

Batch Separation

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Agenda

◆ Batch block layout

- Setup forms
- Heat transfer form
- Initial conditions
- Column setup form

◆ Operating steps

- Charge
- Distil

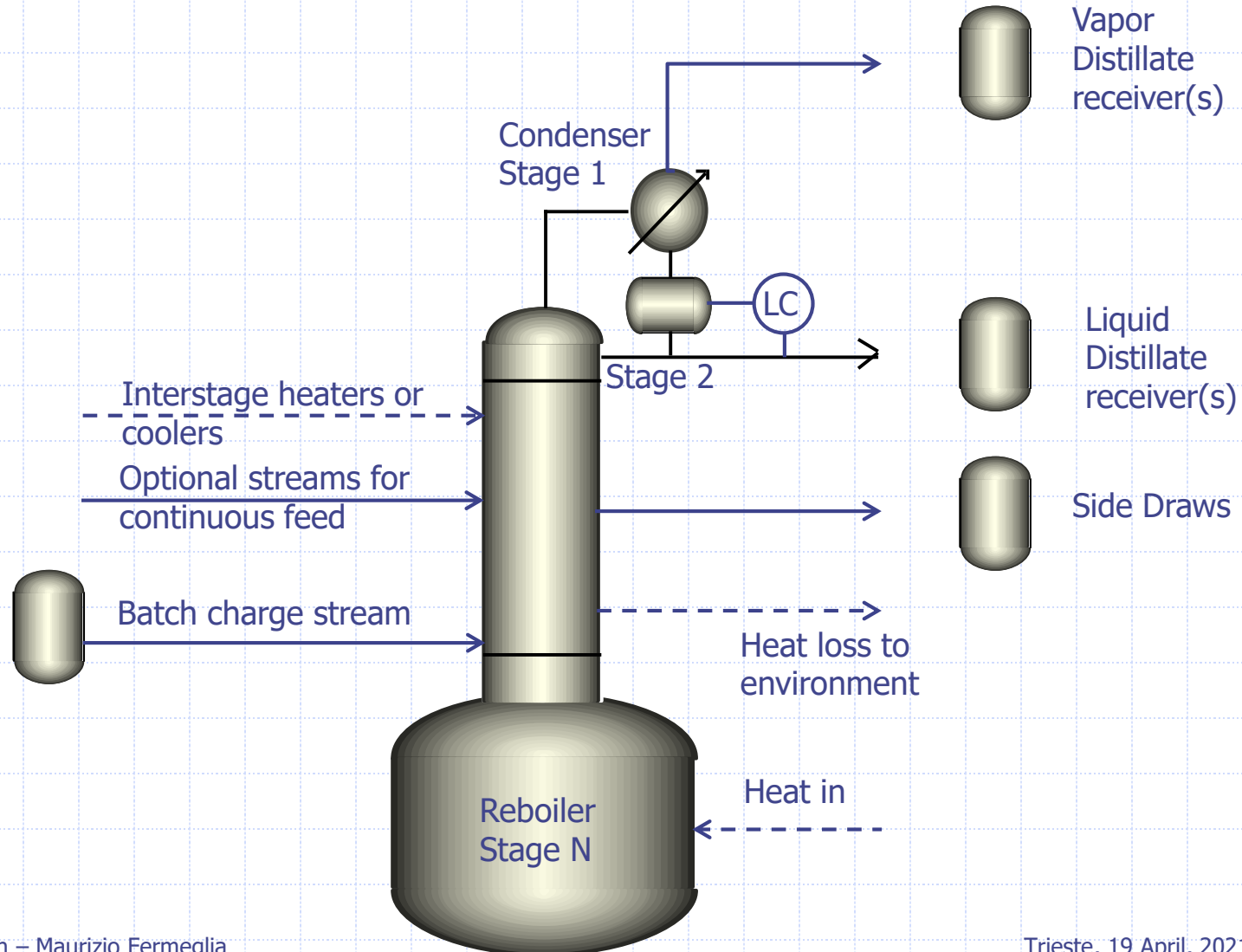
◆ Results and profiles

Objectives

- ◆ Learn how to setup basic specifications for batch distillation and reactor
- ◆ Recognize how to interpret and review result for a batch distillation simulation
- ◆ Setup a simulation of a batch procedure



BatchSep Block Layout



Capabilities

- ◆ Startup from total reflux, empty column or initial charge
- ◆ 2- or 3-phase calculation anywhere in the column
- ◆ Feeds to the column at any time, any stage including the pot and reflux drum
- ◆ Switch distillate or side draws to one of any number of receivers at any time during simulation
- ◆ Simulate multiple batches with recycle of material to the next batch
- ◆ Reactive distillation using rate based or equilibrium reactions
- ◆ Various modes for holdups and pressure profile
- ◆ Methods for estimating pressure drop and holdup for trays or packing
- ◆ Realistic modeling of heat transfer in pot and condenser
- ◆ Interstage heaters and coolers
- ◆ Heat loss to environment
- ◆ Dynamic effect of the heat capacity of the column materials
- ◆ Ability to include and configure controllers to manipulate operating conditions

Demo BatchSep

Batch separation of a mixture benzene/toluene

Components:

Benzene

Toluene

Nitrogen

Charge

100 kmol

Mole Frac:

Benzene 0.5

Toluene 0.5

Pot

Geometry:

