# Getting started with BatchColumn®

#### Use Case 1: Simulation of solvents mixture separation

Software & Services In Process Simulation



We guide You to efficiency

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# Introduction

This document presents the different steps to follow in order to simulate a batch distillation using BatchColumn software.

This presentation is based on an example of separation of the following solvents mixture: methanol / acetone / dichloromethane / diacetone alcohol. This example is available on ProSim website (<u>www.prosim.net</u>) or in the BatchColumn example directory.

The summary of this Getting Started is:

- Part 1 Description of the example
- Part 2 General points on the software interface
- Part 3 Description of the different simulation steps

### Part 1

- Description of the example:
  - Objective of the distillation
  - Compounds and thermodynamic model
  - Description of the equipment
  - Operating scenario

# **Objective of the distillation**

The boiler is loaded with a solvent mixture including methanol (19.45 wt%), acetone (21.96 wt%), dichloromethane (56.29 wt%) and diacetone alcohol (2.3 wt%). The initial load is 6090 kg.

The objective is to simulate the recovering of:

- Dichloromethane with a purity of 95 wt  $\!\!\!\!\%$
- Acetone with a purity of 90 wt%
- Methanol with a purity of 98 wt%

### **Compounds and thermodynamic model**

The compounds involved in this distillation are:

- -Methanol
- -Acetone
- -Dichloromethane
- -Diacetone alcohol

The thermodynamic model selected is NRTL.

The binary interaction parameters of the methanol - acetone binary are automatically loaded. For a better accuracy, they should be replaced by those of the table below. There are also the other binaries to fill in. The binary interaction parameters, expressed in cal/mol.

Methanol-Acetone	-12.37	290.51	0.3085
Methanol-Dichloromethane	74.14	1517.35	0.4830
Acetone-Dichloromethane	-725.20	641.70	0.35
Acetone-Diacetone alcohol	2127.96	-1624.17	0.2908

# **Description of the equipment**

Four tanks are connected to the condenser for distillation recovery: tank 1, tank 2, tank 3, tank 4.

The column characteristics are:

- 32 theoretical plates (including boiler and condenser)
- Liquid holdups are 15 l for the condenser and 2.5 l per tray
- The heat duty is assumed to be constant at 500 000 kcal/hr
- The condenser is an ideal total condenser.

### **Operating mode**

The column head pressure is 100 mmHg. Pressure drop is 10 mmHg. <u>Dichloromethane recovery</u>

- Step 1: Filling-up the column. Initial load temperature is 0°C
- Step 2: Distillate to tank 1 with a reflux ratio = 2 Final event: 2000 kg of product in tank 1
- Step 3: Distillate to tank 1 with a reflux ratio = 5 Final event: 2800 kg of product in tank 1
- Step 4: Infinite reflux

Final event: time duration = 30 minutes

Step 5: Distillate to tank 1 with a reflux ratio = 5

Final event: dichloromethane weight fraction in tank 1 < 0.96

Step 6: Infinite reflux

Final event: time duration = 30 minutes

Step 7: Distillate to tank 1 with a reflux ratio = 5

Final event: dichloromethane weight fraction in tank 1 < 0.95

## **Operating mode**

#### Intermediate cut

Step 8: Distillate to tank 2 with a reflux ratio = 5

Final event: acetone weight fraction in distillate > 0.96

Acetone recovery

Step 9: Distillate to tank 3 with a reflux ratio = 5 Final event: 800 kg of product in tank 3

Step 10: Infinite reflux

Final event: time duration = 30 minutes

Step 11: Distillate to tank 3 with a reflux ratio = 5

Final event: acetone weight fraction in tank 3 < 0.90

Methanol recovery

Step 12: Distillate to tank 4 with a reflux ratio = 2 Final event: residual load in the boiler < 150 kg

# Part 2

- General points on the software interface:
  - The main window
  - Using the toolbar
  - Choosing the unit system
  - Creating a new simulation file

