ProSimPlus Application Example

CO_2 CAPTURE USING AN AMINE SOLUTION

EXAMPLE PURPOSE
This example presents the simulation of a CO_2 capture process by absorption using an amine solution. The flue gas is first cooled in a direct contact cooler with water before to be CO_2 impoverished in an absorber (absorption column) using an amine solution. The amine is then regenerated in a desorber (distillation column) to be reused in the absorber. The desorber gas outlet composed of CO_2 and water is then cooled and put in a drum to separate water from CO_2. This example especially illustrates the use of the ProSimPlus "Script" module for make-up amine and make-up water flowrates calculation.

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CORRESPONDING PROSIMPLUS FILES	*PSPS_E19_EN –CO2 capture process with amine.pmp3*

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. 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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1. INTRODUCTION

This example presents a CO_2 capture process by absorption using an amine solution. The unit can be placed at a fossil fuel combustion process outlet and allow to decrease the CO_2 amount rejected in the atmosphere. In a context of environmental norms reinforcement and further to the COP21 agreements aiming at limiting the climate change, this process is a conceivable solution to decrease CO_2 (a greenhouse gas) rejects at the outlet of the combustion units.

One of the difficulty to simulate this process is the presence of recycling, a wake-up amine and a wake-up water. The ProSimPlus “Script” module allows to easily calculate the make-ups and to model recycling in order to obtain the simulation convergence.

2. PROCESS MODELING

2.1. Process presentation

CO_2 absorption:

The stream to be threated is a flue gas at 100°C and atmospheric pressure. It contains dinitrogen, carbon dioxide and water. To obtain the optimal conditions for the CO_2 absorption, the gas is cooled at around 40°C through a Direct Contact Cooler (DCC) using water. It is then put in touch with amine in an absorption column (absorber) to extract CO_2.

Amine regeneration and recycling:

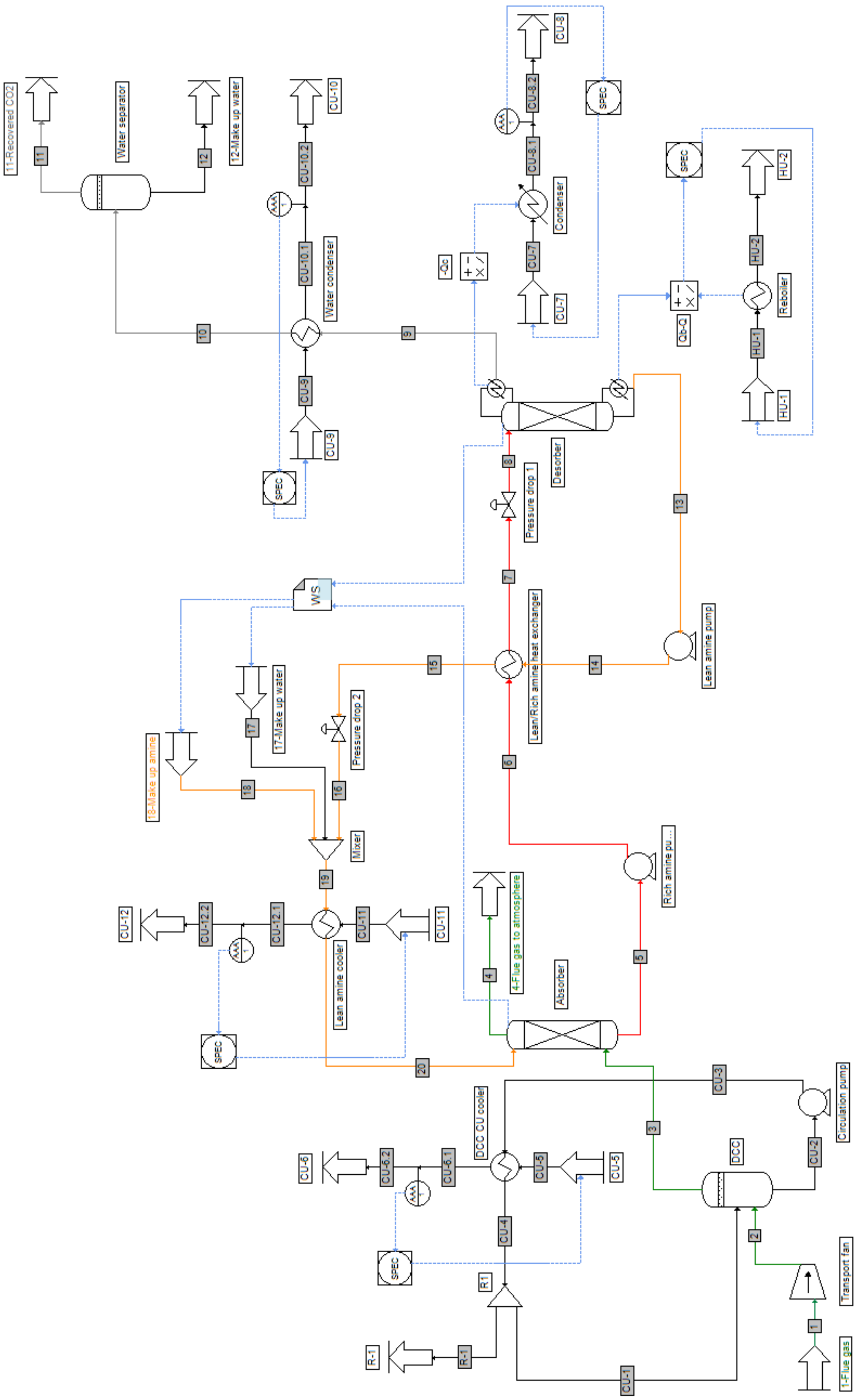
The CO_2 rich amine at the outlet of the absorber is regenerated (separated from the CO_2) in a distillation column (desorber) in order to be reused in the absorber. To compensate the amine losses in the vapor outlets of the absorber and the desorber, an amine make-up is added to the recycling stream.

In the same way, a water make-up is required to complete the mass balance.

CO_2 recovery:

The desorber vapor outlet contains CO_2 and water. To separate these compounds, the stream is cooled and sent to a separation drum. The drum vapor outlet is mainly composed of CO_2 that will be stocked and the liquid outlet is composed of water that could be recycled as make-up.

2.2. Process flowsheet



Flowsheet of the CO_2 capture unit

To improve the process flowsheet readability, the flue gas is in green, the rich amine is in red, the lean amine is in orange, the recovered CO_2 is in grey and the water is in black.