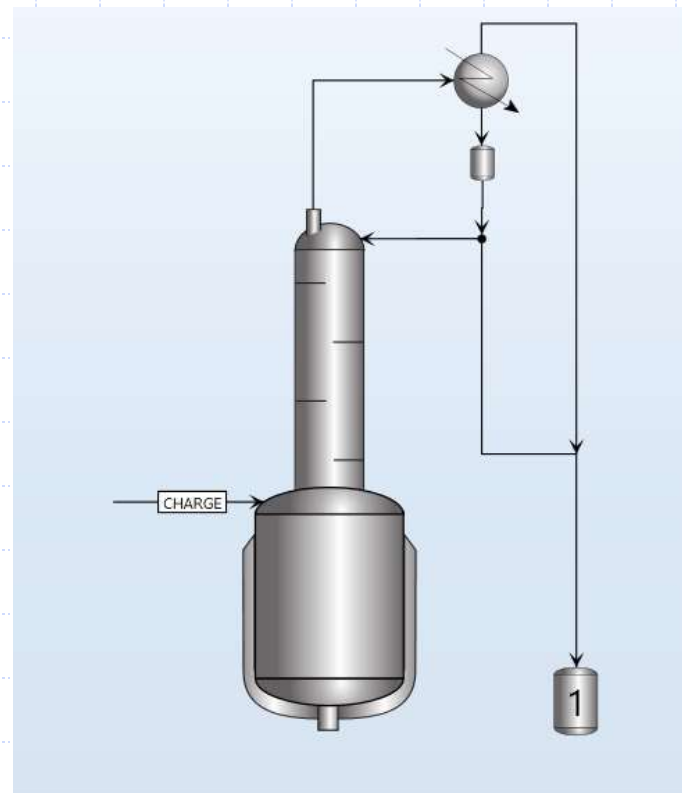
Diameter 3m

Height 2m

Reflux Drum

1.0472 cum

Reflux Ratio: 5



Column

Design:

4 Trays with

spacing 0.5 m

Heat Transfer:

Jacket Heating Medium

Temperature 200 °C

Operate until benzene mole fraction in pot becomes less than 0.1% mol

Setup form

◆ Configuration tab enables the user to specify:

Number of Stages
(Trays + 2)

Number of phases

The screenshot shows the 'B1 (BatchSep) - Setup' configuration window. The 'Configuration' tab is active. The 'Number of stages' is set to 6, and 'Valid phases' is set to 'Vapor-Liquid'. Under 'Overhead', 'Condenser' is set to 'Partial'. Under 'Distillate receivers', the number of receivers is 1, and a table shows 1 receiver for both Liquid and Vapor phases. Under 'Pressure & Holdups', 'Calculated from tray or packing hydraulics' is selected. Under 'Pot heat transfer', 'Rigorous' is selected. Under 'Initial condition', 'Empty' is selected.

Phase	Condenser Receiver
Liquid	1
Vapor	1

Type of condenser.
If incondensable are present,
Total must not be selected

Pressure calculation

Initial conditions

Setup form

The screenshot shows the 'Streams' tab of the 'B1 (BatchSep) - Setup' window. It includes sections for 'Pot charge' (Stream: CHARGE, Flow rate basis: Mole), 'Continuous Feeds' (No continuous feeds present), 'Distillate Receivers' (Number of receivers: 1, with a table showing Receiver 1 and Product Stream DIST), and 'Side Draw Receivers'.

Receiver	Product Stream
1	DIST

◆ **Streams tab** enables the user to specify the inlet and outlet streams of the column. Remember to specify the correct receiver

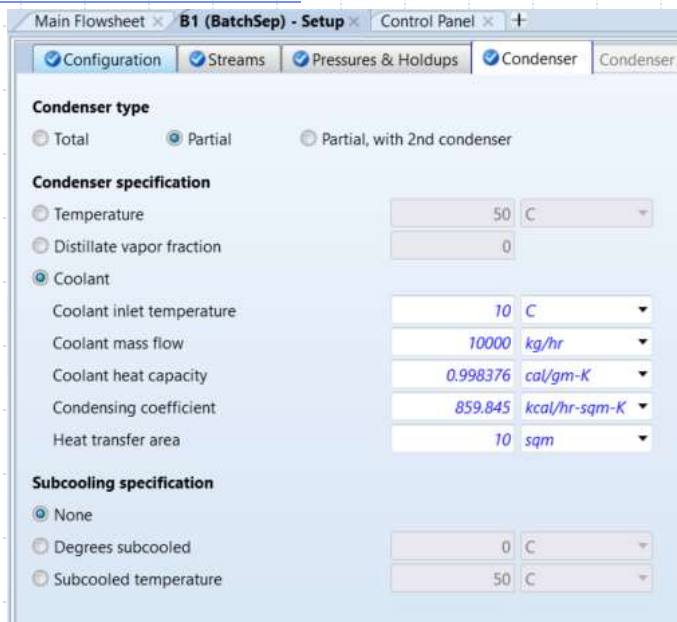
◆ **Pressure & Holdups tab** enables the user to specify the pressure of the column:

- If "Specified", pressure drop and holdups must be specified
- If "Calculated", condenser and internals characteristics must be specified

The screenshot shows the 'Pressure & Holdups' tab of the 'B1 (BatchSep) - Setup' window. It includes sections for 'Pressure & Holdups Calculation Option' (Specified or Calculated from tray or packing hydraulics), 'Overhead' (Condenser pressure: 1.01325 bar, Second condenser pressure: 1.01325 bar, Condenser inlet diameter: 0.1 meter), 'Pressure drop' (Pressure drop specification: Column Pressure drop), and 'Holdups' (Holdup basis: Mole, Reflux drum liquid holdup: kmol, with a table for Stage Holdup).

