Batch Separation

Maurizio Fermeglia
Maurizio.fermeglia@units.it
Department of Engineering & Architecture
University of Trieste

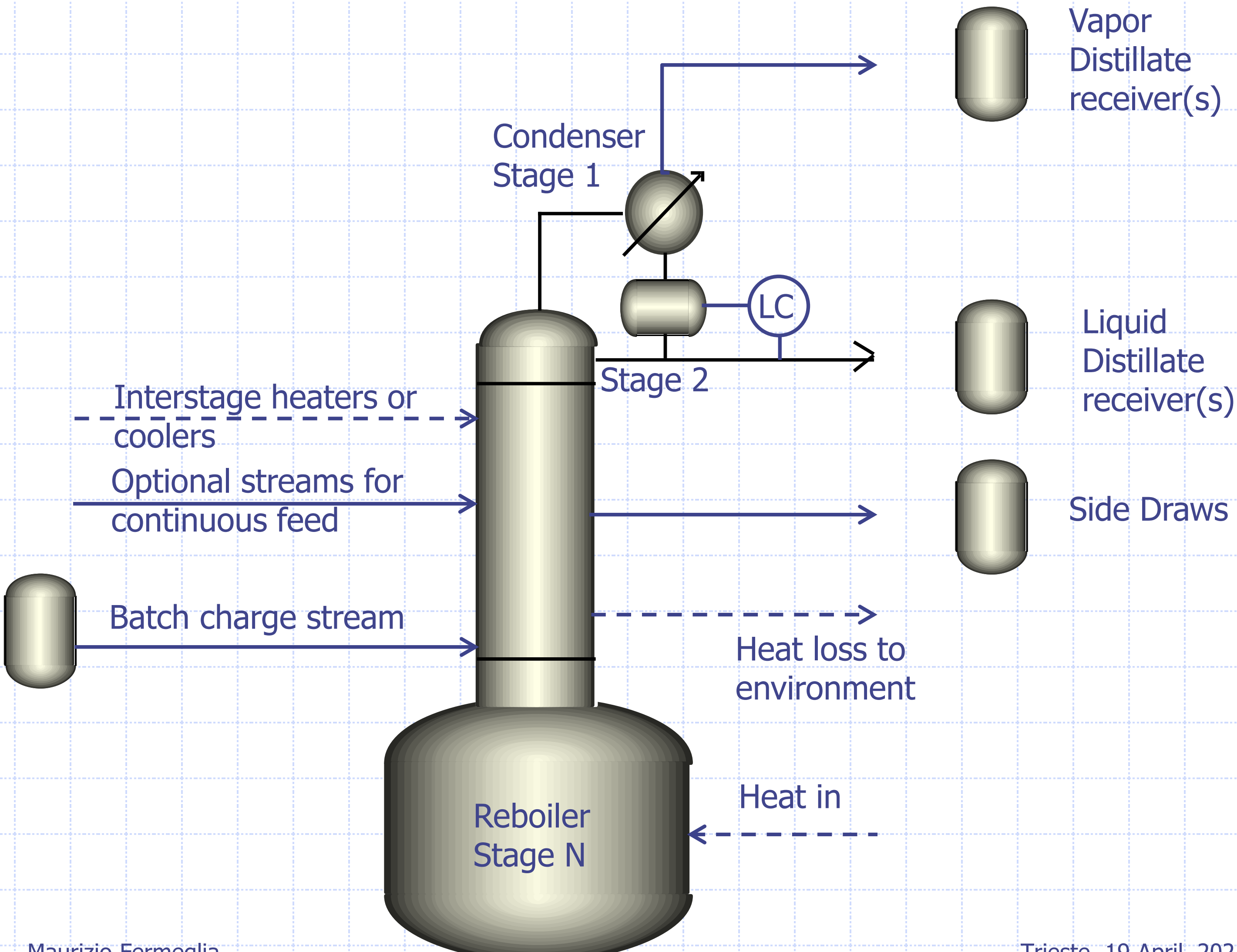
Agenda

- 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

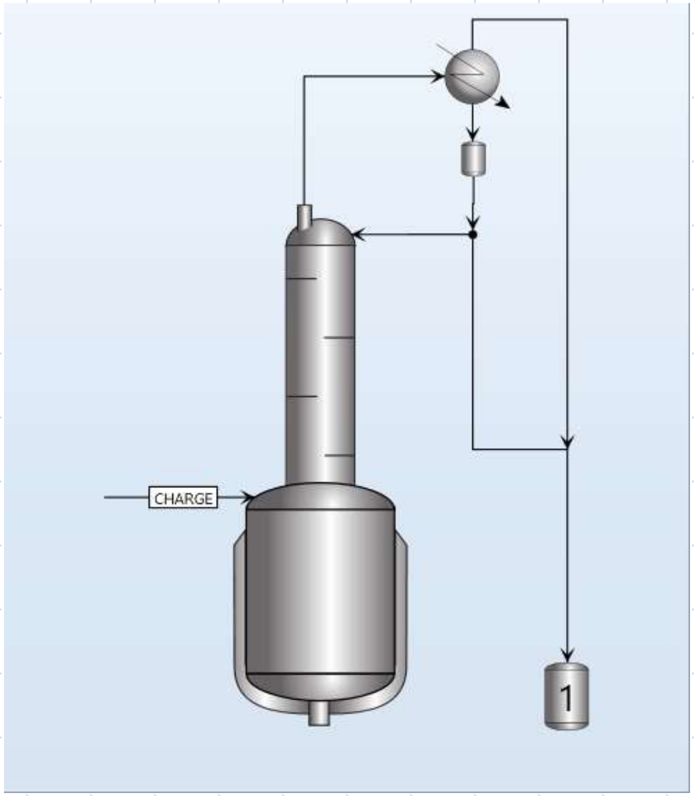
Batch separation of a mixture benzene/toluene

