coefficients. These can be calculated or provided, as in this example. The value for the gas-adsorbent transfer is due to the fact that this transfer should not be limiting in this example.

Thermal transfer	Value
Enthalpy balances	Taken into account
Gas – Adsorbent	1 000 000 W/m <sup>2</sup> /K
Gas – Wall	3 W/m <sup>2</sup> /K

The screenshot below shows the information of paragraphs 1.5.3.10. and 1.5.3.11. entered in the module's interface: "Parameters" tab, "Transfer" sub-tab.

Identification
Parameters
Scripts
Report
Streams
Profiles
Notes
Advanced parameters

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

**Mass transfer**

Transfer type Gas and solid transfer ▾

**Gas mass transfer**

Gas transfer type No resistance ▾

**Solid mass transfer**

Solid transfer type kf supplied ▾

Mass transfer coefficients of solid phase (s<sup>-1</sup>)

1	AIR	0
2	CARBON DIOXIDE	0.0002
3	WATER	0.001

**Thermal transfer**

Enthalpy balances ?

Gas-adsorbent Supplied ▾

Exchange coefficient 1000000 W/m2/K ▾

Gas-wall Supplied ▾

Exchange coefficient 3 W/m2/K ▾

**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 ▾

### 1.5.3.12. Adsorption thermodynamic model

For this example, the thermodynamic adsorption model of Stampi – Bombelli is used. This model takes into account the positive effect of the stream humidity on the adsorption of carbon dioxide. This model is more specifically developed to correct two of the parameters of the generalized Toth isotherm by a function of the adsorbed quantity of water.

$$q_{s,wet} = q_s \left( \frac{1}{1 - \Psi q_{H_2O}} \right)$$

$$b_{wet} = b(1 + \beta q_{H_2O})$$

<b>Main adsorbent</b>	Carbon dioxide
<b>Co-adsorbent</b>	Water
<b>ψ (kg/mol)</b>	0.00958
<b>β (kg/mol)</b>	3.448

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: Stampi - Bombelli

Main adsorbent: CARBON DIOXIDE

Co-adsorbent: WATER

ψ (Psi): 0,00958 kg/mol

β (Beta): 3,448 kg/mol

### 1.5.3.13. Sequence

The "Adsorption / Regeneration" sub-tab of the "Parameters" tab allows you to choose the type of cycle to simulate among 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 "Adsorption + pressure regeneration + thermal regeneration" cycle is used in this example to model a VTSA (Vacuum Thermal Swing Adsorption) process as shown in the screenshot below.

The screenshot displays the 'Adsorption and regeneration' configuration window. At the top, there are tabs for 'Identification', 'Parameters', 'Scripts', 'Report', 'Streams', 'Notes', and 'Advanced parameters'. Below these, there are sub-tabs for 'Streams', 'Characteristics', 'Compounds', 'Transfer', 'Others', 'Adsorption / Regeneration', 'Financial results', 'Prints', and 'Parameters'. The 'Adsorption / Regeneration' sub-tab is selected.

The main area is titled 'Adsorption and regeneration'. It features a 'Sequence type' dropdown menu set to 'Adsorption + pressure regeneration + thermal regeneration'. Below this, there are four sections: 'Adsorption', 'Pressure regeneration', 'Thermal regeneration', and 'End of simulation'. Each section has an 'Events...' button and a 'Parameters...' button.

On the right side, a flowchart illustrates the cycle: EVA (Stop adsorption events) -> RP (Pressure regeneration) -> EVP (Stop pressure regeneration events) -> RT (Thermal regeneration) -> EVT (Stop thermal regeneration events) -> back to EVA. A legend on the right explains the abbreviations: EVA: Stop adsorption events, RP: Pressure regeneration, EVP: Stop pressure regeneration events, RT: Thermal regeneration, and EVT: Stop thermal regeneration events.