Start stage	End stage	Stage Holdup
		kmol

Setup form



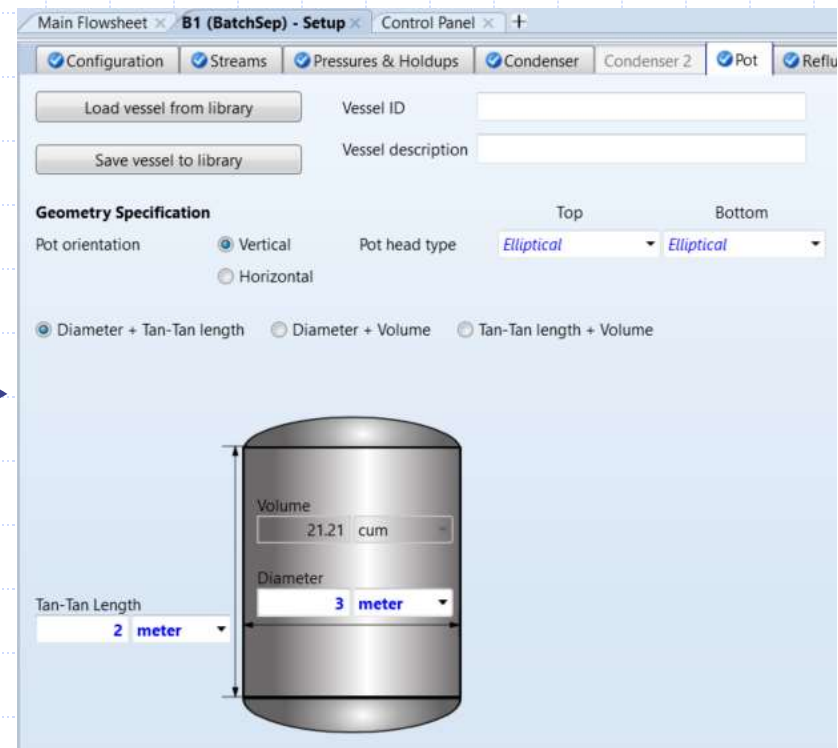
The screenshot shows the 'Condenser' tab of the software interface. It includes the following sections:

- Condenser type:** Radio buttons for 'Total', 'Partial' (selected), and 'Partial, with 2nd condenser'.
- Condenser specification:** Fields for 'Temperature' (50 C), 'Distillate vapor fraction' (0), 'Coolant' (selected), 'Coolant inlet temperature' (10 C), 'Coolant mass flow' (10000 kg/hr), 'Coolant heat capacity' (0.998376 cal/gm-K), 'Condensing coefficient' (859.845 kcal/hr-sqm-K), and 'Heat transfer area' (10 sqm).
- Subcooling specification:** Radio buttons for 'None' (selected), 'Degrees subcooled' (0 C), and 'Subcooled temperature' (50 C).

◆ **Condenser tab** enables the user to specify information regarding the condenser and the condensation specifications

◆ **Pot tab** enables the user to define the dimension of the pot using commercial vessels from library or specifying the specific dimension defining two out of:

- Diameter
- Height
- Volume



The screenshot shows the 'Pot' tab of the software interface. It includes the following sections:

- Buttons:** 'Load vessel from library' and 'Save vessel to library'.
- Fields:** 'Vessel ID' and 'Vessel description'.
- Geometry Specification:** Radio buttons for 'Vertical' (selected) and 'Horizontal'. 'Pot head type' has dropdowns for 'Top' (Elliptical) and 'Bottom' (Elliptical).
- Dimensioning:** Radio buttons for 'Diameter + Tan-Tan length' (selected), 'Diameter + Volume', and 'Tan-Tan length + Volume'.
- Visuals:** A 3D rendering of a pot with 'Volume' (21.21 cum) and 'Diameter' (3 meter) displayed. 'Tan-Tan Length' is set to 2 meter.

Setup form

The screenshot shows the 'Reflux' tab in the software interface. It includes sections for 'Reflux specification', 'Reflux drum geometry', and 'Reflux level'. The 'Reflux specification' section has a 'Reflux ratio' dropdown set to '3'. The 'Reflux drum geometry' section has 'Orientation' set to 'Vertical' and 'Head type' set to 'Cylindrical'. The 'Geometry Specification' section has 'Diameter + Volume' selected. A 3D model of a reflux drum is shown with 'Volume' set to '1.047 m³' and 'Diameter' set to '1 meter'. The 'Reflux level' section has a table with the following data:

	Liquid 1	Liquid 2
Set Point	meter	meter
Gain	10	10
Integral time	0.333333 hr	0.333333 hr
Derivative time	0 hr	0 hr
Maximum outlet flow	3.6e+07 kg/hr	3.6e+07 kg/hr

◆ Reflux tab enables the user to specify the reflux ratio or other specifications regarding the distillation operation variables. It allows to define the dimension of the reflux drum and the level control parameters

◆ Reactions tab enables the user to specify if a reaction is occurring inside the vessel or the entire column

The screenshot shows the 'Reactions' tab in the software interface. It includes a 'Reaction model' dropdown and two radio button options: 'Reactions occur in all stages' and 'Reactions occur in pot only', with the latter being selected.