2.3. Compounds

The compounds considered in this example are listed in the table below:

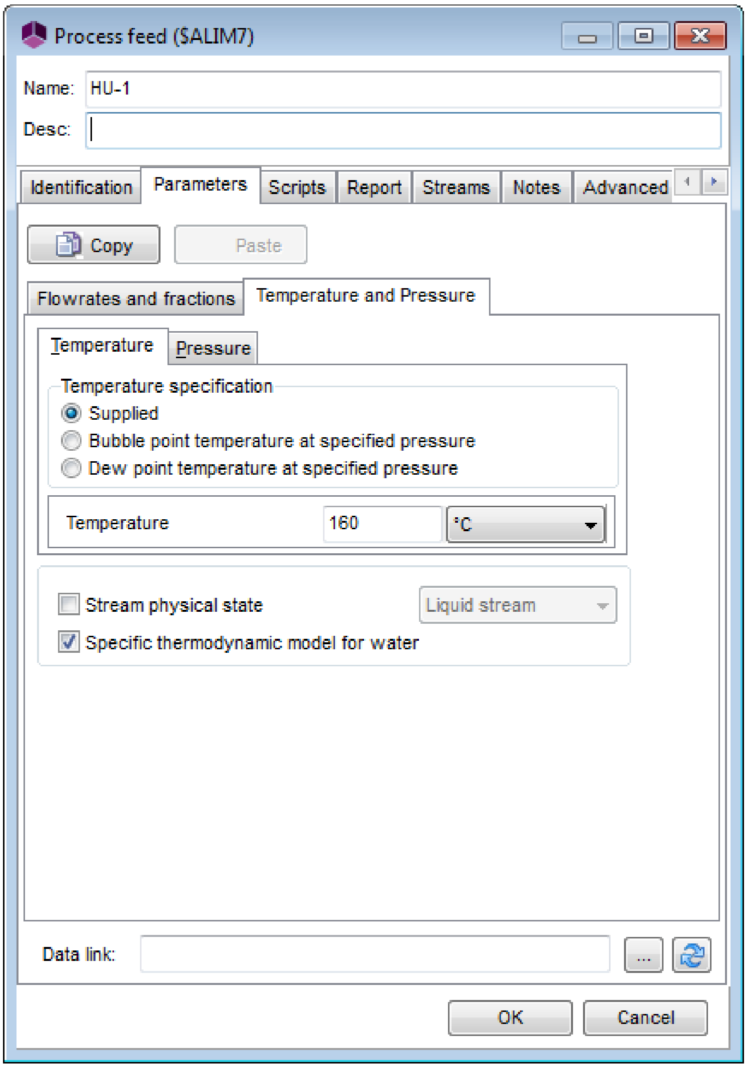
Name	Chemical formulae	CAS number
Carbon dioxide	CO_2	124-38-9
Monoethanolamine	C_2H_7NO	141-43-5
Water	H_2O	7732-18-5
Dinitrogen	N_2	7727-37-9

Monoethanolamine is noted MEA in the rest of this document.

2.4. Thermodynamic model

The system considered contains an alkanolamine, CO_2 (acid gas) and water. The working pressure never exceeds 100 bars. As a consequence, the "Amine and acid gas" model has been chosen [DES81], [WEI93].

The specific thermodynamic model for water is used for the hot and cold utilities calculation (HU and CU). To use this model, the "Specific thermodynamic model for water" box has been ticked in the utility streams (HU-1 and CU-5, 7, 9 and 11) as shown below:



2.5. Operating conditions

All the operating conditions required to define the process are summarized in this part. The data in green are initial values:

- ✓ Flue gas

	Flue gas
CO_2 mass fraction	0.059
H_2O mass fraction	0.043
N_2 mass fraction	0.898
Total mass flowrate (t/h)	3073
Temperature (°C)	100
Pressure (kPa)	101

- ✓ Make-up water

	Make-up water
H_2O mass fraction	1
Total mass flowrate (t/h)	100
Temperature (°C)	15
Pressure (kPa)	301

- ✓ Make-up amine

	Make-up amine
MEA mass fraction	1
Total mass flowrate (t/h)	1
Temperature (°C)	15
Pressure (kPa)	301

✓ Cold utilities (CU) and hot utility (HU)

	DCC CU cooler ***CU-5***	***Desorber condenser*** ***CU-7***	***Water condenser*** ***CU-9***	***Lean amine cooler*** ***CU-11***	***Desorber reboiler*** ***HU-1***
H_2O mass fraction	1	1	1	1	1
Total mass flow rate (t/h)	10 000	1 000	1 500	3 000	1 000
Pressure (kPa)	101	101	101	101	500
Temperature (°C)	15	15	15	15	160

✓ Columns

Operating parameters	***Absorber***	***Desorber***
Column type	Absorber	2-phase distillation column with partial condenser
Number of theoretical stages	5	12
Feed stage	-	2
Vapor distillate flow rate (t/h)	-	189.2
Molar reflux ratio	-	0.4
Reboiler heat duty (kcal/h)	-	Calculated
Column head pressure (kPa)	106	200
Column bottom pressure (kPa)	121	200
Stages efficiency	0.48	0.5*

*: except for the condenser which efficiency is 1

Desorber further specifications:

Specification		***Product type***	***Compound***	***Value***	***Type***	***Action***
1:	Partial flowrate	Vapor distillate	CO_2	154.47 t/h	Mass	Vapor distillate flowrate

To assure the desorber convergence, the maximum damping factor (that can be changed in the numerical parameters in the “Further specifications” tab) has been set to 0.5. The other numerical parameters are the default ones.

✓ Separators

Operating parameters	*Direct Contact Cooler DCC*	*Water separator*
Separator type	Liquid-vapor separator	Liquid-vapor separator
Pressure (kPa)	121	The lowest of the feed streams
Pressure drop (kPa)	0	0
Heat duty (kcal/h)	Adiabatic	Adiabatic

✓ Generalized heat exchangers

Name	*Type*	*Specification type*	*Specification value*	*Pressure drop (kPa)*	
				1st stream	*2nd stream*
DCC CU cooler	Counter current or multipasses	Hot stream outlet temperature	30°C	179	0
Lean / rich amine heat exchanger	Counter current or multipasses	Minimal internal temperature approach	10°C	300	100
Lean amine exchanger	Counter current or multipasses	Hot stream outlet temperature	40°C	49	0
Water condenser	Counter current or multipasses	Hot stream outlet temperature	60°C	0	0

✓ Other heat exchangers

Name	*Type*	*Outlet temperature (°C)*	*Pressure drop (kPa)*
Reboiler	Cooler/Heater	Bubble temperature	0
Condenser	Simple heat exchanger	25	0

✓ *Compressors*

Operating parameters	*Transport fan*
Exhaust pressure (kPa)	121
Isentropic efficiency	0.8
Mechanical efficiency	1
Electrical efficiency	1

