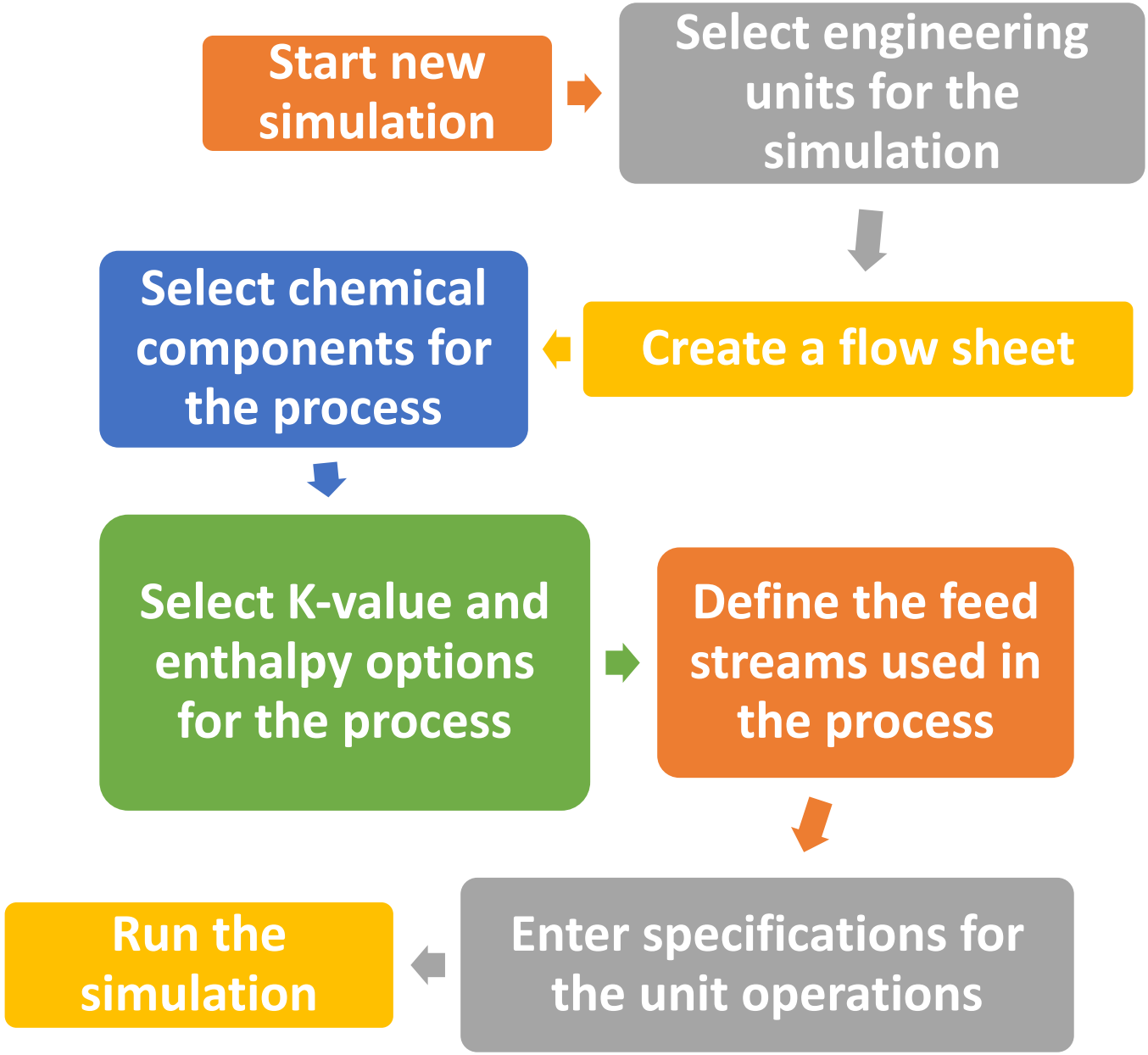
Introduction to CHEMCAD

Getting Started with CHEMCAD

- Creating flowsheets and running simulations is fast and easy with CHEMCAD
- The program is highly customizable to fit your needs and the way you work.
- The basic procedure for creating a simulation can be broken down into the following common steps ➔