# The main window



#### **Configuration panel**

Validation system

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# Using the toolbar

Preferences of the software



# Using the toolbar



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# Choosing the unit system



- 1- Select the predefined system "ISO" and click on "Apply system"
- 2- For a given quantity you can change the default unit to another one by clicking on its name

3- Click on "OK" to validate

	Use this window to modify the un application. Quantity	it system used by you △ Unit	Jr
Choose a predefined unit system in this list and	(Obsolete - Not used) Heat capaci	tv J/kg/K	+
click "Apply system" to use theses units in your	Amount of substance	mol	
	Angle	•	
ISO	Area	m2	
ProSim	Density	kg/m3	
British	Dipole moment	D	
Application default	Dynamic viscosity	Pa.s	
	Electric current	А	
	Electric potential	V	
	Electric resistance	Ohm	
	Energy	eV	
Apply system	Enthalpic flow	J/s	
	Entropic flow	J/s/K	
00ls ——— 🔺	Frequency	Hz	
Copy to the cliphoard	Heat exchange coefficient	W/m2/K	
Copy to the cipboard	Henry constant	mol/l/atm	
Paste from the clipboard	Joule-Thomson coefficient	K/atm	

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# Creating a new simulation file



## Description of the different simulation steps

- 1: Selecting the compounds
- 2: Selecting the thermodynamic model
- 3: Describing the chemical reactions
- 4: Describing the distillation system
- 5: Describing the operating steps
- 6: Running the simulation
- 7: Reviewing the simulation results

# **1-Selecting the compounds**



# **1-Selecting the compounds**



# **1-Selecting the compounds**

7- The compounds imported from the database are listed here.



#### 2-Selecting the thermodynamic model

1- Click on the "Model" tab to open the thermodynamic models configuration window.

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

COMPOUNDS MODEL PARAMETERS

2- All thermodynamic models available are listed here. — Use the scroll bar to go through the complete list. Select NRTL as the model to be used in this example.



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### 2-Selecting the thermodynamic model



### 2-Selecting the thermodynamic model

Thermodynamic calculator editor										-		×
	This window help	os you to define the co	ontext of yo	ur thermodyna PARAMETEF	mic calculator RS							
Save as	These parameter profile)	s correspond to the g	eneral value	es and are used	if the user ha	s not provide	d specific para	meters (buttons	to the right of	f each option in the th	ermodynam	ic
PACKAGE	Binaries view:		atrix		272 15)							_
SERVICES	Compound	- gjj = cij0 + cij1 (i -	275.15), alj 1		- 2/5.15)	CUT	CIT	aiiT		BINARIES		
Calculate	METHANOL	ACETONE	-12.37	290.51	0.3085	0	0	0	ACTI	ONS		
Fyport as a DSE file	METHANOL	DICHLOROMETHAI	74,14	1517,35	0,483	0	0	0	6	Import hiparies		
	METHANOL	DIACETONE ALCOH	0	0	0	0	0	0				
Diagrams	ACETONE	DICHLOROMETHAI	-725,2	641,7	0,35	0	0	0	<b>U</b>	Clear all binaries		
🔀 Residue	ACETONE	DIACETONE ALCOH	2127,96	-1624,17	0,2908	0	0	0	画	Estimate binaries		
👍 Export as a PVT file	DICHLOROMETH	A DIACETONE ALCOH	0	0	0	0	0	0	- 6	Save the binaries		
Stream									OPTI	IONS		
🧏 Sigma profiles									Unit			
MODIFICATIONS									cal/	mole	•	
									p	arameters will be igno	ored	
									<b>M</b> p	arameters are automa	ticcaly loade	d
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Comments												
Calculator type												
Native												
Show the expert mode	Not supplied	Supplied	mported	Estimated	i Erro	Dr						
										Ok	Cancel	

5- You can enter your binary interaction parameters.

Click on "OK" at the bottom to exit the thermodynamic calculator



For more information about the compounds selection and the configuration of the thermodynamic profile, please consult "Getting started with Simulis Thermodynamics" documents.