Heat Transfer form

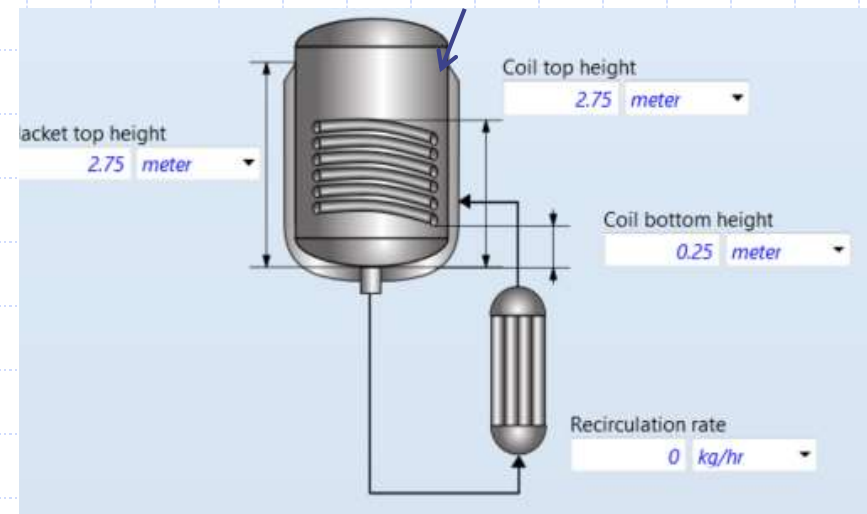
The screenshot shows a software window titled "B1 (BatchSep) - Heat Transfer" with a "Configuration" tab selected. The form is divided into several sections:

- Heat Transfer Model:** Includes radio buttons for "Shortcut" and "Rigorous" (selected). A "Specification" section shows a dropdown for "Duty" and a value of "1" with units "Gcal/hr". There are also checkboxes for "Model heat loss to the environment" and "Model vessel heat capacities", both of which are unchecked.
- Jacket:** Includes checkboxes for "Heating" (checked) and "Cooling" (unchecked). A "Jacket covers bottom" checkbox is also checked.
- Coils:** Includes checkboxes for "Heating" and "Cooling", both unchecked. A "Heat transfer area" field is set to "1 sqm".
- External Exchanger:** Includes checkboxes for "Heating" and "Cooling", both unchecked. A "Heat transfer area" field is set to "1 sqm".

At the bottom, there is a 3D diagram of a vessel with a jacket and a coil. A "Jacket top height" dropdown is set to "2.75 meter".

◆ Configuration tab enables the user to specify the approach to heat transfer calculation:

- Shortcut: Duty must be specified. Eventually, any side duties require further specification regarding their stage location
- Rigorous: it allows to specify the existent heating device (Jacket, Coils, External Exchanger) and its purpose.



Heat Transfer form

Main Flowsheet × B1 (BatchSep) - Heat Transfer × Control Panel × +

Configuration Jacket Heating Side Duty Process Side Heat Transfer Coeff.

Heating option *specified medium temperature*

Medium temperature 200 C

Heat transfer coefficient

Use overall heat transfer coefficient 429.923 kcal/hr-sqm-K

Compute using process side and service side film heat transfer coefficients

specified medium temperature

LMTD

Mass Boilup rate

Mole boilup rate

Specified duty

specified medium temperature

Steam heating

- ◆ Jacket Heating, Coils Heating, External Exchanger Heating tabs enables the user to specify the working condition of the heating/cooling device:
 - LMTD: Logarithmic mean temperature difference
 - Mass/mole boilup rate: mass/molar flow of boilup from pot to column
 - Specified Duty: Net duty given/removed from the pot depending on the purpose of the device
 - Specified medium temperature: temperature of the utility adopted for the heat transfer
 - Steam heating: condition (T or P, mass flowrate) of the steam adopted for heating up the pot

Initial Condition form

◆ Main tab enables the user to specify the initial condition among:

- Total reflux: the column is charged and heated up using total reflux until steady state is reached. Temperature and pressure must be "calculated"
- Empty: The column contains Pad Gas only (usually Nitrogen or Air) and the user must specify initial temperature and pressure.
- Initial charge: The column already contains some reactants and pad gas.

◆ Distillate Receivers tab enables the user to specify the composition of mixture inside distillate containers, if present.