Start new simulation
Select engineering units for the simulation
Create a flow sheet
Select chemical components for the process
Select K-value and enthalpy options for the process
Define the feed streams used in the process
Enter specifications for the unit operations
Run the simulation

Simple Example 1

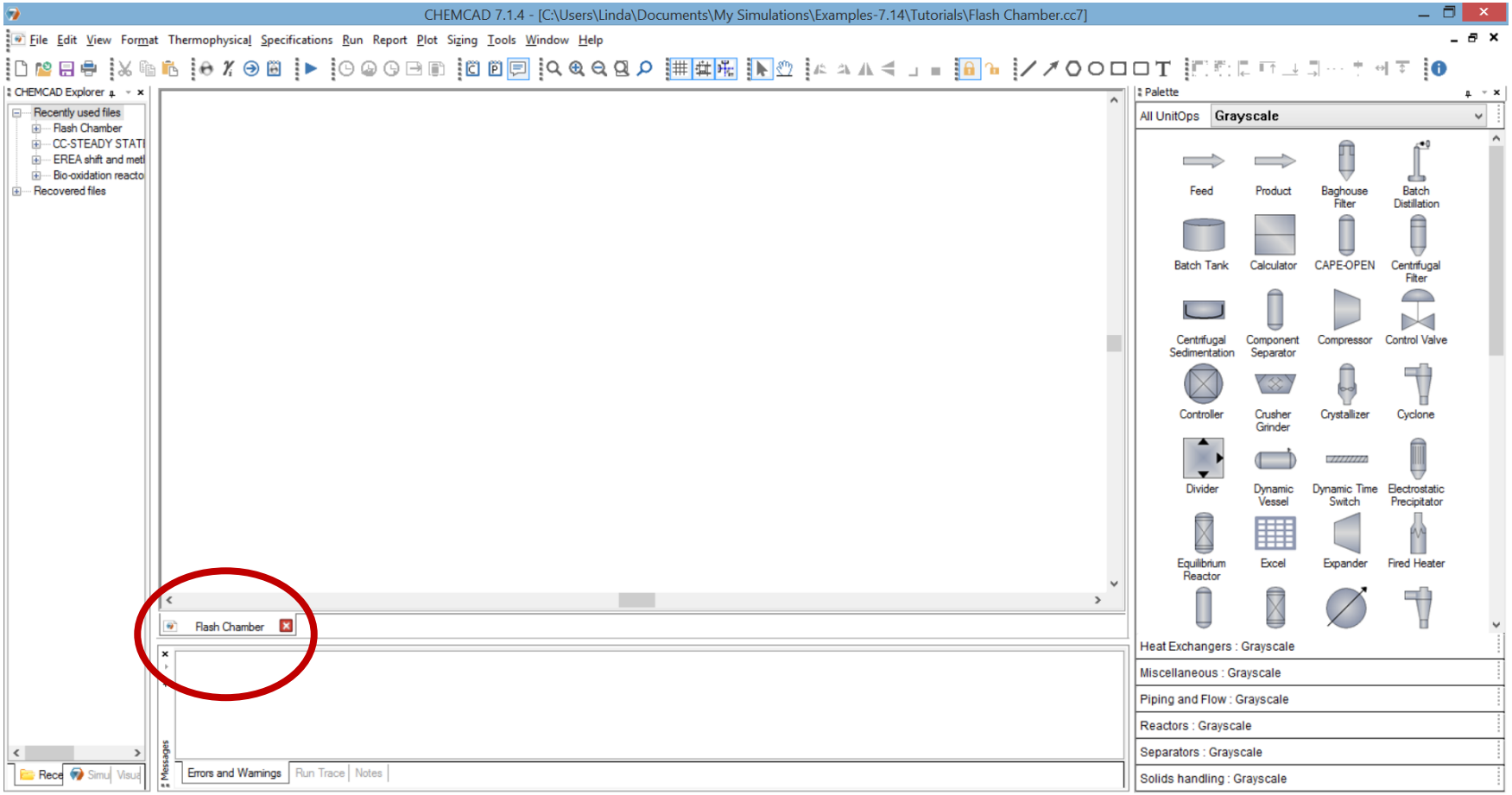
- A flash chamber operating at 80 °C (176 ° F) and 500 kPa (72.5 psia) is separating 1000 kg/hr (2204 lb/hr) of a feed that is 10 mol% Ethane, 5% Propane, 15% n-Butane, 10% n-Pentane, 12% iso-Pentane, 8% n-Hexane, 30% Heptane and 10% Nonane.
  - What are the product compositions and flow rates? Feed conditions are the same as that of the flash chamber.