# **3-Describing the chemical reactions**

There is no chemical reaction involved in this example. But if it is the case, they can be described as follows.

- 1- Click on "Edit the chemical reactions..." to open the chemical reactions editor
- 2- Select "Add a reaction"





The main flowsheet window allows to display the distillation system (inlet and outlet storages, boiler, column and condensing system) and directly access the different configuration windows.

1- Enter the number of theoretical

stages

File	Edit View Configuration Simulation Element:	Shapes Tools Help	
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2	🍭 🛶 🤹 🔁 🔁 🔶 - 🗎	Image: The step in	
	Flowsheet		
	Flowsheet 🗵		
3	Number of theorical stages	100	
	32		
	Internals		
	Plate 💌		
	Use of middle-vessels		
	Vith a decanter		
	Vessel bottom geometry is known		
	Torispherical		
	Vith a mixing device		
	4 straight flat-blades turbine		
	Vith an external heat exchanger		
	Vith an helical coil		
	With a wall neat exchanger		
	External Jacket		
		Tachta ann	

#### 2- Select the main items of the column:

$\backslash$	Flowsheet		
	Flowsheet 🗙		
	Number of theorical stages		
$\backslash$	32		
$\backslash$	Internals		
4	Plate 💌		$\square$
	Use of middle-vessels		
	└─ /Vith a decanter		
	Vessel bottom geometry is known		
	Torispherical		
	Vith a mixing device		
	4 straight flat-blades turbine		
	With an external heat exchanger		
	└ /\/ith an helical coil		
	└ With a wall heat exchanger		
	VVith an inductor		M
	External jacket		
			BalchColumn

#### 4.1- Liquid tanks

1- Double click on the first liquid tank to open the configuration window and add the other tanks TL02, TL03, TL04

Name:	Available liquid tanks (Top)			Condenser
Paramet Tanks Type I	ers Notes Validation	st		
TL01			^	
TL03				
TL04				
<u> </u>			 _	
			_	



1 - Double click on the column icon



2 - Click on "Hold-up"



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4.2- Column

	Nold-up Parameters	/alidation			-		×
Entor hold up for the	Hold-up type Condenser		Volume 15 I	~	Use of middle-vessels		
condenser and the stages (hold-up per stage)	Stage 1 2	Stage 2 31	Value 2.5 I		Stage		
	Restore				<u>о</u> к	<u>C</u> an	cel

#### 4.2- Column





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(Warning: in any case, the boiler efficiency should be kept equal to 1)

#### 4.2- Column 🔔 Initial load × Initial load Fractions Mass V Click on "Initial load" p • h 4 = x/Σ Column -× Name: Column Compound Fraction Parameters Notes Advanced parameters 🚱 Validation METHANOL 0.1945 Stage ACETONE 0.2196 umber of theoretical stages 33 DICHLOROMETHANE 0.5629 DIACETONE ALCOHOL 0.023 Hold-up Pressure profile Consta Gas sidestreams Liquid sidestreams Efficiencies Liquid tank Stage 1.00000 QK Cancel Restore 6090 kg Total mass load -<u>o</u>ĸ Restore Cancel Enter composition and mass of the initial load

#### 4.2- Column

ļ	Column —							
1	Name: C	olumn						
F	Parameters	Notes	Advanced parameters	Validation				
				1				
	Path					Message		

Select the validation tab.

This tab displays the warning and error messages. If the input data is correctly provided, this tab should be empty and the distillation icon should not be highlighted anymore.

The distillation icon is not

#### 4.2- Column



The global validation system reports other missing or inconsistent information. It is normal since your file is still being configured.







1- Select the first step (dout A new tab appears, for the	3- Double click on the column icor	
	2- Change the default name t	by Step 1
Scenario	Flowsheet Step 1          Filling step         Step name:         Plate         Use of middle-vessels         With a decanter         Vessel bottom geometry is known         Torispherical         With a mixing device         4 straight flat-blades turbine         With an external heat exchanger         With an inductor         External jacket	
		Burricham.