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

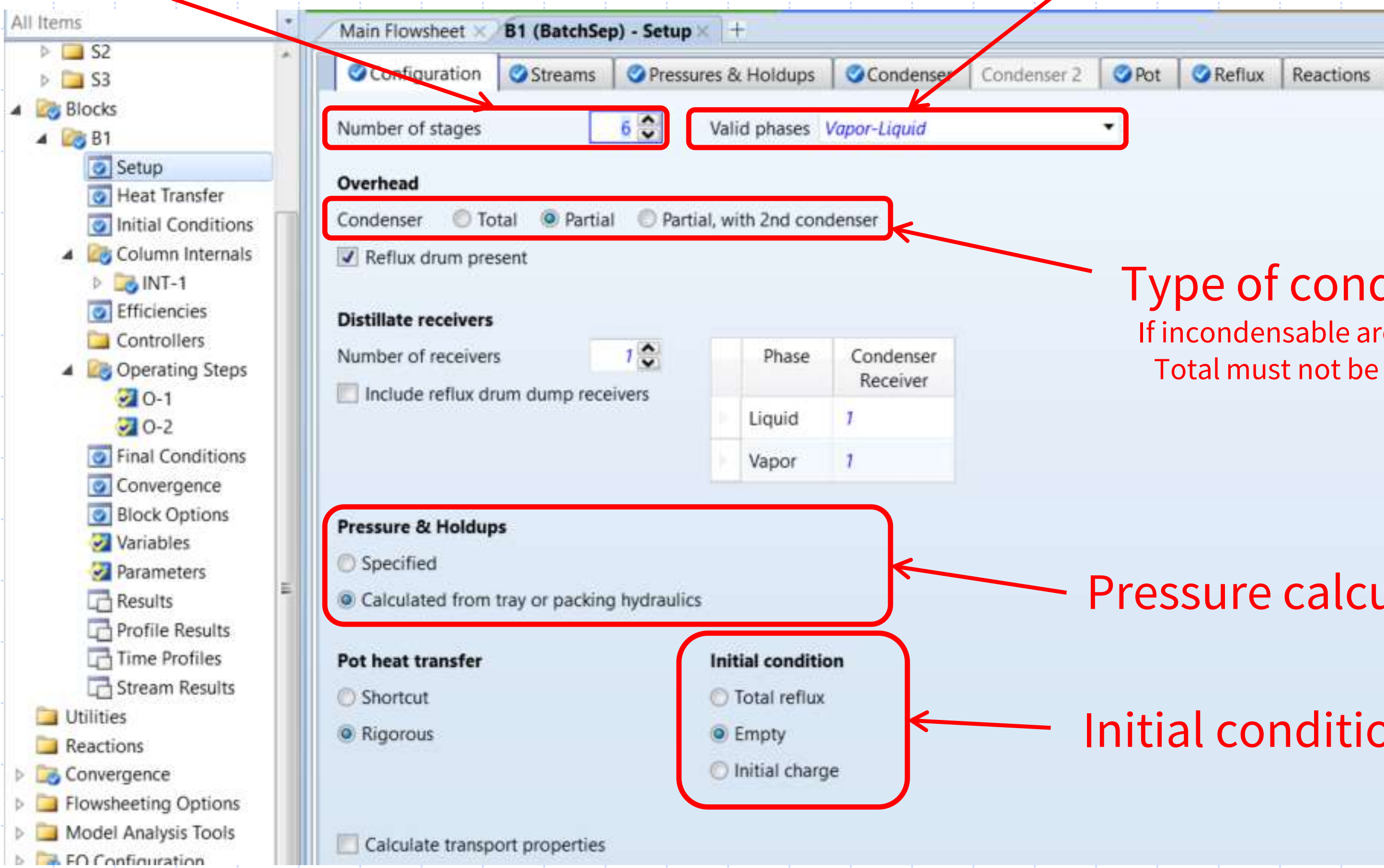
Operate until benzene mole fraction in pot becomes less than 0.1% mol

Setup form

- Configuration tab enables the user to specify:

Number of Stages
(Trays + 2)

Number of phases



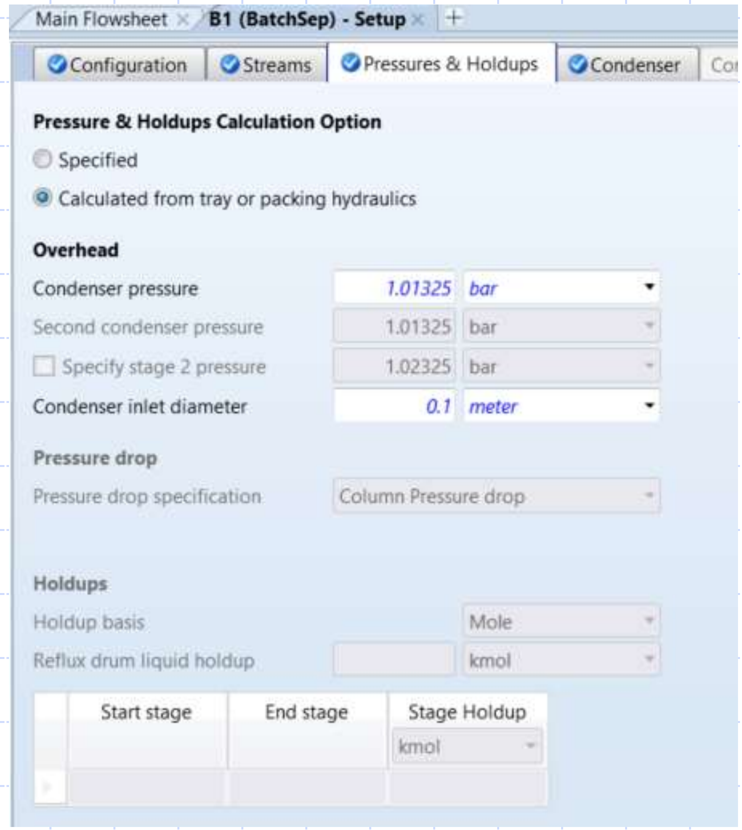
Type of condenser.
If incondensable are present,
Total must not be selected