Simple Example 1

- What are the product compositions and flow rates? Feed conditions are the same as that of the flash chamber.

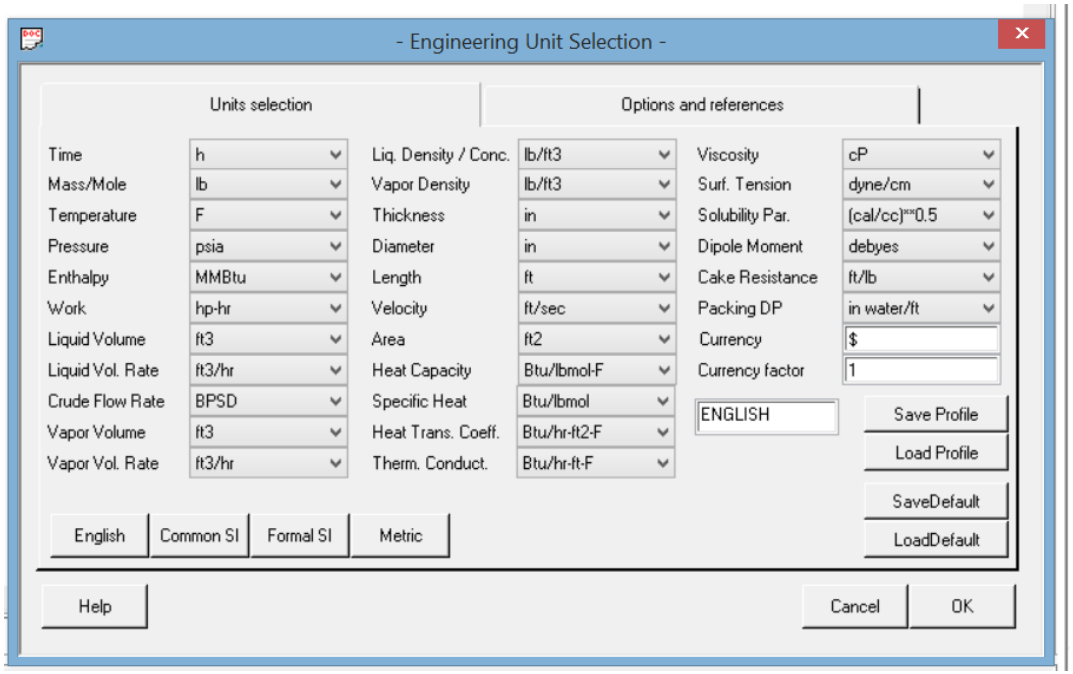
- **Solution Methodology**
  - **Step 1:**

    After you Start up CHEMCAD , start new simulation, how?
  - Select File>>Save as, then name your simulation Flash Chamber.


CHEMCAD 7.1.4 - [C:\Users\Linda\Documents\My Simulations\Examples-7.14\Tutorials\Flash Chamber.cc7]
File Edit View Format Thermophysical Specifications Run Report Plot Sizing Tools Window Help
CHEMCAD Explorer
Recently used files
Flash Chamber
CC-STEADY STATI
EREA shift and metl
Bio-oxidation reacto
Recovered files
Flash Chamber
Messages
Errors and Warnings
Run Trace
Notes
Palette
All UnitOps
Grayscale
Feed
Product
Baghouse Filter
Batch Distillation
Batch Tank
Calculator
CAPE-OPEN
Centrifugal Filter
Centrifugal Sedimentation
Component Separator
Compressor
Control Valve
Controller
Crusher Grinder
Crystallizer
Cyclone
Divider
Dynamic Vessel
Dynamic Time Switch
Electrostatic Precipitator
Equilibrium Reactor
Excel
Expander
Fired Heater
Heat Exchangers : Grayscale
Miscellaneous : Grayscale
Piping and Flow : Grayscale
Reactors : Grayscale
Separators : Grayscale
Solids handling : Grayscale