Main Flowsheet × B1 (BatchSep) - Initial Conditions × Control Panel × +

Main Distillate Receivers Side Draw Receivers

Initial Condition

Total reflux Empty Initial charge

Initial temperature: 20 C

Initial pressure: 1.01325 bar

Initial drum liquid volume fraction: 0.5

Pad gas: N2

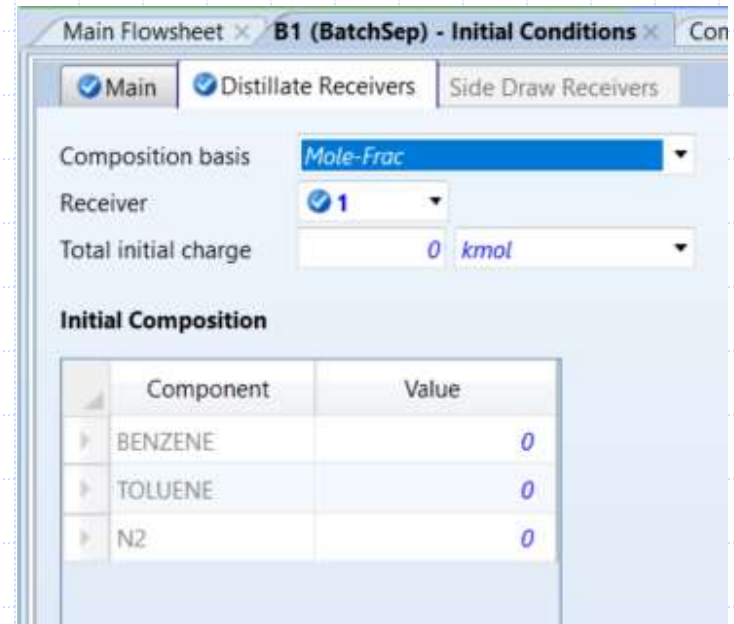
Charge

Specify charge time: 1 hr

Specify total charge

Charge basis: Mole

Total initial charge: kmol



Main Flowsheet × B1 (BatchSep) - Initial Conditions × Con

Main Distillate Receivers Side Draw Receivers

Composition basis: Mole-Frac

Receiver: 1

Total initial charge: 0 kmol

Initial Composition

Component	Value
BENZENE	0
TOLUENE	0
N2	0

Column Internals form

- ◆ Sections and Geometry tab enables the user to specify internal details for specific sections of the separation column
 - Trayed: the user can define specific geometric parameters for sieve trays
 - Packed: the user can define specific parameters for packing internals

The screenshot displays the 'Column Internals' software interface. The 'Sections' tab is active, showing a table with the following data:

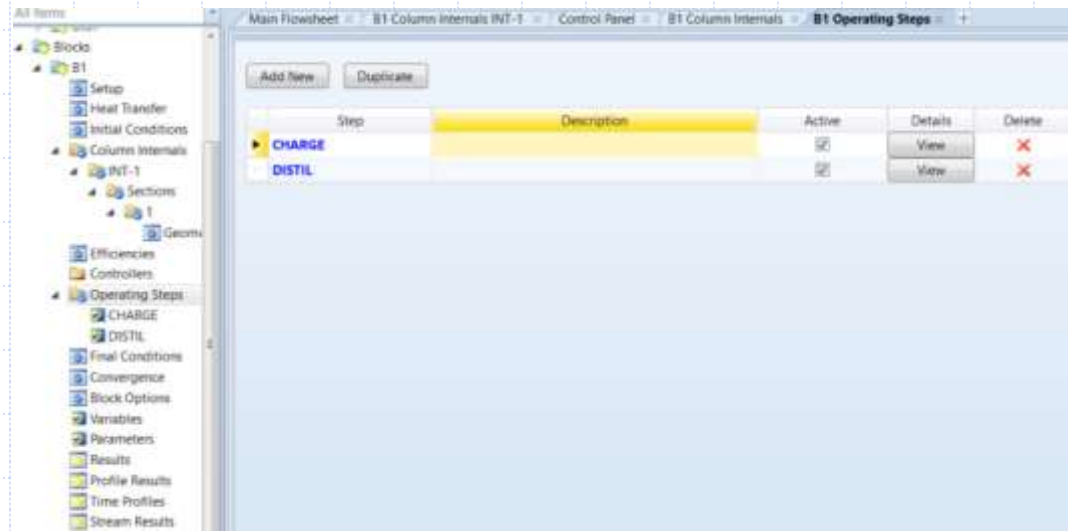
Section Number	Start Stage	End Stage	Internal Type	Tray Spacing/Stage Packed Height	Diameter	Details
1	2	5	Trayed	0.5 meter	1 meter	View

The 'Geometry' tab is also visible, showing a 3D model of a tray and various geometric parameters:

- Hold Diameter: 0 mm
- Fractional active area: 0.9
- Fractional hole area: 0.125
- Discharge coefficient: 0.6
- Side Downcomer Width: Top: 156.2 mm, Bottom: 156.2 mm
- Side Weir Length: 0.228 meter
- Diameter: 1 meter
- Weir height: 50.8 mm
- Tray Spacing: 0.5 meter

Operating Steps form

- ◆ It allows the user to specify the operating steps inside the equipment. Since batch distillation is a dynamic process, different operations need to be specified.
- ◆ Change operating conditions such as charges, reflux ratio, heating, cooling, switch receiver, ...
- ◆ All changes start at the same time
- ◆ A duration time (ramp) can be specified to reach and maintain the specified value
- ◆ In our demo, we need to charge the vessel first and then start the distillation operation.



Charge Operation

- ◆ We need to charge the pot with the continuous stream "CHARGE" until we reach 100 kmol of solution inside the vessel.
- ◆ How long do we need to let the operation last?