Pressure calculation

Initial conditions

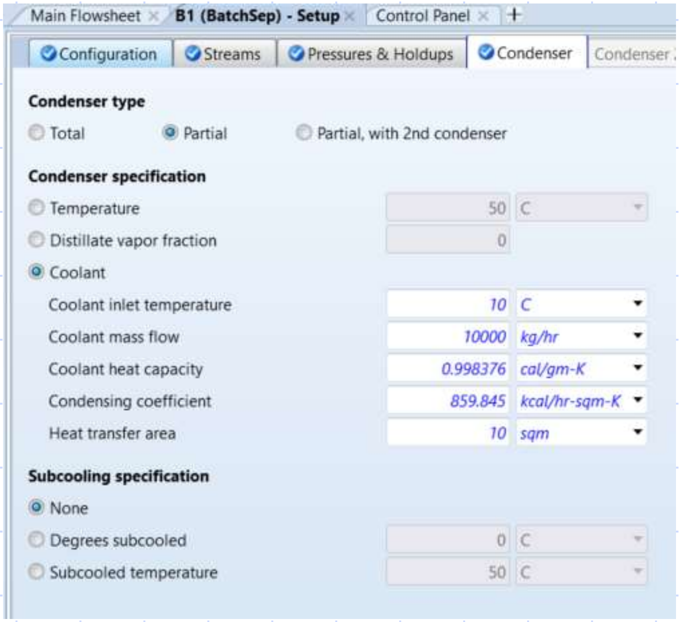
Setup form

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



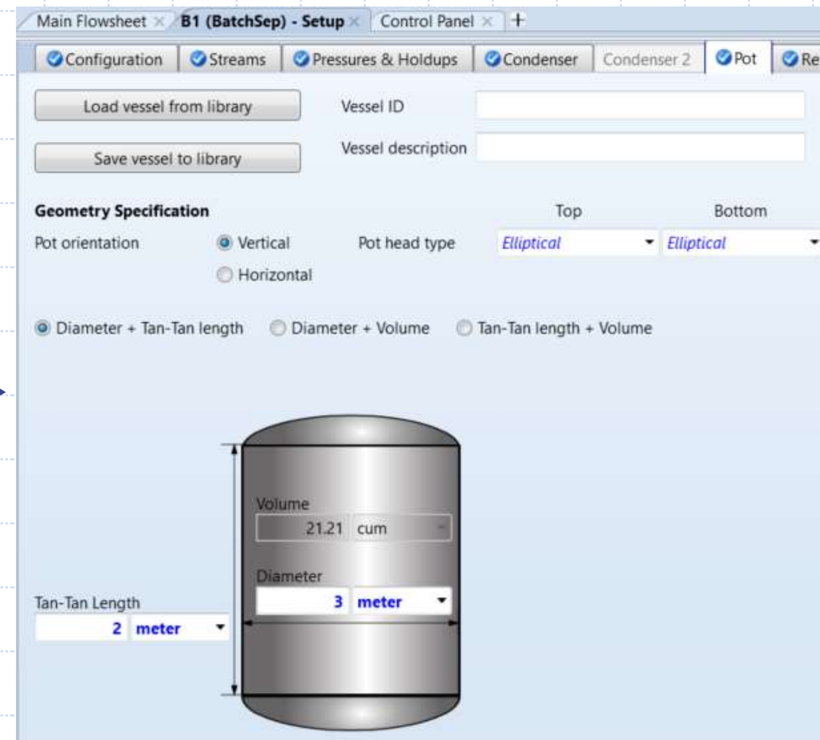
- **Pressure & Holdups tab** enables the user to specify the pressure of the column:
  - If "Specified", pressure drop and holdups must be specified
  - If "Calculated", condenser and internals characteristics must be specified

Setup form

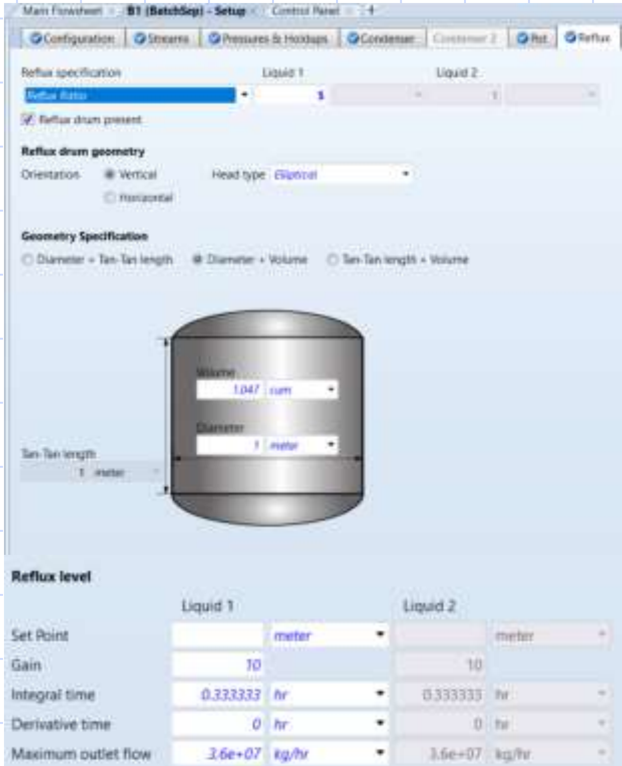


- **Condenser tab** enables the user to specify information regarding the condenser and the condensation specifications