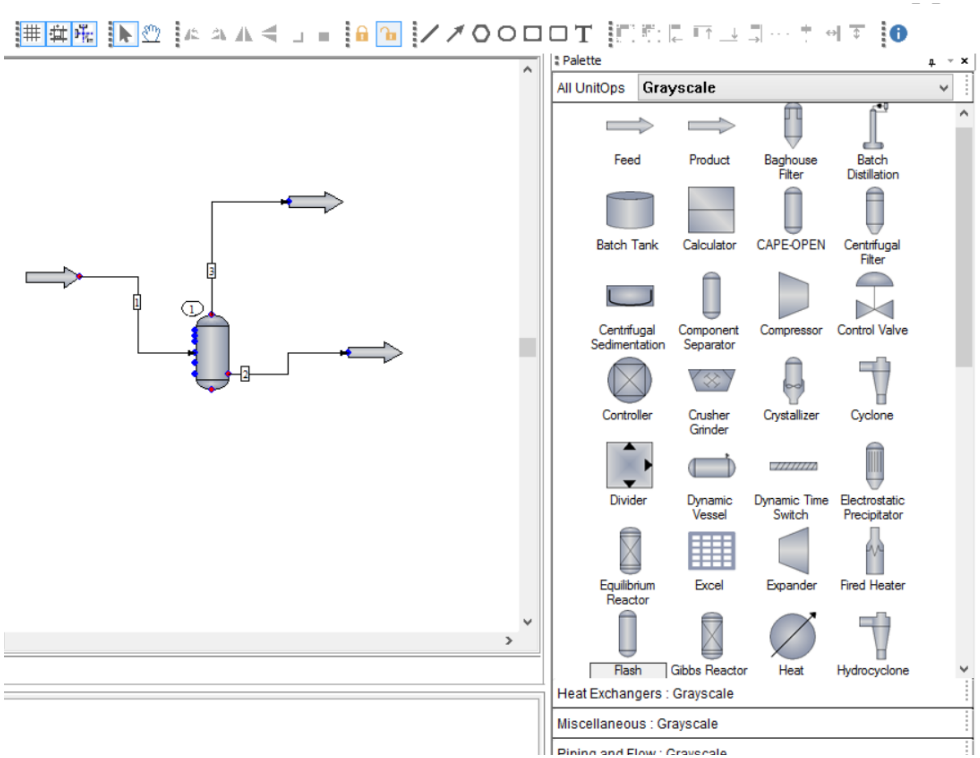
Simple Example 1

- **Step 2:**
  - Select engineering units that you will use for your simulation.
  - Select Format>> Engineering Unit>>
    Select default setting in English units.