✓ *Pumps*

Operating parameters	***Pump***	***Rich amine pump***	***Lean amine pump***
Exhaust pressure (kPa)	301	750	700
Volumetric efficiency	0.75	0.75	0.75
Mechanical efficiency	1	1	1
Electrical efficiency	1	1	1

✓ *Mixers*

Operating parameters	***Mixer***
Outlet pressure (kPa)	150

✓ *Pressure drops (expansion valves)*

Operating parameters	**Pressure drop *1***	**Pressure drop *2***
Pressure drop (kPa)	200	299

✓ *Stream splitters*

Operating parameters	***Stream splitter R1***
CU-1 stream mass flowrate (t/h)	6500
Outlet pressure (kPa)	Equal to the feed pressure

✓ *Stream splitters: Make-ups determination*

To determine the make-up flowrates, a “Script” module has been used. The flowrates are determined by the following formulas (simple mass balance):

$$Make\ up\ amine\ = Absorber\ amine\ outlet\ + Condenser\ amine\ outlet$$

$$Make\ up\ water = Absorber\ water\ outlet + Condenser\ water\ outlet - Absorber\ water\ inlet$$

The code (written in VBS language) in the “Script” module that allows to do this calculation is the following one:

```
'-----------------------------------------------------------------------------'
' COMPOUNDS SEARCH TOOL
'-----------------------------------------------------------------------------'

With CreateObject("Scripting.FileSystemObject")
  ExecuteGlobal .OpenTextFile(Project.ApplicationPath & "Scripts\FindCompound.vbs", 1).ReadAll()
End With

'-----------------------------------------------------------------------------'
' MAKE-UP AMINE AND MAKE-UP WATER CALCULATION
'-----------------------------------------------------------------------------'

Function OnCalculation()

' Compounds search

  iWater = FindCompound("7732-18-5")
  iAmine = FindCompound("141-43-5")

' Partial flowrates recovery

  Absorber_Output = "4"
  Desorber_Output = "9"
  Absorber_Input = "3"

  ' Water
  Water_AbsorberInput = Project.Streams(Absorber_Input).PartialMassFlowrate(iWater)
  Water_AbsorberOutput = Project.Streams(Absorber_Output).PartialMassFlowrate(iWater)
  Water_DesorberOutput = Project.Streams(Desorber_Output).PartialMassFlowrate(iWater)

  ' Amine
  Amine_AbsorberOutput = Project.Streams(Absorber_Output).PartialMassFlowrate(iAmine)
  Amine_DesorberOutput = Project.Streams(Desorber_Output).PartialMassFlowrate(iAmine)

' Make-up flowrates calculation

  With Module
  ' Water
   .Parameter(1) = (Water_AbsorberOutput + Water_DesorberOutput) - Water_AbsorberInput
   if .Parameter(1) < 0 Then
      .Parameter(1) = 0
      Msgbox "Débit d'appoint d'eau calculé négatif"
   end if
   ' Amine
   .Parameter(2) = Amine_AbsorberOutput + Amine_DesorberOutput
  End With

' Calculation validation
  Oncalculation = True

End Function
```

A part of the data required for the elaboration of this example comes from the KALLEVIK work [KAL10]. The specifications to calculate the utility flowrates are given in the **2.6 Utility consumption determination** part.

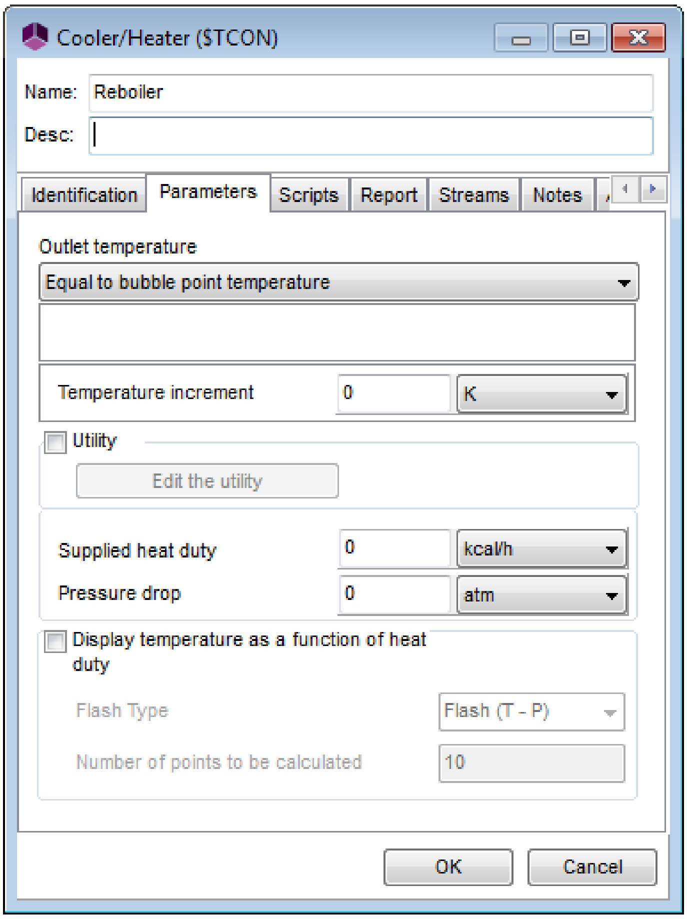
2.6. Utility consumption determination

The physical characteristics of the utility feeds are gathered in the corresponding table of the **2.5 Operating conditions** part.

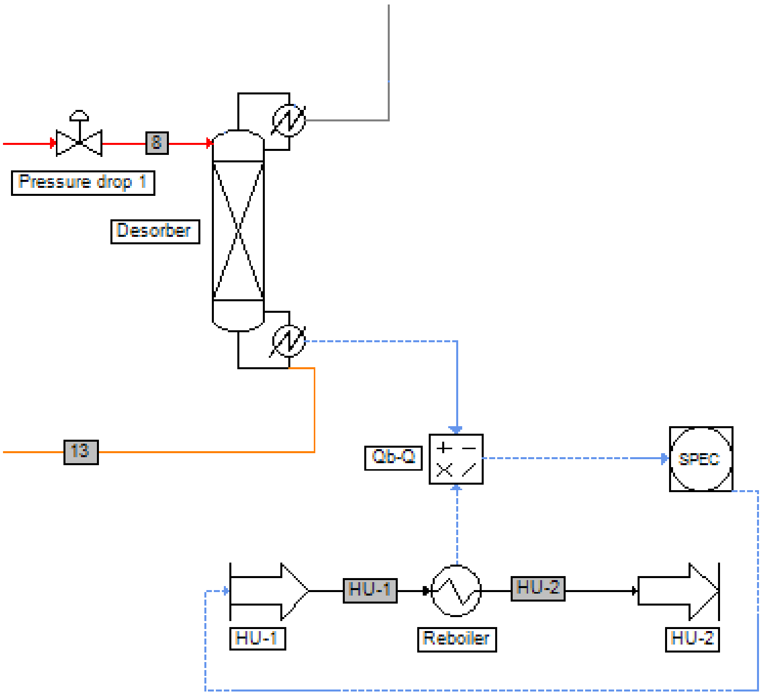
Hot utility

The desorber reboiler has been simulated with a “Cooler/Heater” unit operation. We use overheated water vapor at 160°C and 500 kPa. At the reboiler outlet, we impose the temperature to be the bubble temperature.