Configuration

Operating Changes

Process Variable being changed		New Value		Units	Ramp Time
Location	ID	Name	Mode/Receiver	Value	
Continuous feed	CHARGE	Mole flow rate		100 kmol/hr	0 hr
Jacket heating		Medium temperature		25 C	0 hr

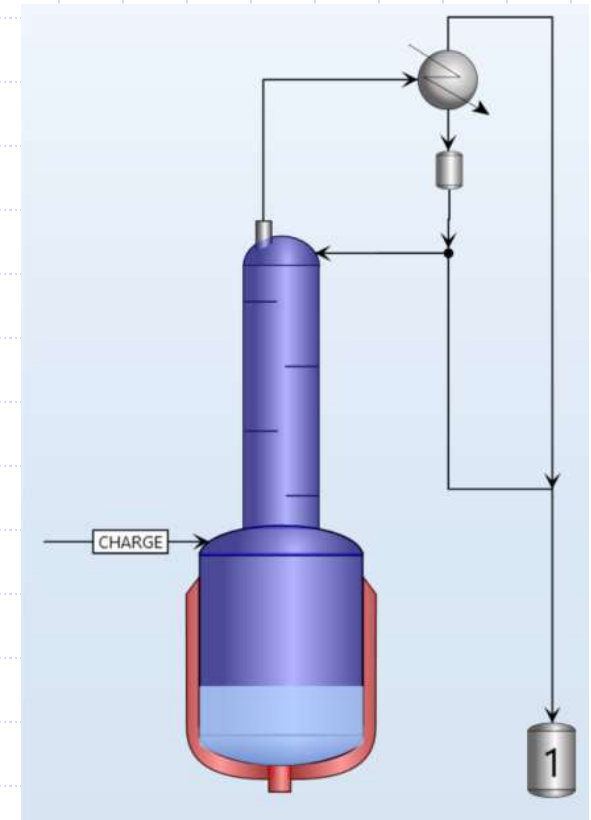
Stop Criteria

Duration Process variable

1 hr

Location	Receiver/Stage	Process Variable	Component	Trigger Value	Approach From
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Stop if process variable trigger value not reached in 24 hr



Distil Operation

- ◆ We need to stop charging the vessel!
- ◆ Since we defined just the coolant conditions, we need to specify the flow of this utility involved in the cooling operation
- ◆ Now we want to heat up the vessel! What should we modify?
- ◆ How can we define the duration of this operation?

Configuration

Operating Changes

Process Variable being changed			New Value		Units	Ramp Time
Location	ID	Name	Mode/Receiver	Value		
Continuous feed	CHARGE	Mole flow rate		0 kmol/hr		0 hr
Condenser		Coolant mass flow		30000 kg/hr		0 hr
Jacket heating		Medium temperature		200 C		0 hr

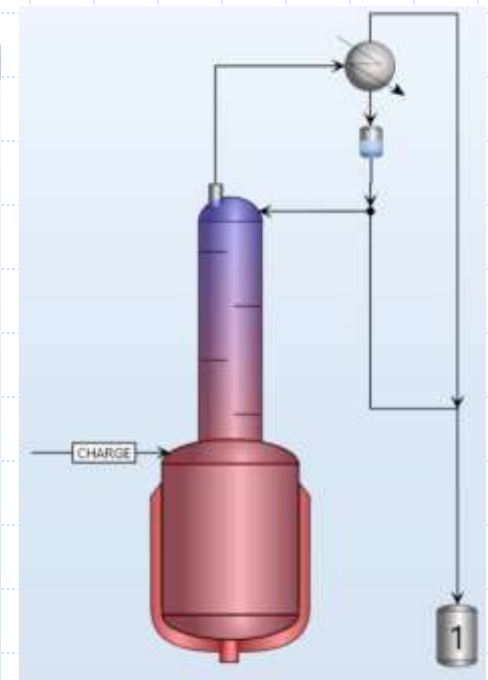
Stop Criteria

Duration hr

Process variable

Location	Receiver/Stage	Process Variable	Component	Trigger Value	Approach From	
Pot		Liquid mole fraction	BENZENE	0.001 fraction	Above	✗

Stop if process variable trigger value not reached in hr



Final Conditions

◆ Define what to do with the material in the column at the end of the batch:

- Leave in place
- Dump to Distillate receiver
- Leave in place and recycle

Option	Description
Leave in place	At the end of the batch show the material where it is, but the material will not be recycled to the next batch in case of multiple batches
Leave in place and recycle	When simulating multiple batches and using Total reflux as the initial condition. At the end of the batch show the material where it is, then recycles it to the initial charge of the next batch
Dump to distillate receiver	Useful when simulating multiple batches with recycle and using Empty as the initial condition. Material left in pot, reflux drum, trays/packing is discarded before next batch starts. If any of it must be recycled, specify on the Initial Conditions form how this material will be used in the next batch

Results

- ◆ **Results form:** contains the steady state information, not related to column profile or time. This information will be sent to the rest of the flowsheet...

Step	Step End Time	Units	Value at Step End	Units	Threshold	Units
CHARGE	1.00001	hr				
- DISTIL	7.4984	hr				
POT L-MOLEFRAC BENZ...			0.001	fraction	0.001	fraction

Name	Value	Units
Liquid level	0.622885	meter
Total mole holdup	22.9608	kmol
Total mass holdup	2115.29	kg
Liquid volume	2.84506	ccm
Mole holdup rate	40.0973	kmol/hr
Mass holdup rate	3893.28	kg/hr
Temperature	113.297	C
Duty for heat transfer with environment	0	Gcal/hr
Net duty	0.318461	Gcal/hr

Name	Units	Total	Vapor	Liquid
Total holdup	kmol	22.9608	0.626932	22.3339

Name	Total	Vapor	Liquid
BENZENE	0.0237938	0.00545794	0.0223359
TOLUENE	22.937	0.629474	22.3116
N2	0	0	0