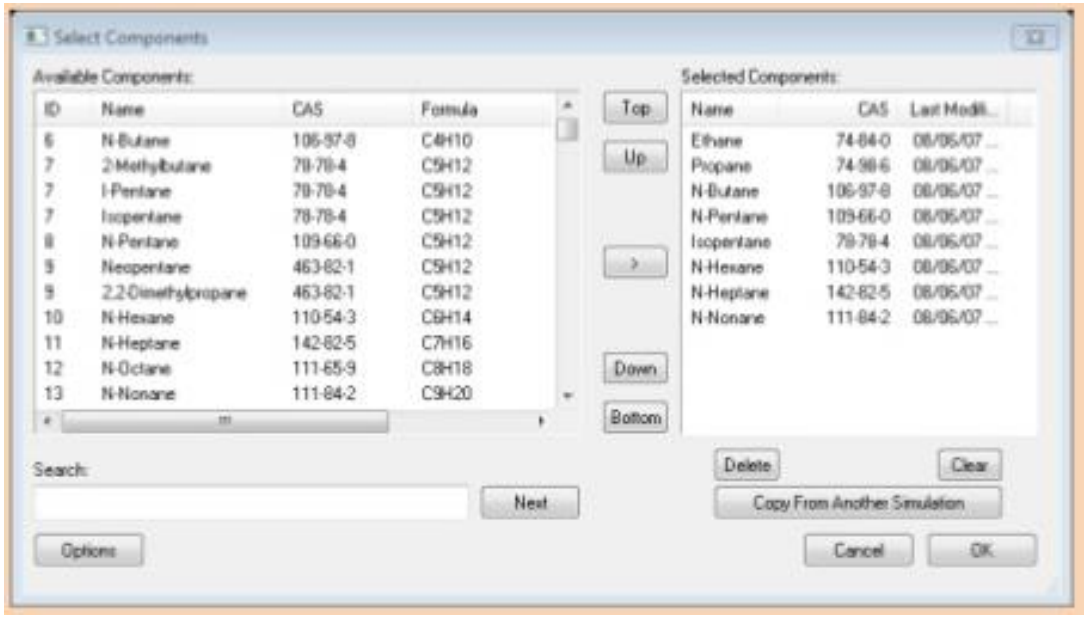
Simple Example 1

- **Step3: Create flowsheet**
  - First you need to select the piece(s) of equipment you desire, from **All UnitOps** tap select **Feed arrow**, two **product arrows** , and **Flash**.
  - Then select Stream to connect Flash with in and outputs arrows.
  - After connecting press ESC



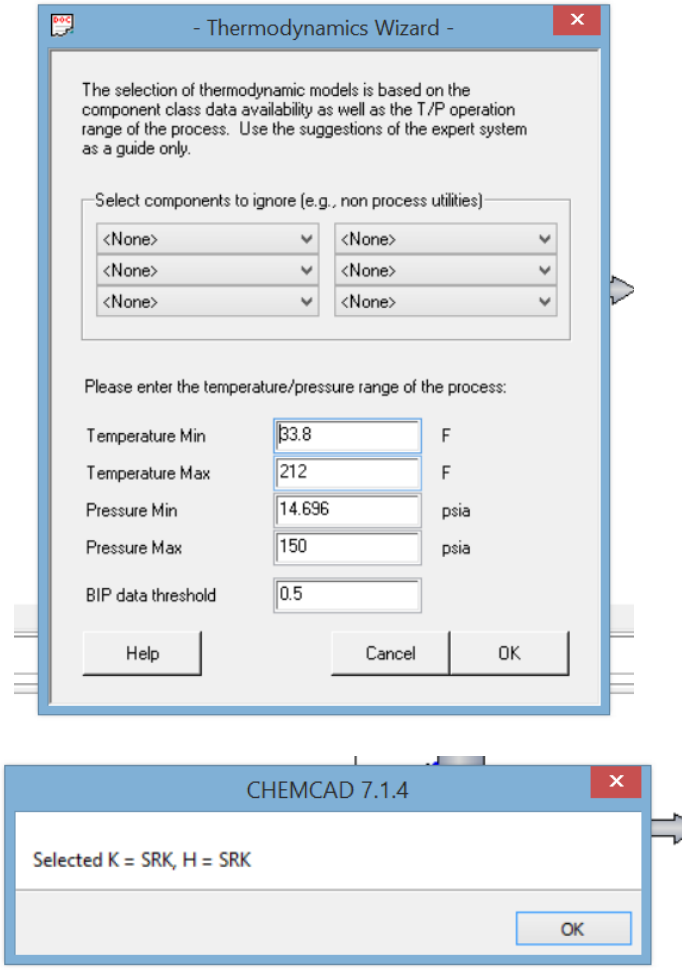
Simple Example 1

- **Step 4: Select chemical components for the process**
  - Here we have (Ethane, Propane, n-Butane, n-Pentane, iso-Pentane, n-Hexane, Heptane and Nonane)
  - From toolbar select ,or select Thermophysical>>Select components.. from available component select desired components and then press OK