The parameters of the adsorption step are:

Adsorption	
Column cooling through the wall	Yes
Wall temperature	20°C
Other parameters	Default value
Event	Duration = 13 772 s

The parameters of the pressure regeneration step are:

Pressure regeneration	
Pressure to reach	50 mbar
Pressure down duration	80 s
Pressure up duration	0 s
Valve coefficient	10 <sup>-6</sup>
Other parameters	Default value
Event	Duration = 80 s

The parameters of the thermal regeneration step are:

Thermal regeneration	
Regeneration type	Co-curent
Other parameters	Default value
Event	Duration = 22 148 s

The simulation end event is:

End of simulation	
Event	Temps de fin de simulation

#### 1.5.3.14. Financial balance

*ProSim DAC* carries out a financial balance on the regeneration steps. If the user is interested, it is possible to change the default parameters in the "Financial balance" sub-tab of the "Parameters" tab.

### 1.5.3.15. Printings

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

Parameters	Value
Print result files	Frequency = 10 s
Print outlet stream with time step of the module	Yes
Printing of input data	Yes
Type of results	Molar
Other parameters	Default value

The screenshot below shows their specification in the "Parameters" tab, "Impressions" sub-tab.

The screenshot displays the software's parameter configuration window. At the top, there are several tabs: Identification, Parameters (selected), Scripts, Report, Streams, Notes, and Advanced parameters. Below these, a sub-menu is open for 'Parameters', showing options like Streams, Characteristics, Compounds, Transfer, Others, Adsorption / Regeneration, Financial results, Prints (highlighted with a dashed box), and Parameters. The main area is titled 'Print' and contains the following settings:

- Print results files
  - Frequency: 10 s
- Print 3D plots
  - Frequency: 0,1 h
- Print outlet stream with time step of the module
- Printing of input data
- Type of results: Molar
- Inert detection
  - Threshold: 1E-6 kmol

### 1.5.3.16. Parameters

ProSim DAC provides an access to a given number of numerical and models parameters. The model is based on time integration and spatial discretization. The column is here discretized into 15 cells in order to obtain a "fine" solution of the problem.

Model parameters	Value
Number of discretization cells	15
Solid transfer during regeneration	Given
Mass transfer coefficients of solid phase	
Air	0 s <sup>-1</sup>
Carbon dioxide	0.0002 s <sup>-1</sup>
Water	0.002 s <sup>-1</sup>
Other parameters	
Default value	

The screenshot below shows their specifications in the "Parameters" tab, "Parameters" sub-tab.

The screenshot displays the 'Parameters' sub-tab in the ProSim DAC software. The interface includes several sections:

- Integration:**
  - Max. integration step: 500 s
  - Initial integration step: 0,005 s
  - Integration method: Sparse matrix, analytical evaluation
  - Step count: 2
  - Derivatives: calculated analytically
- Model parameters:**
  - Number of discretization cells: 15
  - Axial dispersion coefficient: 0 m<sup>2</sup>/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 (regeneration): Given
  - Mass transfer coefficients of solide phase - regeneration (s-1):

1	AIR	0
2	CARBON DIOXIDE	0,0002
3	WATER	0,002
- Tolerances (adsorption):**
  - Partial concentrations: Relative 1E-5, Absolute 1E-5 mol/m<sup>3</sup>
  - Concentrations: Relative 0,0001, Absolute 0,0001 mol/m<sup>3</sup>
  - Temperatures: Relative 0,001, Absolute 0,001 K
  - Pressures: Relative 0,001, Absolute 0,001 atm
  - Enthalpies: Relative 0,1, Absolute 0,1 J/kg
  - Speed: Relative 0,1, Absolute 0,1 m/s
  - Production: Relative 0,0001, Absolute 0,0001
- Tolerances (regeneration):**
  - Partial concentrations: Relative 1E-5, Absolute 1E-5 mol/m<sup>3</sup>
  - Concentrations: Relative 0,0001, Absolute 0,0001 mol/m<sup>3</sup>
  - Temperatures: Relative 0,001, Absolute 0,001 K
  - Pressures: Relative 0,001, Absolute 0,001 atm
  - Enthalpies: Relative 0,1, Absolute 0,1 J/kg
  - Speed: Relative 0,1, Absolute 0,1 m/s
  - Production: Relative 0,0001, Absolute 0,0001

## 2. RESULTS

### 2.1. Adsorption column simulation report

The adsorption column simulation report ("Report") presents overall results (integrated over time), initial characteristics of the column, amount adsorbed, amount recovered during regeneration, etc.