Name	Value	Units
Receiver taking liquid	1	
Receiver taking vapor	1	
Liquid flow rate	4.95039	kmol/hr
Vapor flow rate	0	kmol/hr

Name	Receiver 1
BENZENE	0.89448
TOLUENE	0.292532
N2	0.0132799

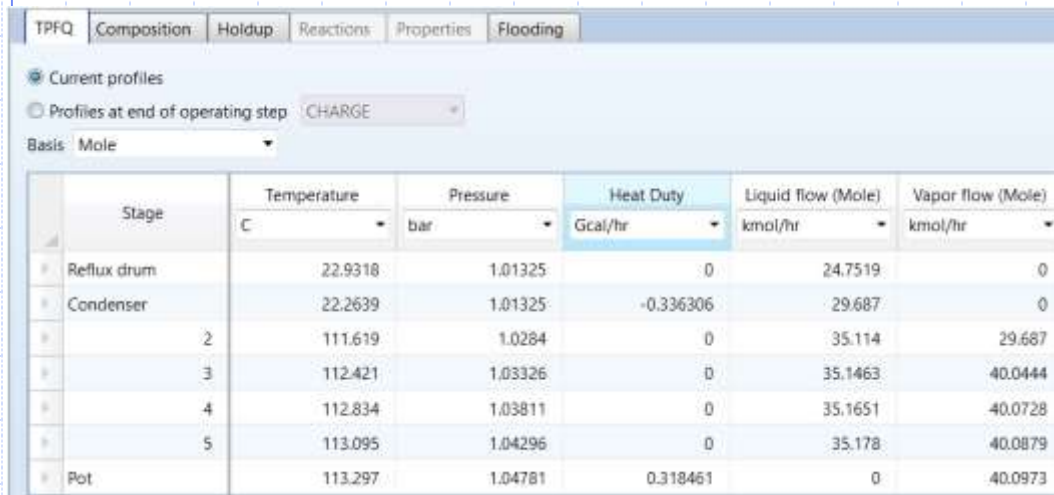
Name	Value	Units
Duty	-0.336306	Gcal/hr
Inlet temperature	111.619	C
Outlet temperature	22.2639	C
Outlet pressure	1.01325	bar
Outlet vapor fraction	0	
Outlet liquid fraction	1	
Outlet liquid flow rate	29.687	kmol/hr
Outlet vapor flow rate	0	kmol/hr

	BENZENE	TOLUENE	N2
Inlet composition	0.0490512	0.950949	0
Liquid composition	0.0490512	0.950949	0
Vapor composition			

... and so on

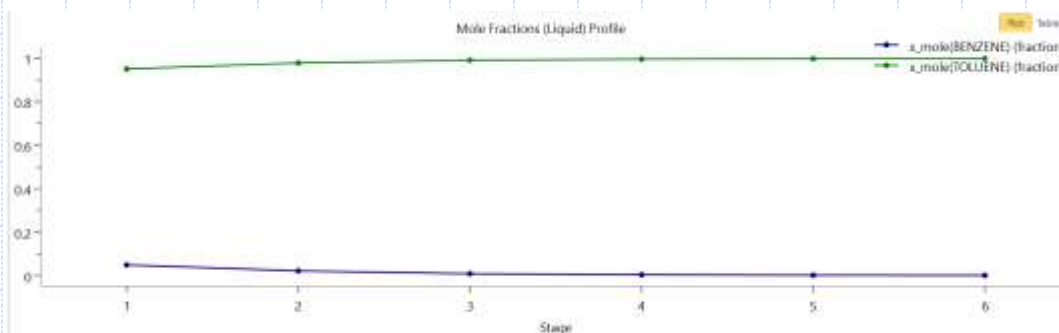
Profile Results

- ◆ **Profile Results form:** contains information related to column profile for composition, temperature, pressure, holdup, duty, etc...



Stage	Temperature (C)	Pressure (bar)	Heat Duty (Gcal/hr)	Liquid flow (Mole) (kmol/hr)	Vapor flow (Mole) (kmol/hr)
Reflux drum	22.9318	1.01325	0	24.7519	0
Condenser	22.2639	1.01325	-0.336306	29.687	0
2	111.619	1.0284	0	35.114	29.687
3	112.421	1.03326	0	35.1463	40.0444
4	112.834	1.03811	0	35.1651	40.0728
5	113.095	1.04296	0	35.178	40.0879
Pot	113.297	1.04781	0.318461	0	40.0973

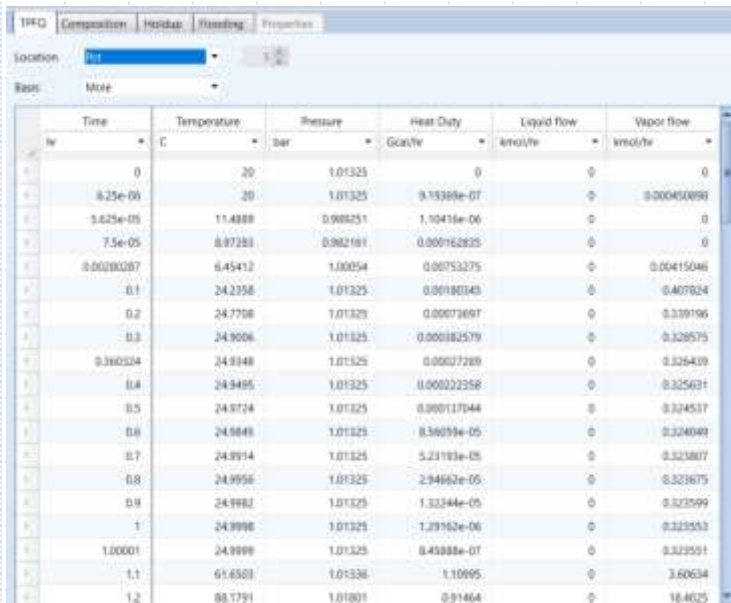
Stage	Temperature (C)
1	22.2639
2	111.619
3	112.421
4	112.834
5	113.095
6	113.297