- **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

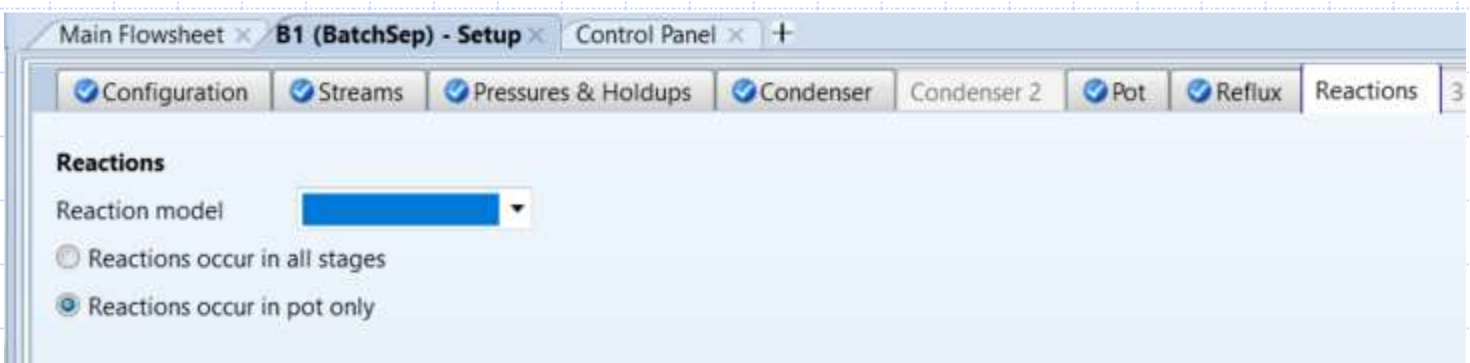


Setup form

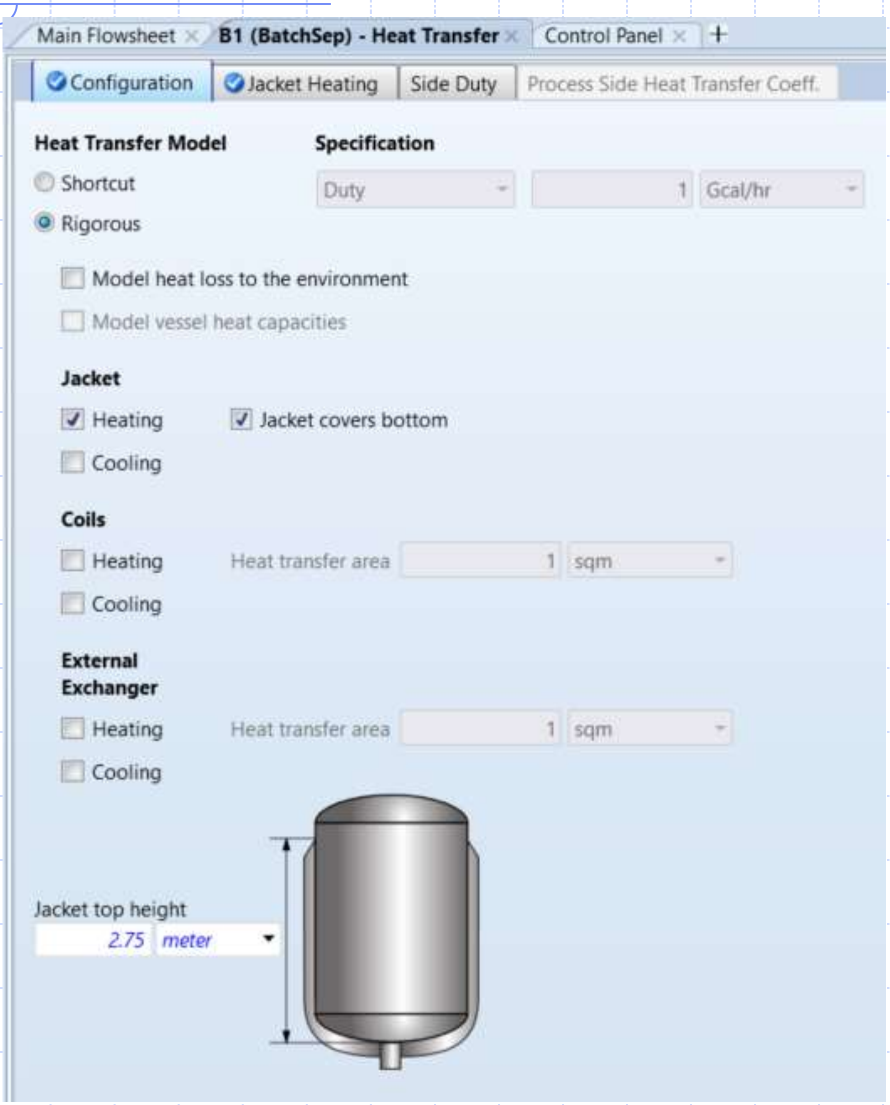


- Reflux tab enables the user to specify the reflux ratio or other specifications regarding the distillation operation variables. It allows to define the dimension of the reflux drum and the level control parameters

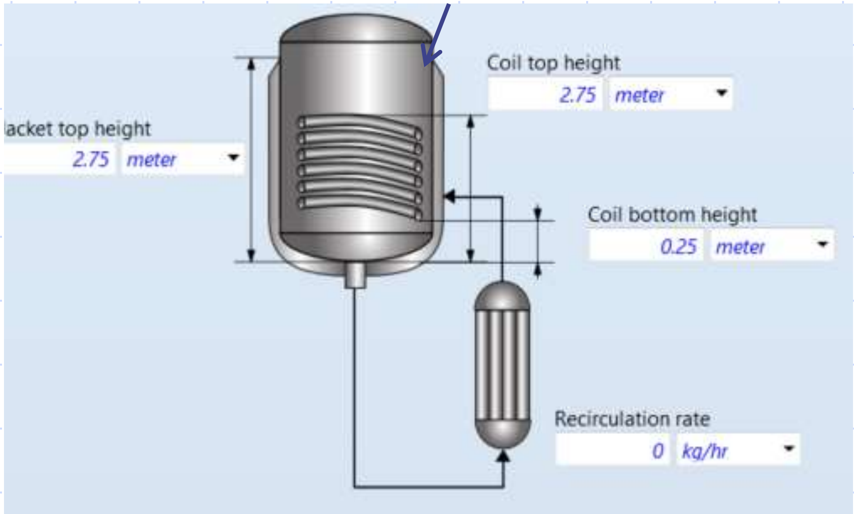
- Reactions tab enables the user to specify if a reaction is occurring inside the vessel or the entire column