	Condenser			-	×
Condenser	Name: Condenser				
	Parameters Notes 📀 Validation				
	State parameters				
	Condenser type Idea	l total condenser	~		
	In use stages 1	×			
ect "Ideal total condenser"	1st used stage				
ault option)	Calculation type At specified area and exchange coefficient:		coefficient	✓ Duplicate	
	Exchange coefficient	0 W/m2/K	Number of calculation steps	10	
	Exchange area	0 m2	Fouling factor (TUBES side)	0 W/m2/K	
	Pressure drop	0 Pa	Fouling factor (SHELL side)	0 W/m2/K	
	Utility fluid				
	Fluid type	Water 🗸	Point number	2	
	Inlet temperature	298.15 K	Mass flowrate	0 kg/s	
	Point #1		Point #2		
	Reference temperature	298.15 K	Reference temperature	298.15 K	
	Mass specific heat	0 J/kg/K	Mass specific heat	0 J/kg/K	
	Density	0 kg/m3	Density	0 kg/m3	
	Dynamic viscosity	0 Pa.s	Dynamic viscosity	0 Pa.s	
	Thermal conductivity	0 W/m/K	Thermal conductivity	0 W/m/K	
	Technology				
	P		-		





Right click on the first step, select "Duplicate to" sub-menu and then select "Distillation step".

This copy avoids to specify again most of the input parameters for this new step.

Connect appropriately the new step to the ending event of the first step













Right click on the second step and select "Duplicate"

This copy avoids to specify again most of the parameters for this new step.

Connect the new step to the ending event of the second step



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4- Select "constant value" and enter the reflux ratio









Right click on the third step and select "Duplicate to", then select "Step at infinite reflux".

This copy avoids to specify again most of the parameters for this new step.

Connect the new step to the ending event of the third step.





🔔 Column \_ × Name: Parameters Notes Advanced parameters 🚫 Validation Step at infinite reflux Operating mode Reflux flowrate Constant heat duty  $\sim$ 4- Nothing to change in this window since this Profile of heat losses step has been duplicated Gas sidestreams Liquid sidestreams Profile of heat inputs Flowrates Molar from the previous one, Reactive stages Liquid tank Used Flowrate the boiler duty is already defined as for the step 3 Volume Controls Boiler duty Constant value ~ - 500000 kcal/h -Tolerances Thermodynamic calculator Default calculator Restore <u>0</u>K Cancel





Right click on the third step and select "Duplicate".

This copy avoids to specify again most of the parameters for this new step.

Connect the new step to the ending event of the fourth step









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Right click on the fourth step and select "Duplicate".

This copy avoids to specify again most of the parameters for this new step.

Connect the new step to the ending event of the fifth step



ouble click on the last ste	p 2- Enter the name: STEP 6	3- Double click on the colu
	$\backslash$	$\backslash$
Scenario	Flowsheet STEP 6	
	Step at infinite reflux       Step name:       STEP 6       Number of theorical stages       32       Internals       Plate	
	Use of middle-vessels With a decanter Vessel bottom geometry is known Torispherical With a mixing device	
STEP 4	4 straight flat-blades turbine      With an external heat exchanger      With an helical coil      With a wall heat exchanger      With an inductor      External jacket	
		isenficiare.

🕭 Column \_ × Name: Parameters Notes Advanced parameters 🐼 Validation Step at infinite reflux Reflux flowrate Operating mode Constant heat duty  $\sim$ 3- Nothing to change in this window since this step has Profile of heat losses been duplicated from step Gas sidestreams Liquid sidestreams Profile of heat inputs 4, which is identical to Flowrates Molar  $\sim$ Reactive stages step 6. The boiler duty is Liquid tank Flowrate Used already defined. Volume Controls ~ - 500000 kcal/h -Tolerances Boiler duty Constant value Thermodynamic calculator Default calculator ~ Restore <u>0</u>K Cancel





Right click on the fifth step and select "Duplicate".

This copy avoids to specify again most of the parameters for this new step.