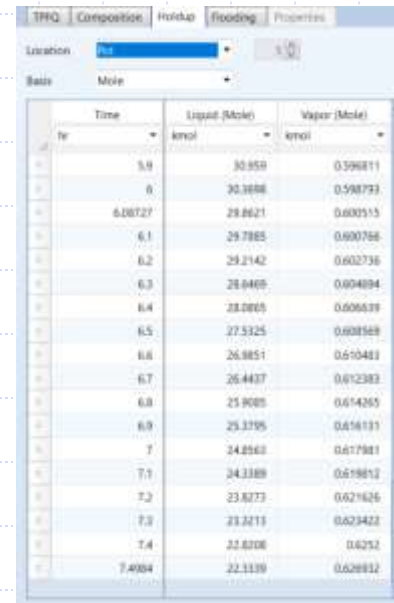
... and so on

Time Results

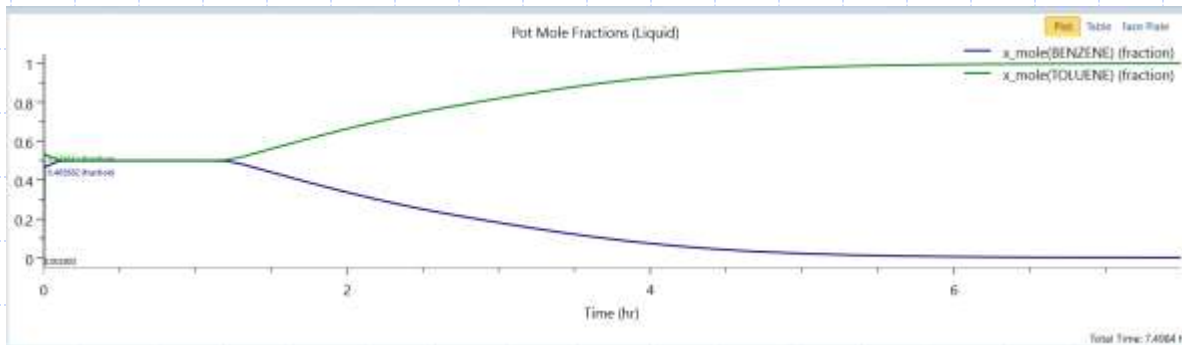
- ◆ **Time Results form:** contains information related to dynamic behavior of the column for composition, temperature, pressure, holdup, duty, etc...



Time	Temperature	Pressure	Heat Duty	Liquid flow	Vapor flow
hr	°C	bar	Gcal/hr	kmol/hr	kmol/hr
0	20	1.01325	0	0	0
6.25e-06	20	1.01325	9.15399e-07	0	0.000450086
3.625e-05	11.4288	0.989251	1.70416e-06	0	0
7.5e-05	8.97281	0.982181	0.000162825	0	0
0.000180287	6.45412	1.00054	0.00753275	0	0.00415048
0.1	24.2358	1.01325	0.00180043	0	0.407824
0.2	24.7708	1.01325	0.00073697	0	0.339196
0.3	24.9006	1.01325	0.00082579	0	0.328575
0.380524	24.9148	1.01325	0.00077269	0	0.325439
0.4	24.9495	1.01325	0.00022358	0	0.325631
0.5	24.9724	1.01325	0.000137044	0	0.324537
0.6	24.9848	1.01325	0.36099e-05	0	0.324049
0.7	24.9914	1.01325	5.23193e-05	0	0.323807
0.8	24.9956	1.01325	2.94662e-05	0	0.323675
0.9	24.9982	1.01325	1.32344e-05	0	0.323599
1	24.9998	1.01325	7.29162e-06	0	0.323553
1.00001	24.9999	1.01325	8.45888e-07	0	0.323551
1.1	61.6501	1.01338	1.10895	0	3.60634
1.2	88.1791	1.01801	0.91464	0	18.4025



Time	Liquid (Mole)	Vapor (Mole)
hr	kmol	kmol
0	0	0
3.9	30.959	0.598811
6	30.3888	0.598793
6.08727	28.8621	0.600515
6.1	29.7885	0.600768
6.2	29.2142	0.602736
6.3	28.8405	0.604894
6.4	28.085	0.606879
6.5	27.5325	0.608568
6.6	26.9851	0.610481
6.7	26.4437	0.612383
6.8	25.908	0.614265
6.9	25.3795	0.616131
7	24.8561	0.617981
7.1	24.3389	0.619812
7.2	23.8273	0.621626
7.3	23.3213	0.623422
7.4	22.8208	0.6252
7.4984	22.3139	0.626932



... and so on

Hands-on: batch simulation of benzene - toluene