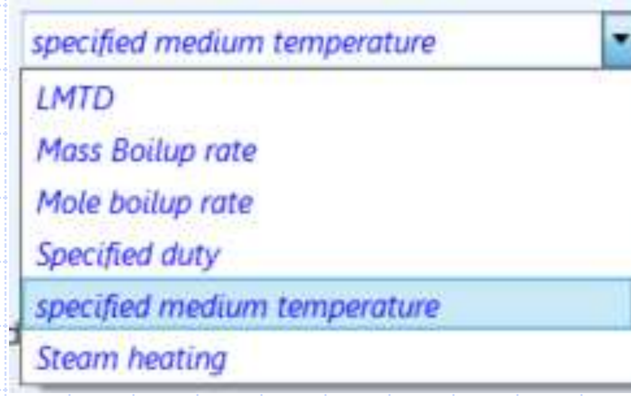
Heat Transfer form



- 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

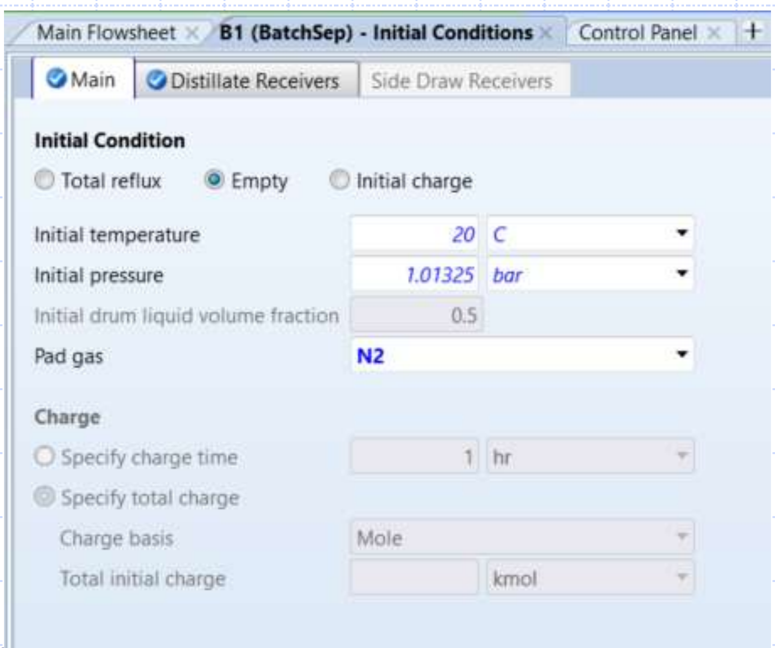


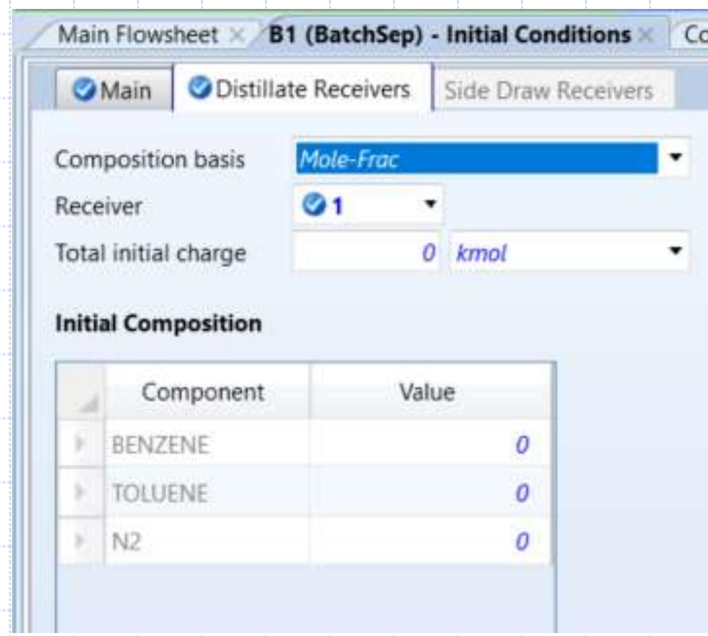
- Jacket Heating, Coils Heating, External Exchanger Heating tabs enables the user to specify the working condition of the heating/cooling device:
  - LMTD: Logarithmic mean temperature difference
  - Mass/mole boilup rate: mass/molar flow of boilup from pot to column
  - Specified Duty: Net duty given/removed 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.

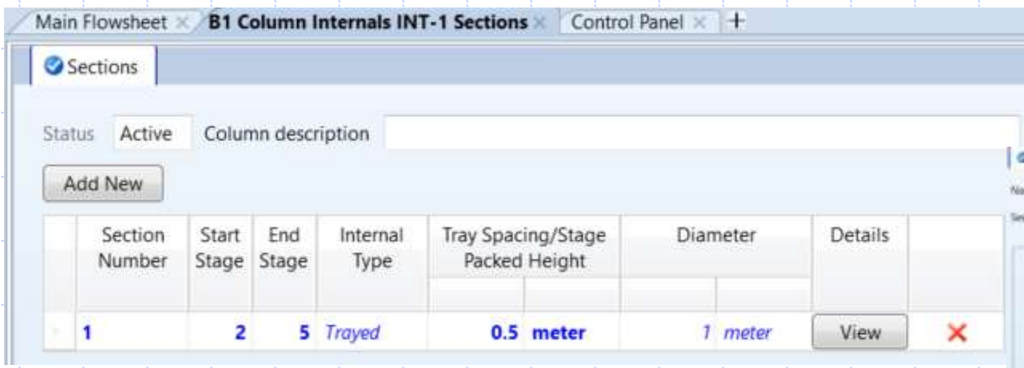
- Distillate Receivers tab enables the user to specify the composition of mixture inside distillate containers, if present.