The mass of adsorbent is not provided directly in the input data. It is calculated by *ProSim DAC* according to the geometric characteristics of the bed and the properties of the adsorbent. It is then interesting to check in the simulation report if the calculated mass of adsorbent corresponds to the one expected. For this example, the mass of adsorbent is just less than 3 g.

#### COLUMN GENERAL CHARACTERISTICS

Adsorbent mass in the column:	2.78410	(g)
Column volume	: 50.2655	(cm3)
Solid volume	: 45.6411	(cm3)
Void volume	: 4.62442	(cm3)

With the selected operating parameters (see § 1.5.3. among others), the adsorbent bed is 98% regenerated.

#### AMOUNT ADSORBED (mol)

These values include the inventory of the gas phase of the column.

COMPONENT	Cycle N° 1
AIR	4.807498E-05
CARBON DIOXIDE	4.620825E-03
WATER	7.976939E-03

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

COMPONENT	Cycle N° 1
AIR	0.846638
CARBON DIOXIDE	4.543218E-03
WATER	7.733148E-03

## 2.2. Adsorption column profiles

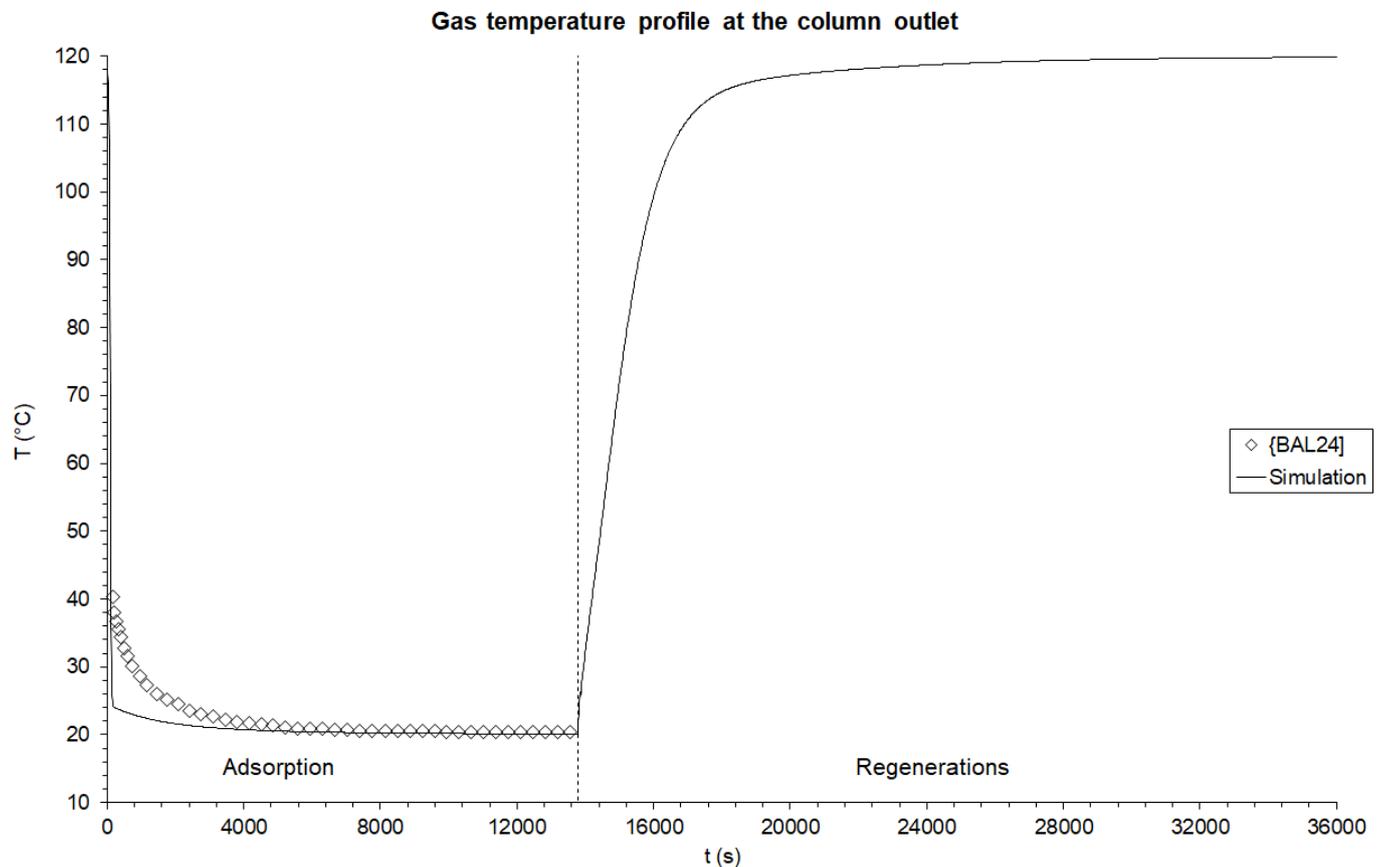
Several profiles in the adsorption column (temperatures, pressures, velocities, molar or mass concentrations, molar or mass fractions and breakthrough curves) are available at the end of the simulation in the editing window (tab "Profiles"). These profiles have two curves:

- ✓ "First cell": Column inlet cell in the direction of adsorption flow
- ✓ "Last cell": Column output cell in the direction of adsorption flow

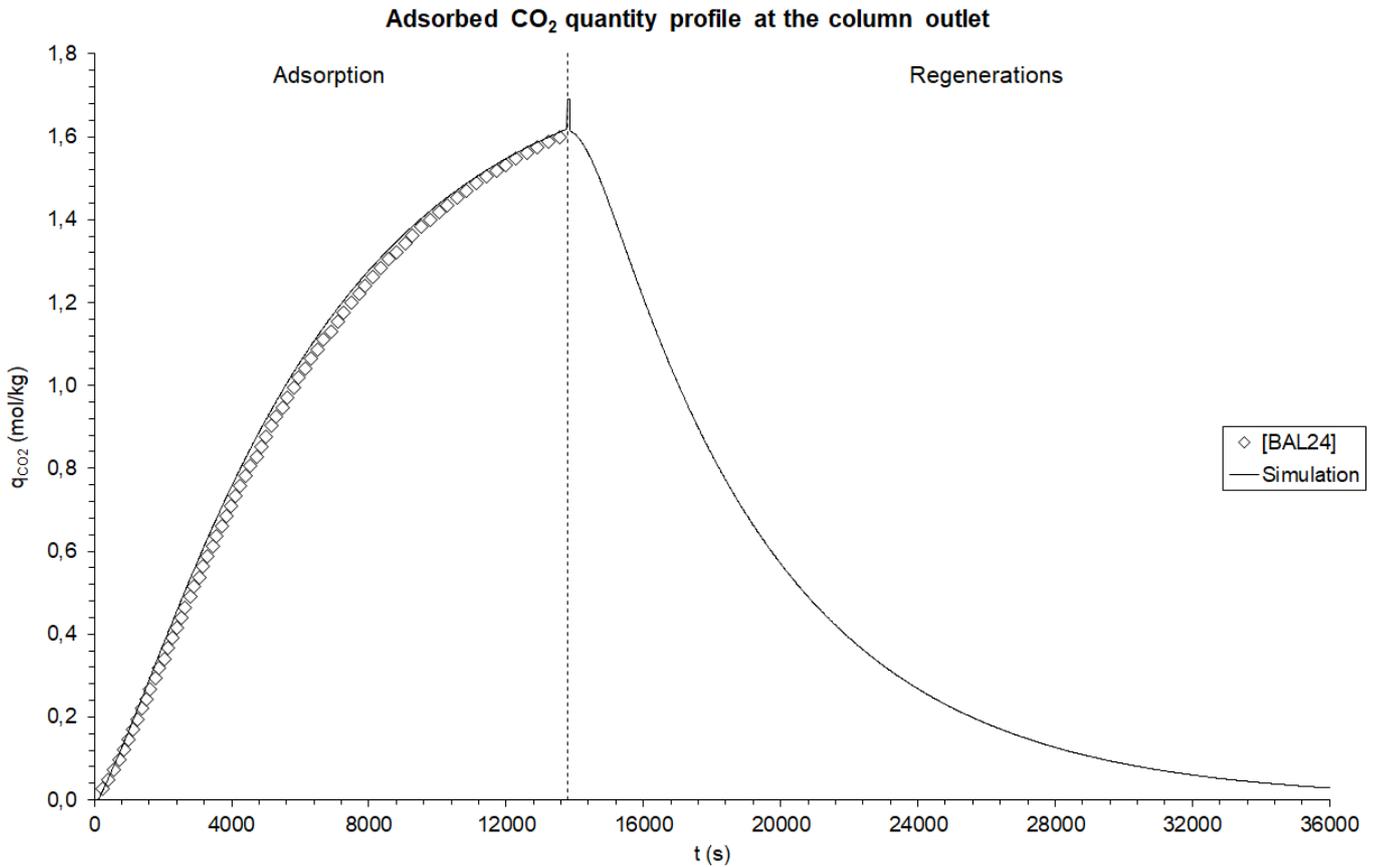
If counter-current regeneration occurs:

- ✓ "First cell": Column outlet cell
- ✓ "Last cell": Column inlet cell

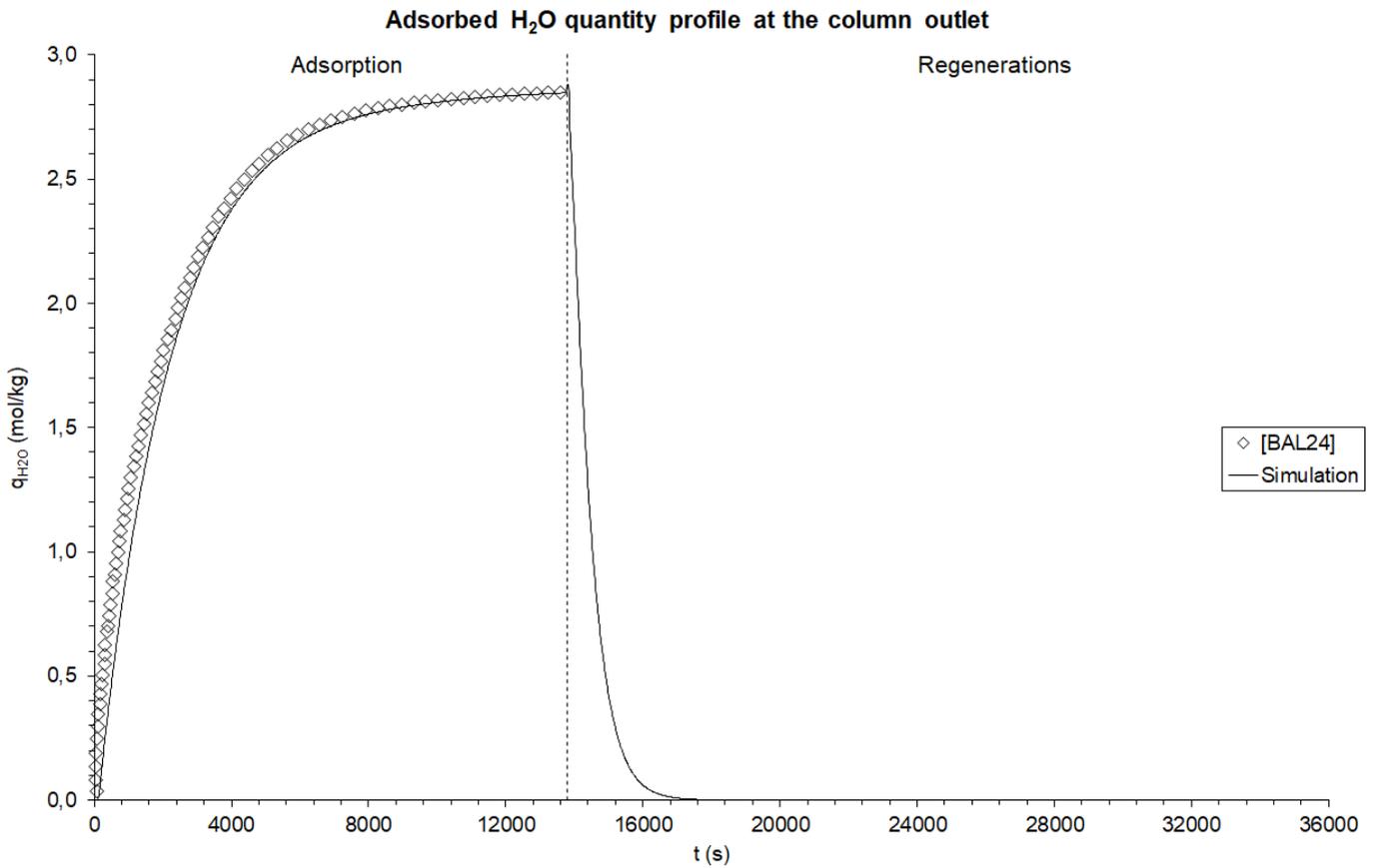
The figure below shows the time evolution of the temperature of the gas at the outlet of the column. A comparison with the results of [BAL24] is made for the adsorption step (the curves published by [BAL24] use a different type of regeneration than the one of this simulation). When the simulation starts, the temperature drops rapidly from the initial temperature of 120°C to the wall temperature specified for this step (20°C). Taking into account the thermal wall inertia would induce a less abrupt profile at the beginning of the adsorption step and corresponding to this of [BAL24]. As the pressure regeneration step is very short (80 s), it is almost invisible on this profile. During the temperature regeneration step, the temperature rise is gradual with the hot inert supply (120°C).



The figure below shows the time evolution of the adsorbed quantity of CO<sub>2</sub> at the outlet of the column. CO<sub>2</sub> adsorbs regularly during the adsorption step. A comparison with the results of [BAL24] is made for the adsorption step (the curves published by [BAL24] use a different type of regeneration than the one of this simulation). This step is stopped when the saturation of the bed with CO<sub>2</sub> is almost reached. The short pressure regeneration results in a peak in CO<sub>2</sub> adsorption. The bed is gradually regenerated during temperature regeneration. The simulation is stopped when the bed is almost completely regenerated.