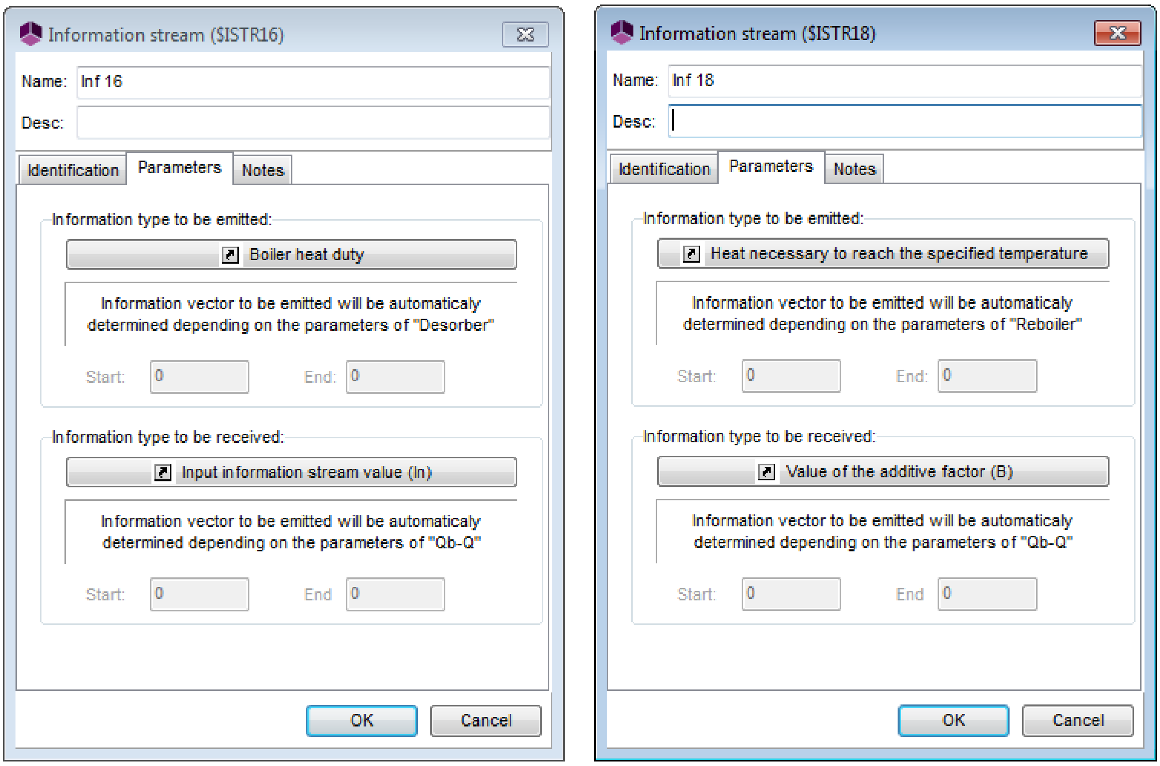
The following screenshot contains the configuration entered in the reboiler:



To determine the necessary hot utility flowrate, we use a SPEC block unit as presented below:

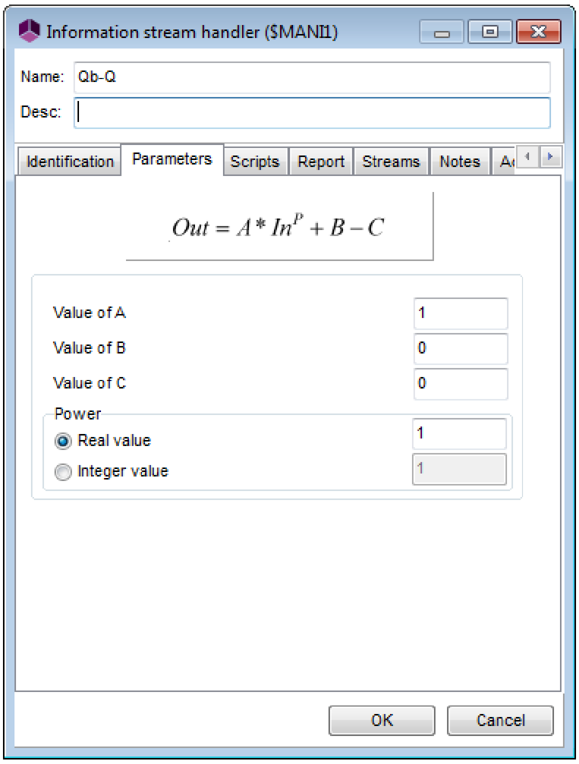


The approach is the following one: we take the heat duty values of the desorber reboiler and the “Cooler/Heater” unit operation using information streams. The configuration of these information streams is presented below:

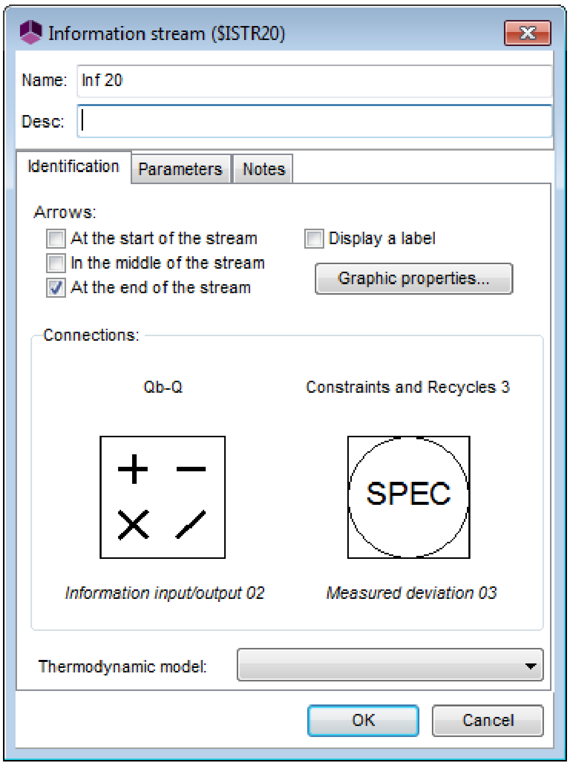


In the information stream handler we want to calculate the difference between the boiler heat duty (In) and the heat duty (B) of the related “Cooler/Heater” unit operation.