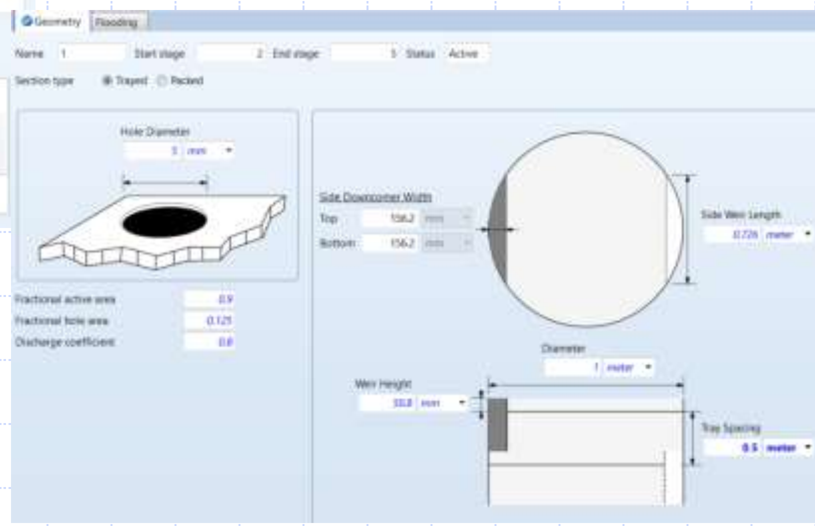




Column Internals form

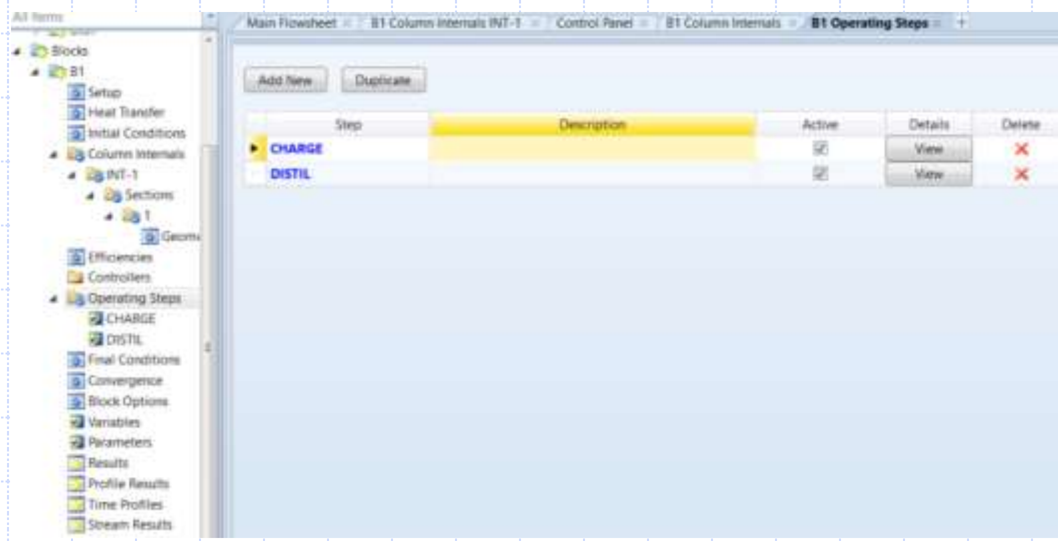
- Sections and Geometry tab enables the user to specify internal details for specific sections of the separation column
  - Trayed: the user can define specific geometric parameters for sieve trays
  - Packed: the user can define specific parameters for packing internals





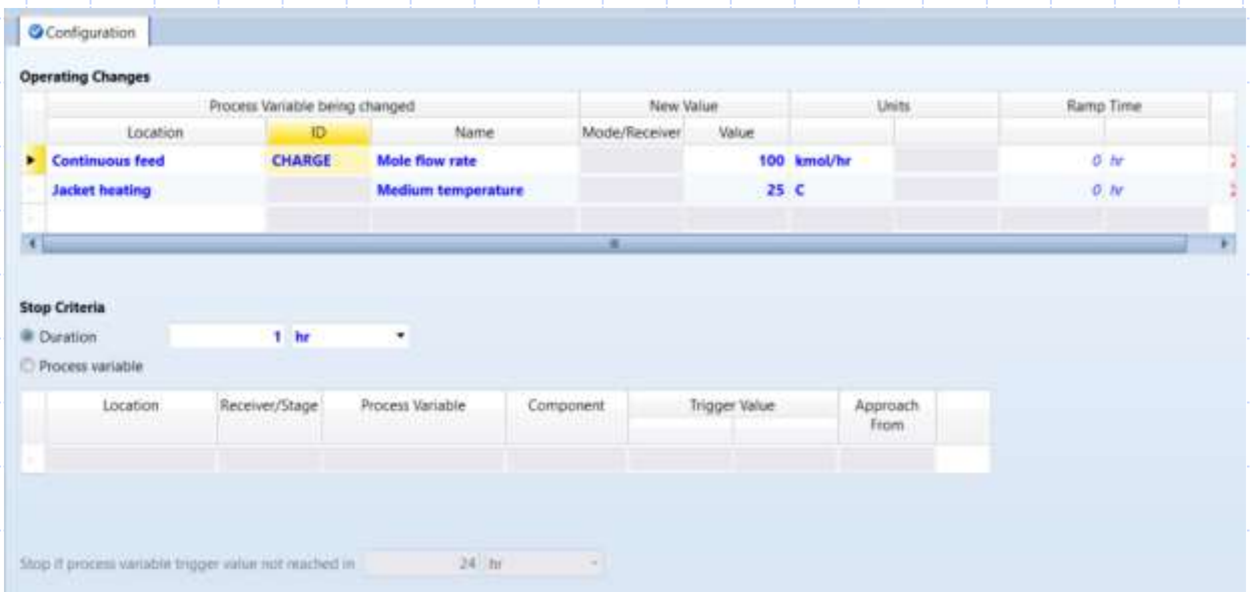
Operating Steps form

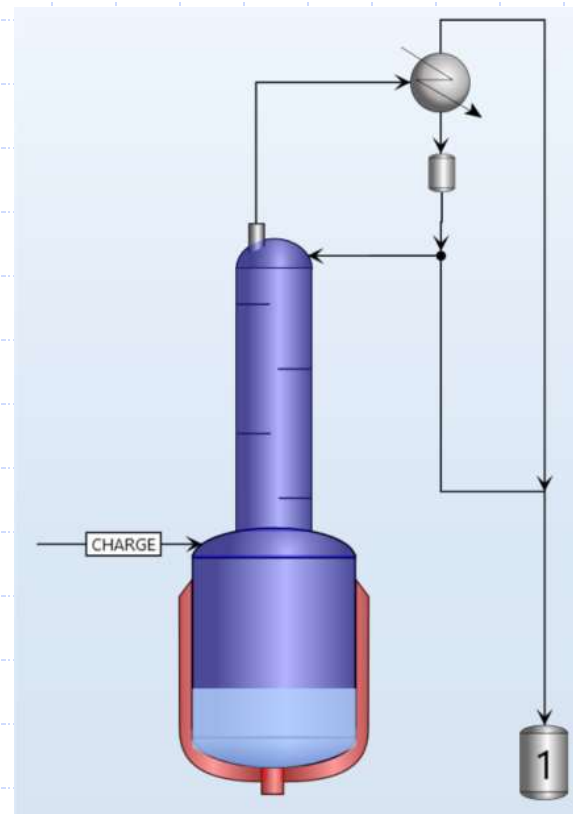
- It allows the user to specify the operating steps inside the equipment. Since batch distillation is a dynamic process, different operations need to be specified.
- Change operationg conditions such as charges, reflux ratio, heating, cooling, switch receiver, …
- All changes start at the same time
- 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