Connect the new step to the ending event of the sixth step



You may want to align the icons on the left side of the window in order to have the new step at the top right side.

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Right click on the step 7 and select "Duplicate ".

This copy avoids to specify again most of the parameters for this new step.
Connect the new step to the ending event of the step 7













Right click on the step 8 and select "Duplicate ". This copy avoids to specify again most of the parameters for this new step.

Connect the new step to the ending event of the step 8













Right click on the step 6 and select "Duplicate".

This copy avoids to specify again most of the parameters for this new step.

Connect the new step to the ending event of the step 9.





🔔 Column \_  $\times$ Name: Notes Advanced parameters 🐼 Validation Parameters Step at infinite reflux Reflux flowrate Operating mode Constant heat duty  $\sim$ 4- Nothing to change in this window since this step has Profile of heat losses been duplicated from step Gas sidestreams Liquid sidestreams Profile of heat inputs 6, which is identical to Flowrates Molar V Reactive stages Liquid tank Used Flowrate step 10. The boiler duty is already defined. Volume Controls -Boiler duty Constant value ~ - 500000 kcal/h Tolerances Thermodynamic calculator Default calculator Restore <u>0</u>K Cancel





Right click on the step 9 and select "Duplicate".

This copy avoids to specify again most of the parameters for this new step.

Connect the new step to the ending event of the step 10





🕭 Column × \_ Name: Parameters Notes Advanced parameters 🐼 Validation Reflux ratio Constant value ~ 5 **Distillation step** Operating mode Reflux flowrate Constant heat duty  $\sim$ 4- Nothing to change in this window since this step has Profile of beat losses been duplicated from step Gas sidestreams Liquid sidestreams Profile of heat inputs 9, which is identical to Flowrates Molar Reactive stages step 11. The boiler duty is Liquid tank Used Flowrate already defined as well as the reflux ratio. Volume Controls -~ - 500000 kcal/h Tolerances Boiler duty Constant value Thermodynamic calculator Default calculator Restore <u>o</u>ĸ Cancel





Right click on the step 11 and select "Duplicate". This copy avoids to specify again most of the parameters for this new step.

Connect the new step to the ending event of the step 11











1- Double click on the event at the end of the step 12

	Parameters Priority Notes 🧭 Validation			
<ul><li>2- Enter a name for the event</li><li>3- Select "total load inside the boiler"</li></ul>	Event type Time spent since beginning of simulation Time spent since beginning of step Reflux ratio Production of a component inside a tank Total production inside a tank Temperature at a stage Fraction inside the distillate			
<ul> <li>4- Enter the desired mass load inside the boiler.</li> <li>Select "&lt;" to indicate that the event should be reached by</li> </ul>	<ul> <li>Fraction inside a tank</li> <li>Fraction inside the boiler</li> <li>Fraction at a stage</li> <li>Load of a component inside the boiler</li> <li>Total load inside the boiler</li> <li>Liquid distillate flowrate</li> </ul>			
decreasing value.	Total load <  V Mass  V 150 kg  V			
5- Click on "OK"	OK Cancel			

Event

Information

×



Finally, connect the last event to the end of the simulation

# 6-Running the simulation



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# 6-Running the simulation

#### The following window displays in real time the process operating parameters:



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# 6-Running the simulation

The following window displays in real time the process operating parameters:



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Condenser temperature Top temperature Boiler temperature

Condenser pressure

Once the simulation is complete, click on "Open the graph report" to analyze the evolution as a function of time of the variable parameters (pressure, temperature, flowrates, compositions, heat duties, physical properties, etc...)