The reboiler heat duty is positive and the related “Cooler/Heater” heat duty is negative. The information stream handler has then to be configured as follows:



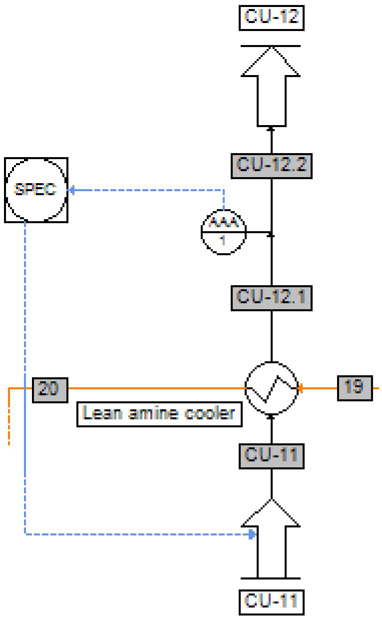
The difference between the reboiler heat duty of the column and the one calculated in the related “Cooler/Heater” unit operation is then sent to the SPEC block unit. This SPEC block unit is linked to the hot utility feed unit operation by an information stream configured as follows:



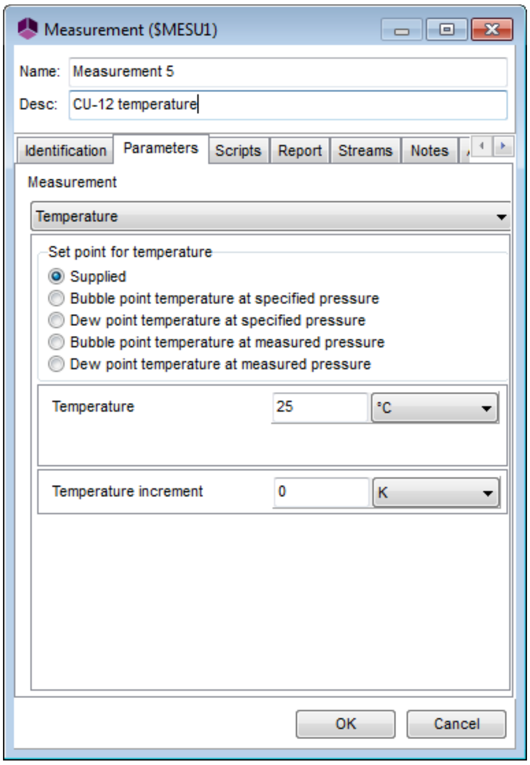
So the SPEC block unit will adjust the hot utility flowrate in order to cancel the difference between the heat duties. This way, the “Cooler/Heater” unit operation will represent the boiler and the calculated utility flowrate will correspond to the utility flowrate circulating in the reboiler.

Cold utilities:

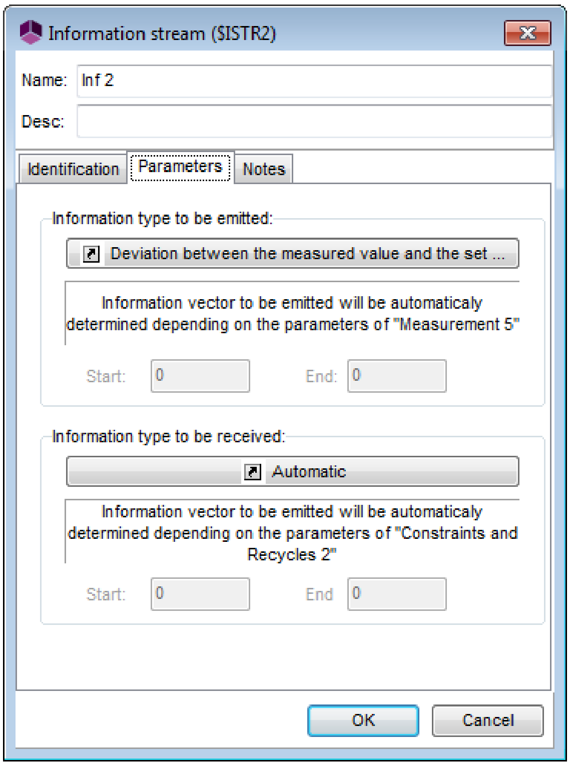
The cold utility used in the process is water at 15°C and 101 kPa. We impose the cold utility temperature at the exchanger outlet to be 25°C. To do so, we use a SPEC block unit as illustrated below in the case of the lean amine cooler:



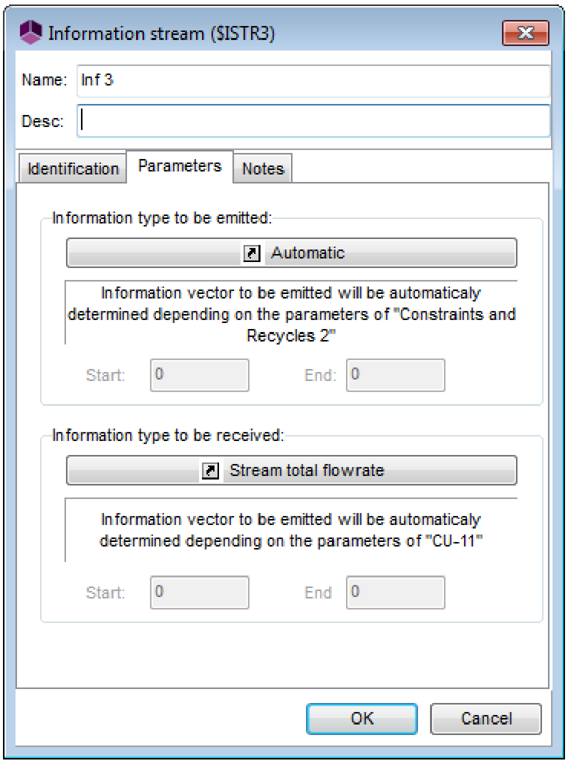
The Measurement block unit contains the set point for the utility outlet temperature and is configured as follows:



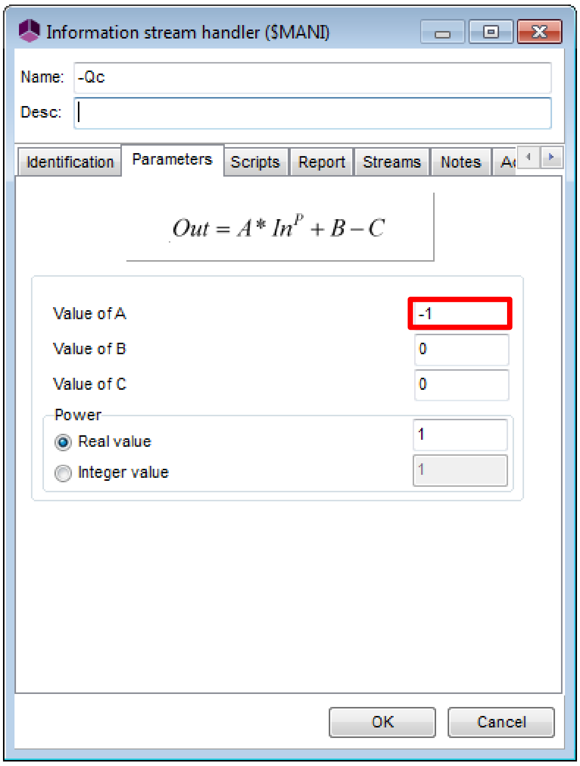
The information stream leaving the measurement block unit and entering in the SPEC block unit conveys the difference between the cold utility stream outlet temperature and the set point for temperature. The configuration of this information stream is then the following one:



In order to adjust the cold utility flowrate to have the set point for temperature at the exchanger outlet, the SPEC block unit is linked to the cold utility feed unit operation with an information stream configured as follows:

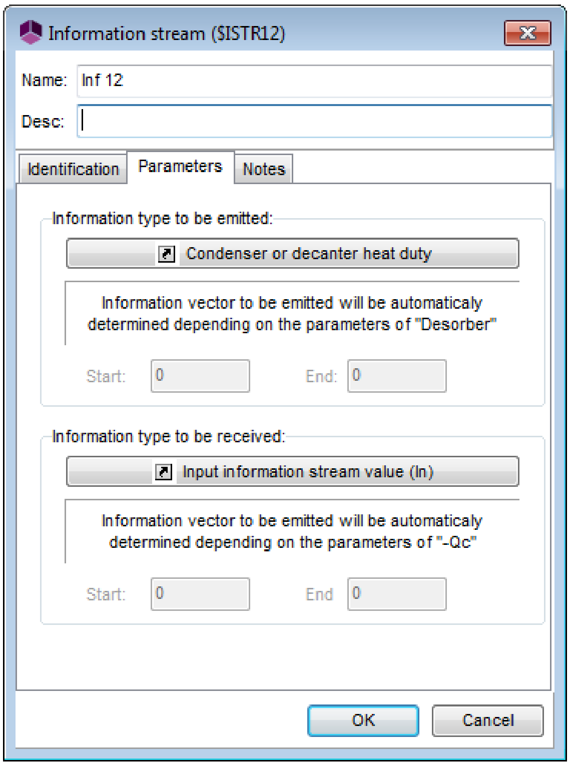


Remark: the condenser has been simulated with a simple heat exchanger. To make this exchanger representative of the condenser, the condenser heat duty value calculated in the desorber has to be sent to the simple heat exchanger. The exchanger requires a negative heat duty in the case of a heating (here cold utility heating) but the value obtained from the desorber is negative. A stream handler has then to be used and configured as follows to respect this sign rule:

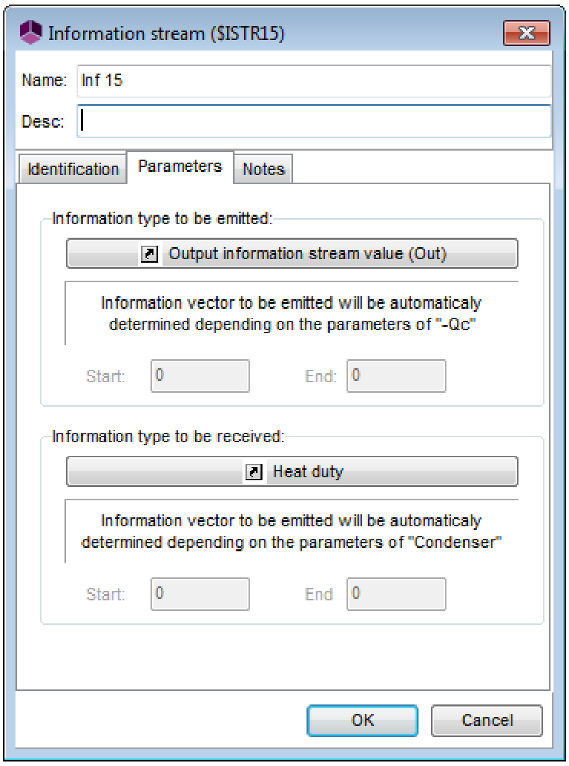


The information streams leaving and entering the stream handler are configured as follows:

Entering stream:



Leaving stream:



3. Simulation results

3.1. Comments on results

The calculation sequence (order of calculation of the unit operations) is automatically generated. The tear streams “14” and “20” are initialized with the following characteristics:

	CU-1	*“14”*	*“20”*
CO_2 mass fraction	0	0.055	0.055
MEA mass fraction	0	0.3	0.29
H_2O mass fraction	1	0.645	0.655
N_2 mass fraction	0	0	0
Total mass flowrate (t/h)	6500	3500	3600
Temperature (°C)	25	115	40
Pressure (kPa)	101.325	700	101

3.2. Mass and energy balances

This document only presents the most relevant stream results. In ProSimPlus, mass and energy balances are provided for every stream. Results are also available at the unit operation level (result tab in the configuration window).

Inlet/outlet stream (except utilities):

Streams		1	4	11	12	17	18	R-1
From		1-Flue gas	Absorber	Water separator	Water separator	17-Make up water	18-Make up amine	R1
To		Transport fan	4-Flue gas to atmosphere	11-Recovered CO2	12-Make up water	Mixer	Mixer	R-1
Partial flows		t/h	t/h	t/h	t/h	t/h	t/h	t/h
CARBON DIOXIDE		181.3	26.8	154.4	0.0	0	0	0
MONOETHANOLAMINE		0	1.0	0	0	0	1	0
WATER		132.1	204.7	7.2	21.6	110.6	0	9
NITROGEN		2759.6	2759.5	0	0	0	0	0
Total flow	t/h	3073.0	2992.0	161.6	21.6	110.6	1.0	9.3
Mass fractions							0	0
CARBON DIOXIDE		0.059	0.009	0.956	0.001	0	0	0
MONOETHANOLAMINE		0	3E-04	0	1E-04	0	1	0
WATER		0.043	0.068	0.044	0.999	1	0	1
NITROGEN		0.898	0.922	2E-04	6E-09	0	0	0
Physical state		Vapor	Vapor	Vapor	Liquid	Liquid	Liquid	Liquid
Temperature	°C	100	46	60	60	15	15	30
Pressure	kPa	101	106	200	200	301	301	122
Enthalpic flow	MW	-874.9	-812.0	-408.9	-94.9	-491.9	-1.1	-41.3
Vapor molar fraction		1	1	1	0	0	0	0