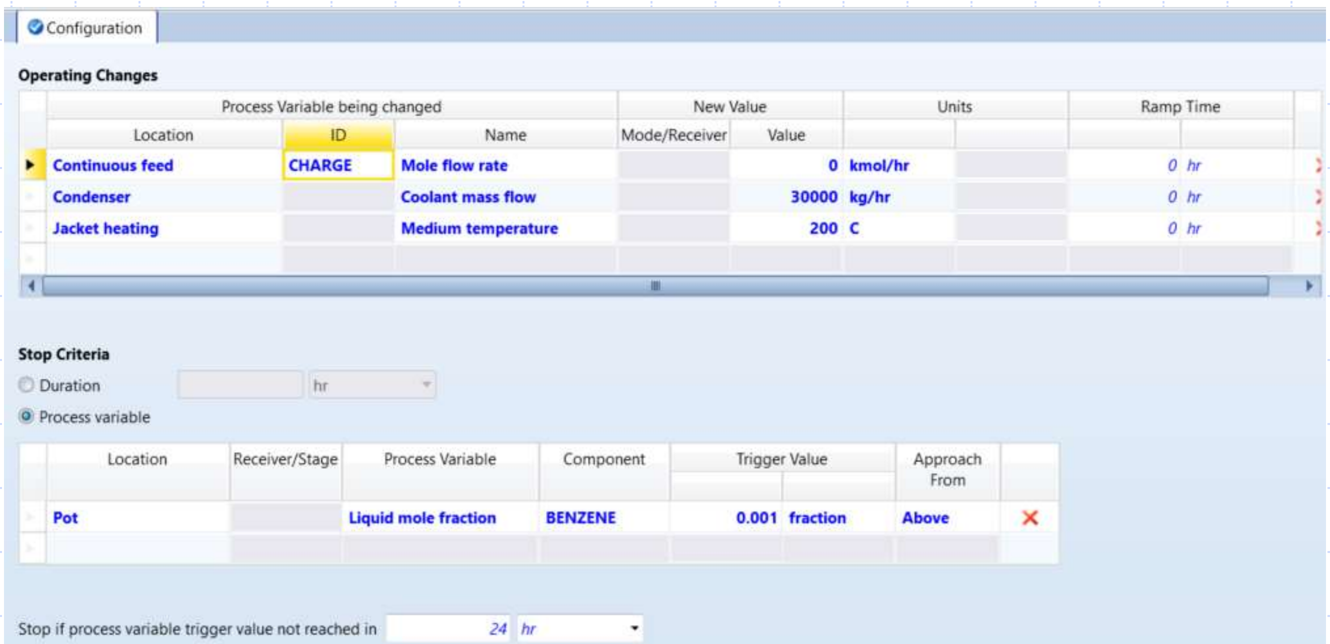
- We need to charge the pot with the continuous stream "CHARGE" until we reach 100 kmol of solution inside the vessel.
- How long do we need to let the operation last?

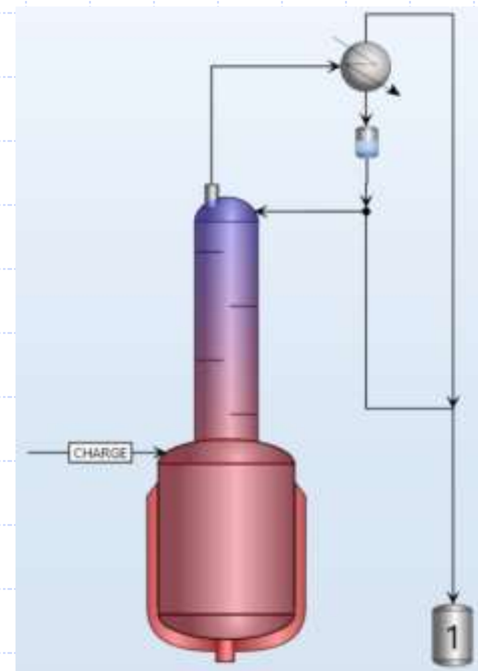




Distil Operation

- 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?





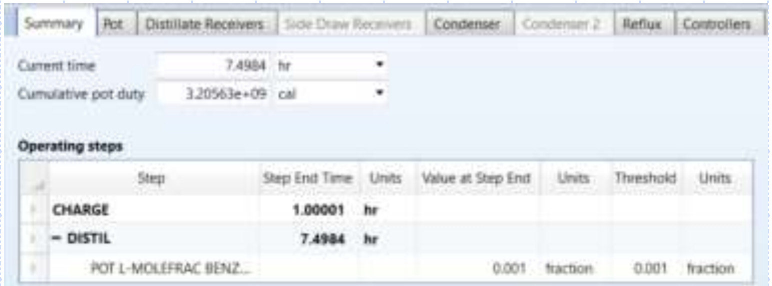
Final Conditions

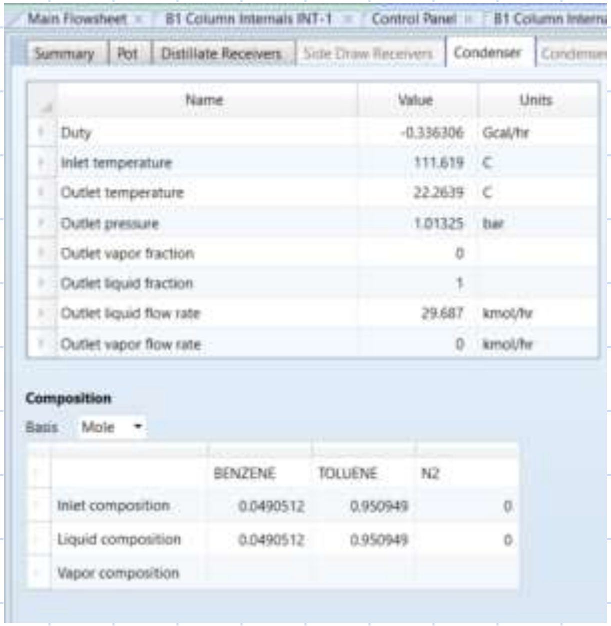
- Define what to do with the material in the column at the end of the batch:
  - Leave in place
  - Dump to Distillate receiver
  - Leave in place and recycle