Temperatures - Pressure

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#### Mass fractions in the distillate







Click here to access the simulation report in MS-Excel format. It includes the evolution of the process variables as a function of time

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2413	Time (h)	Liquid volume (m3)	Feed flowrate (kg/h)	Liquid sidestream (kg/h)	Vapor sidestream (kg/h)	Vapor distillate (kg/h)	liquid distillate (kg/h)	Reflux (kg/h)
2414	1.67E-04	2.2278891	1	0	0	1.0052927	0	2.00E-02
2415	1.67E-02	2.2286754	1	0	0	1.3371409	0	2.73E-02
2416	3.33E-02	2.230627	1	0	0	1.5397891	0	3.36E-02
2417	5.00E-02	2.2332999	1	0	0	1.6559845	0	3.94E-02
2418	6.67E-02	2.2364167	1	0	0	1.7185781	0	4.53E-02
2419	8.33E-02	2.239802	1	0	0	1.7493801	0	5.13E-02
2420	0.1	2.243351	1	0	0	1.7614792	0	5.76E-02
2421	0.116667	2.2470044	1	0	0	1.7625298	0	6.43E-02
2422	0.133333	2.2507285	1	0	0	1.757826	0	7.16E-02
2423	0.15	2.2544892	1	0	0	1.7492106	0	7.94E-02
2424	0.166667	2.2582715	1	0	0	1.7412496	0	8.80E-02
2425	0.183333	2.2620693	1	0	0	1.7278169	0	9.70E-02
2426	0.2	2.2658796	1	0	0	1.7193188	0	0.10702215
2427	0.216667	2.2697004	1	0	0	1.7098734	0	0.11781666
2428	0.233333	2.2735296	1	0	0	1.7007094	0	0.12949264
2429	0.25	2.2773661	1	0	0	1.6923622	0	0.14214939
2430	0.266667	2.2812092	1	0	0	1.6844712	0	0.15582606
2431	0.283333	2.2850585	1	0	0	1.6773023	0	0.17061809
2432	0.3	2.2889139	1	0	0	1.6706803	0	0.18658742
2433	0.316667	2.2927754	1	0	0	1.6645653	0	0.20381152

Several files are automatically generated in the folder containing the simulation file. It includes:

- The simulation file (\*.pbpc)
- The results file in MS-Excel format (\*.csv)
- The evolution as a function of time of the liquid flowrate in the column (\*\_DL.csv)
- The evolution as a function of time of the vapor flowrate in the column (\*\_DV.csv)

BATCHCOL_EX_EN-Solvent-regeneration_files	24/08/2023 08:55	Dossier de fichiers	
BATCHCOL_EX_EN-Solvent-regeneration.cat	24/08/2023 08:55	Catalogue de sécurité	13 Ko
BATCHCOL_EX_EN-Solvent-regeneration.csv	24/08/2023 08:55	Fichier CSV Microsoft E	330 Ko
BATCHCOL_EX_EN-Solvent-regeneration.docx	24/08/2023 08:55	Document Microsoft W	1 806 Ko
BATCHCOL_EX_EN-Solvent-regeneration.don	24/08/2023 08:53	Fichier DON	4 Ko
BATCHCOL_EX_EN-Solvent-regeneration.his	24/08/2023 08:55	txtfile	5 Ko
BATCHCOL_EX_EN-Solvent-regeneration.log	24/08/2023 08:55	Document texte	1 Ko
BATCHCOL_EX_EN-Solvent-regeneration.pbpc	10/09/2020 11:43	Document BatchColumn	9631 Ko
BATCHCOL_EX_EN-Solvent-regeneration.res	24/08/2023 08:55	Compiled Resource Script	620 Ko
BATCHCOL_EX_EN-Solvent-regeneration.xyg	24/08/2023 08:55	Fichier XYG	420 Ko
BATCHCOL_EX_EN-Solvent-regeneration_DL.csv	24/08/2023 08:55	Fichier CSV Microsoft E	60 Ko
BATCHCOL_EX_EN-Solvent-regeneration_DV.csv	24/08/2023 08:55	Fichier CSV Microsoft E	60 Ko

For any questions, please contact ProSim technical support by sending an email to <a href="mailto:support@prosim.net">support@prosim.net</a>, with:

- The objectives of your simulation
- Your simulation file

To facilitate the sending of the simulation file by email, a zip file can be automatically generated by clicking on "send to support"








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