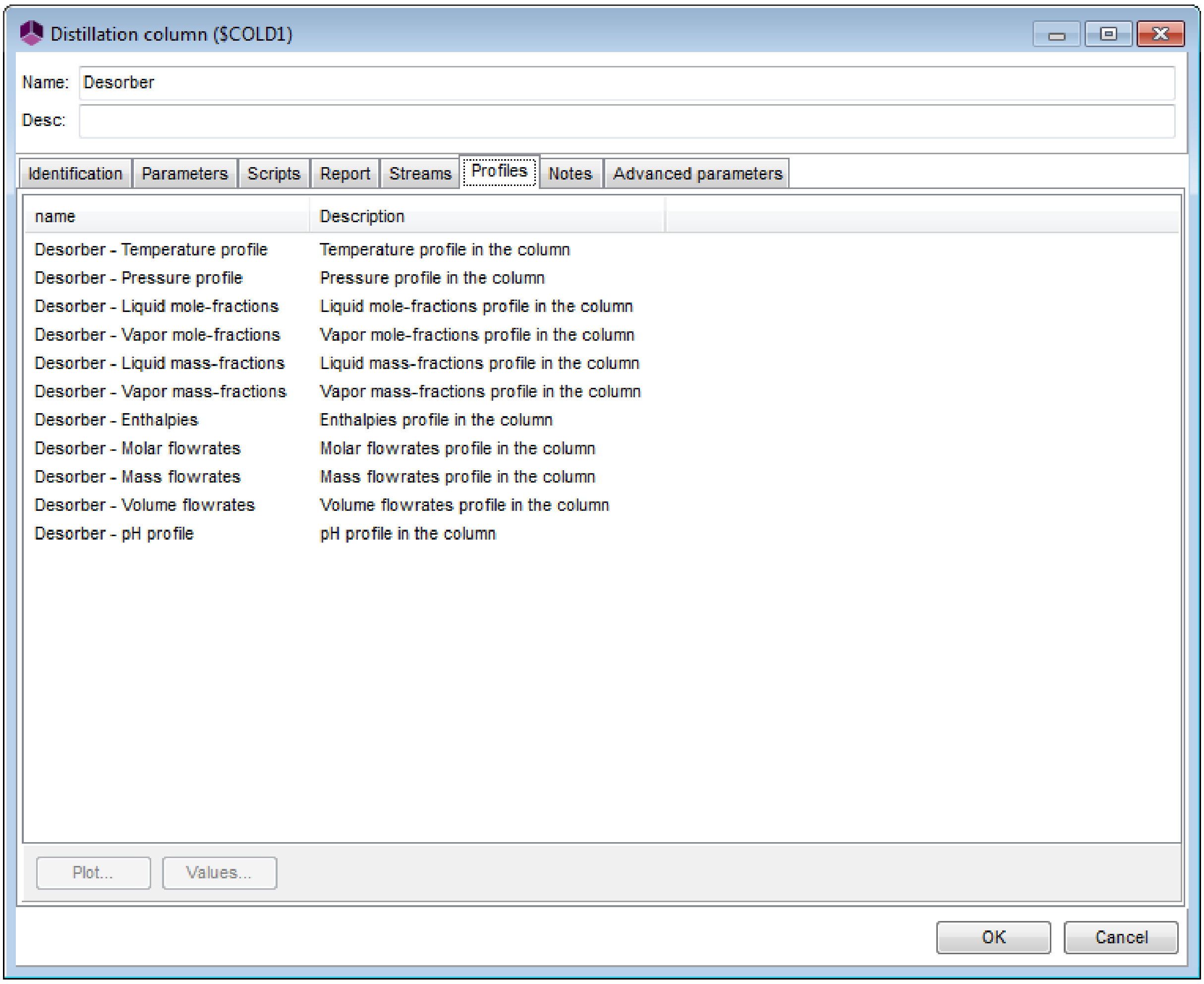
Inlet/outlet stream (utilities):

Streams		CU-5	CU-6.2	CU-7	CU-8.2	CU-9	CU-10.1
From		CU-5	Measurement 2	CU-7	Measurement 7	CU-9	Water condenser
To		DCC CU cooler	CU-6	Condenser	CU-8	Water condenser	Measurement 8
Partial flows		t/h	t/h	t/h	t/h	t/h	t/h
WATER		7 207.8	7 207.8	2 158.0	2 158.0	1 384.5	1 384.5
Total flow	t/h	7207.8	7207.8	2158.0	2158.0	1384.5	1384.5
Mass fractions							
WATER		1	1	1	1	1	1
Physical state		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	°C	15.0	25.0	15.0	25.0	15.0	25.0
Pressure	kPa	101	101	101	101	101	101
Enthalpic flow	MW	-4 974	-4 891	-1 489	-1 464	-955	-939
Vapor molar fraction		0	0	0	0	0	0

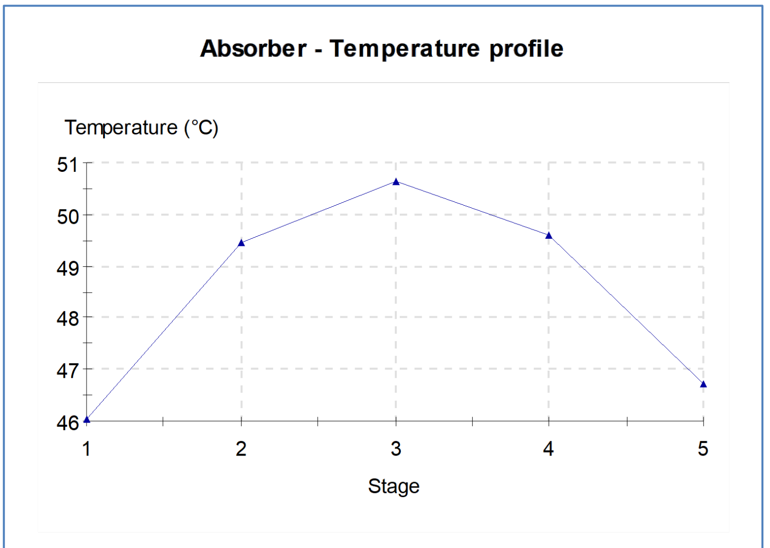
Streams		CU-11	CU-12.2	HU-1	HU-2
From		CU-11	Measurement 5	HU-1	Reboiler
To		Lean amine cooler	CU-12	Reboiler	HU-2
Partial flows		t/h	t/h	t/h	t/h
WATER		4 781.5	4 781.5	283.0	283.0
Total flow	t/h	4781.5	4781.5	283.0	283.0
Mass fractions					
WATER		1	1	1	1
Physical state		Liquid	Liquid	Vapor	Liquid
Temperature	°C	15.0	25.0	160.0	151.9
Pressure	kPa	101	101	500	500
Enthalpic flow	MW	-3 300	-3 244	17	-150
Vapor molar fraction		0	0	1	0