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…

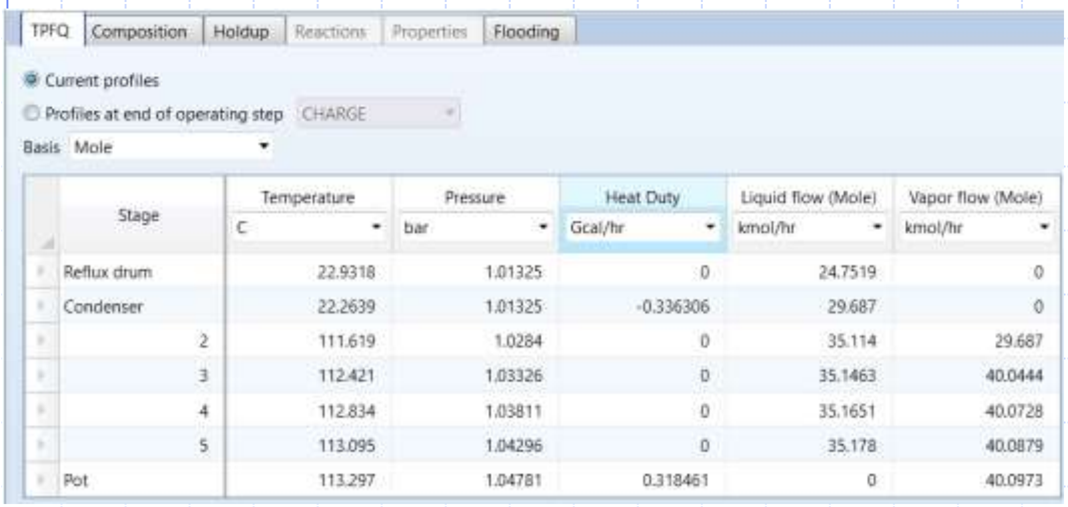




… and so on

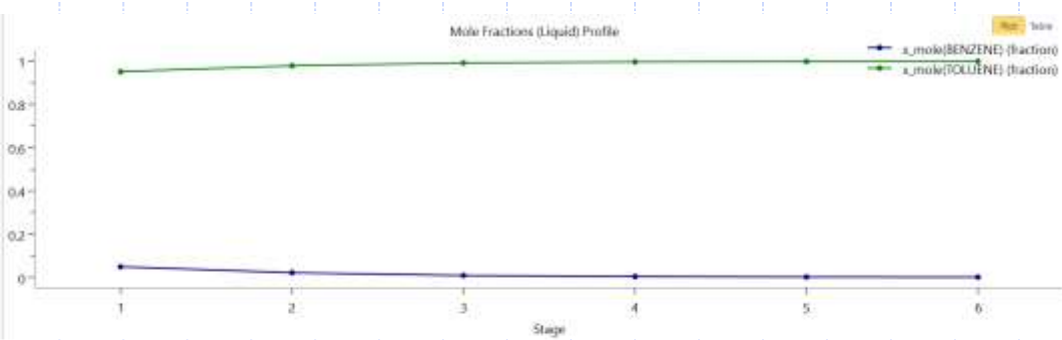
Profile Resuts

- **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

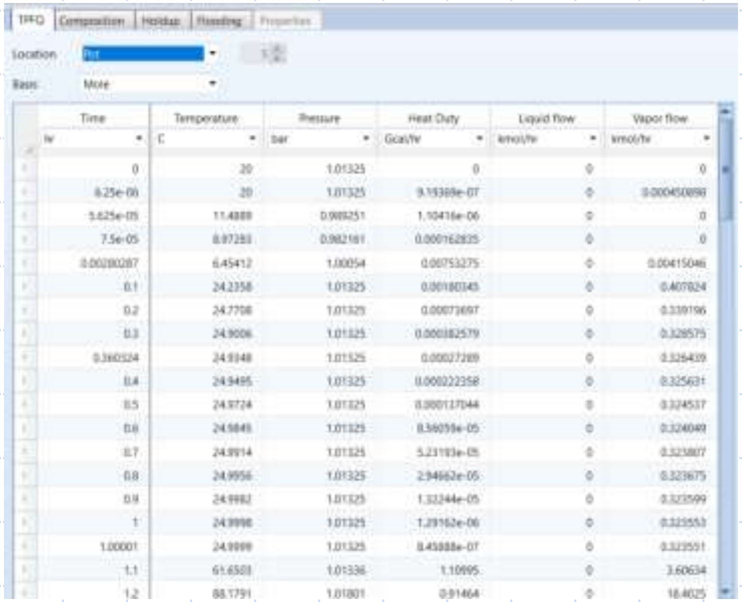
Stage	Temperature (C)
1	22.2639
2	111.619
3	112.421
4	112.834
5	113.095
6	113.297

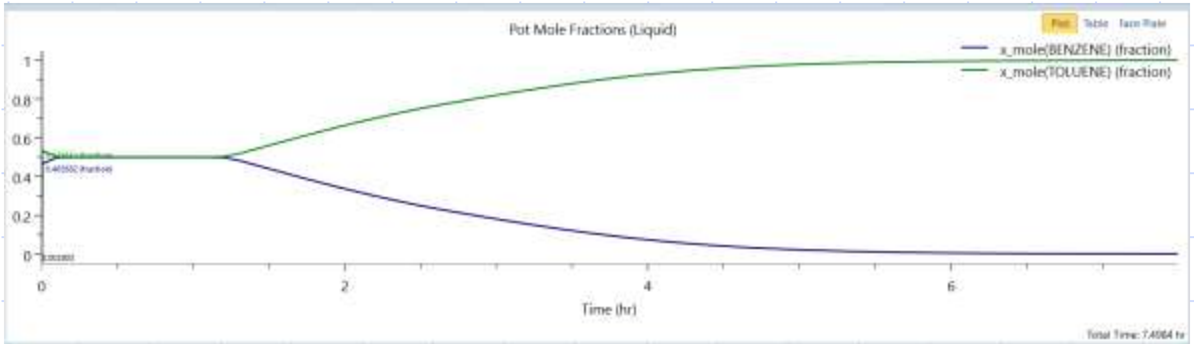


… and so on

Time Results

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





… and so on

Hands-on: batch simulation of benzene - toluene