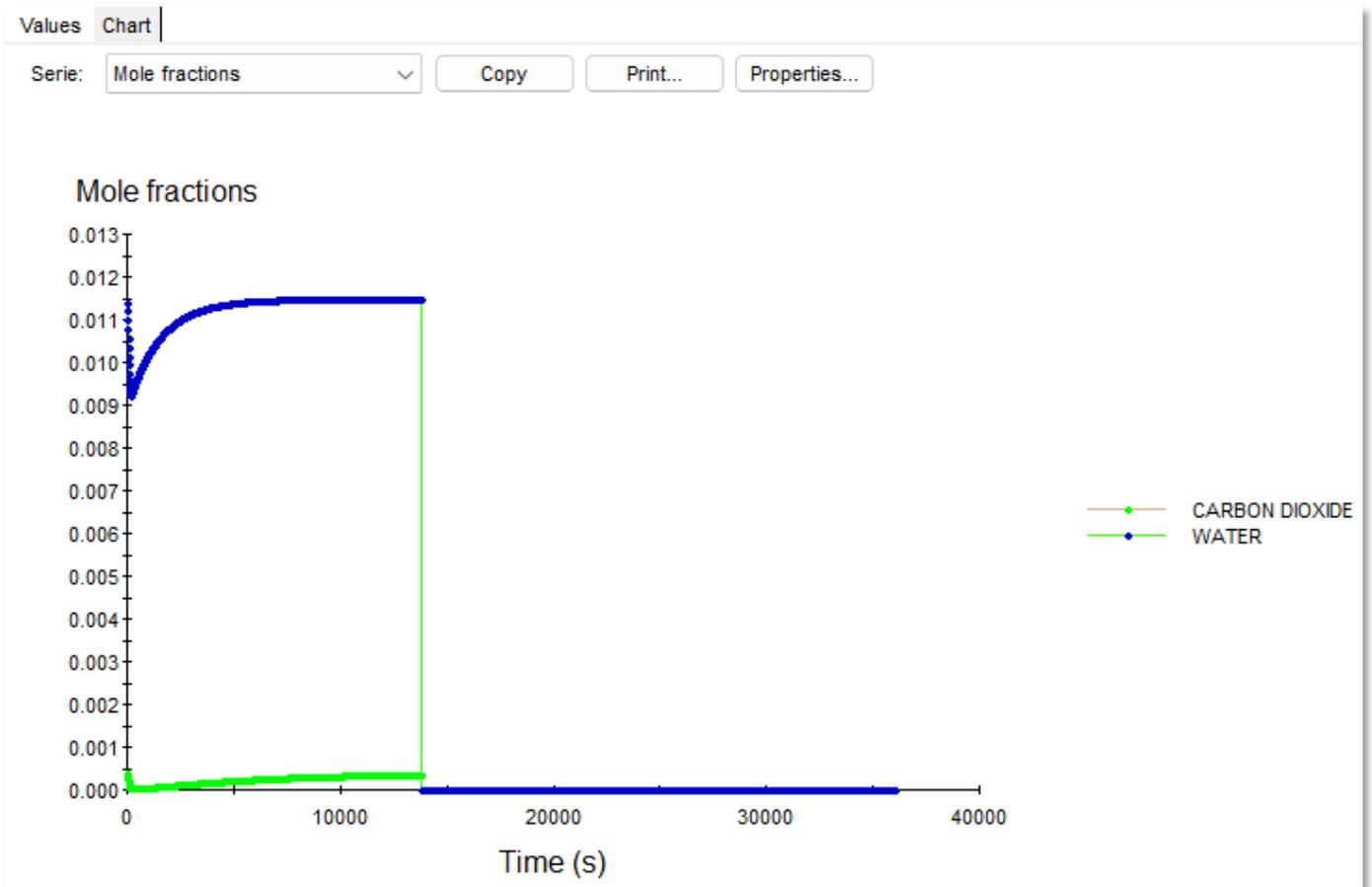


The figure below shows the time evolution of the adsorbed quantity of water at the outlet of the column. Water adsorbs regularly during the adsorption step. A comparison with the results of [BAL24] is made for the adsorption step (the curves published by [BAL24] use a different type of regeneration than the one of this simulation). At the end of this step, the bed is saturated with water. The short regeneration in pressure results in a peak in water adsorption. During temperature regeneration, the bed regenerates quickly. At the end of this step, the adsorbent is dry.



### 2.3. Outlet streams profiles

Temperature, pressure, flow, enthalpy and composition profiles are also available for each adsorption column output streams at the end of the simulation. They can be accessed via the "Tabulated results..." button on the " Parameters" tab of the output stream editing window.



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