3.3. Colum profiles

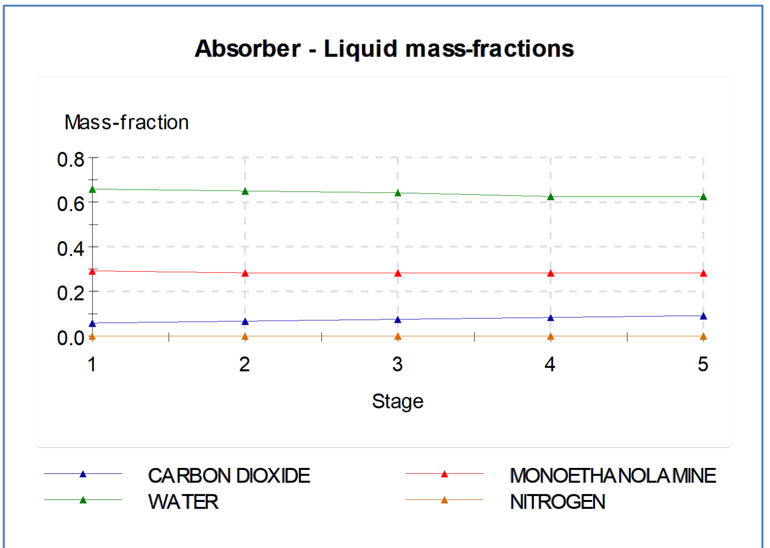
Composition profiles can be accessed after the simulation in each column configuration window, in the "Profiles" tab. Double clicking on the profile will generate the corresponding graph. It is important to note that, in ProSimPlus, the first stage corresponds to the top stage and the last stage to bottom stage (respectively the condenser and the reboiler in the case of a distillation column).



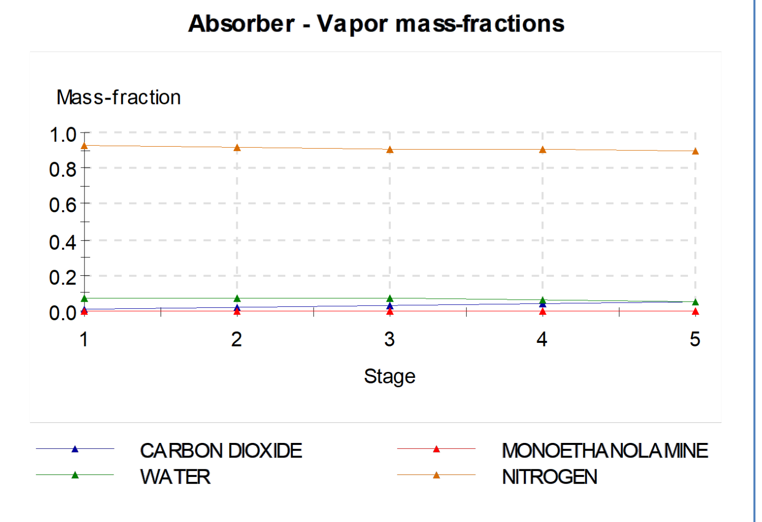
Absorber



Temperature profile in the column



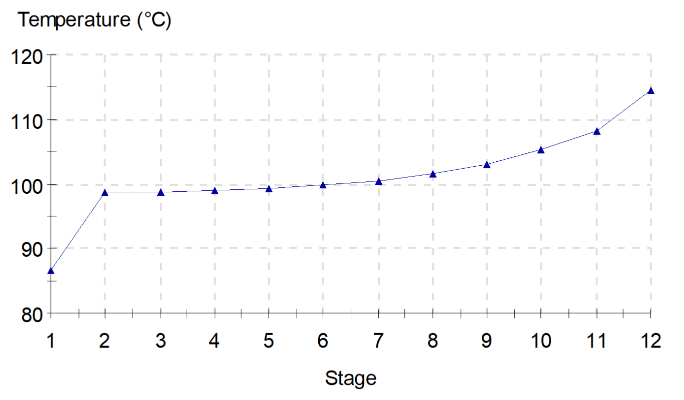
Liquid mass-fractions profile in the column



Vapor mass-fractions profile in the column

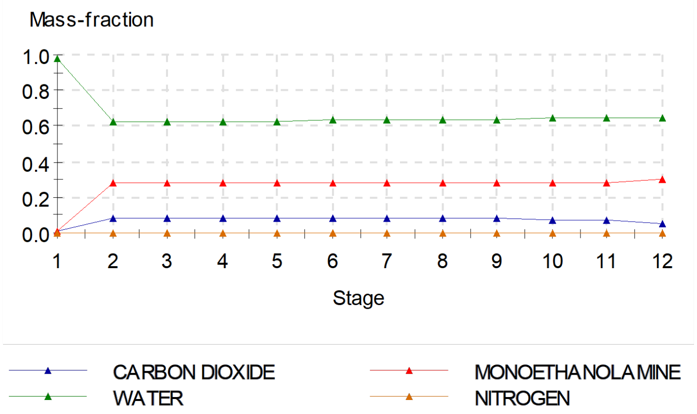
Desorber

Desorber - Temperature profile



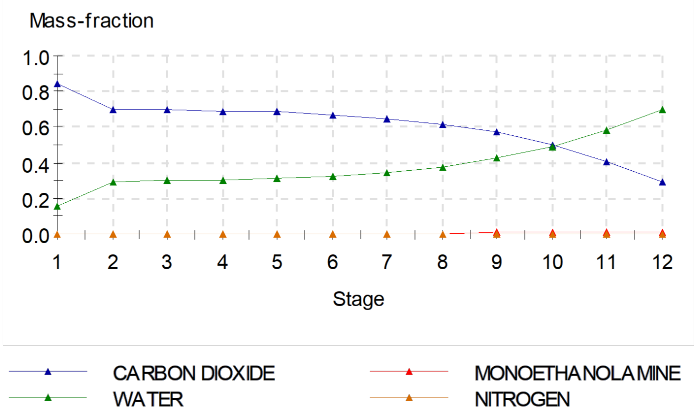
Temperature profile in the column

Desorber - Liquid mass-fractions



Liquid mass-fractions profile in the column

Desorber - Vapor mass-fractions



Vapor mass-fractions profile in the column

4. References

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