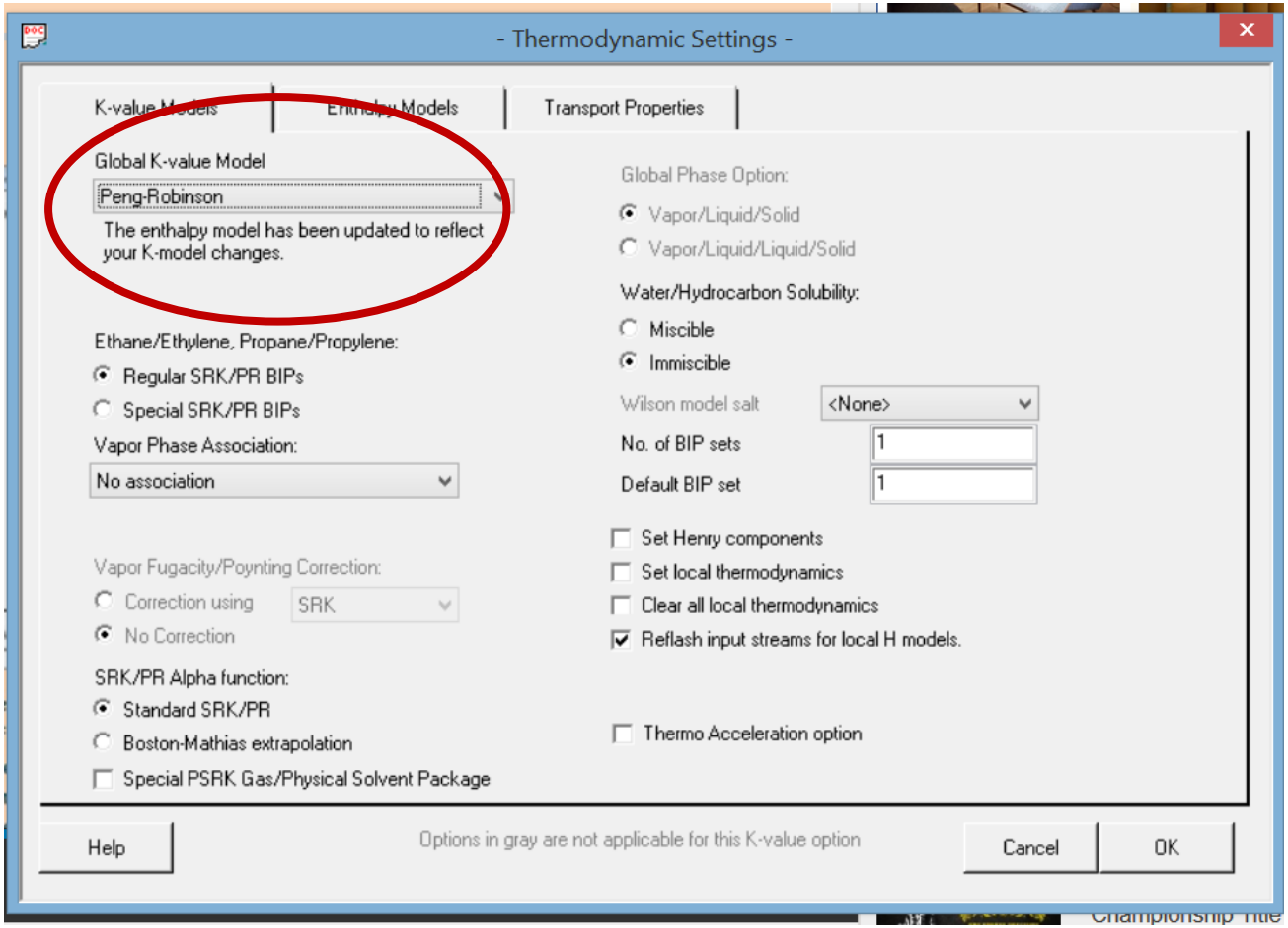
Simple Example 1

- **Step 5: Select K-value and enthalpy options for the process**
  - After selecting the desired components thermodynamic wizard window open to let the user enter pressure/temperature range for the process or you can use the default range;
    - These input let the program choose the suitable thermodynamic models.



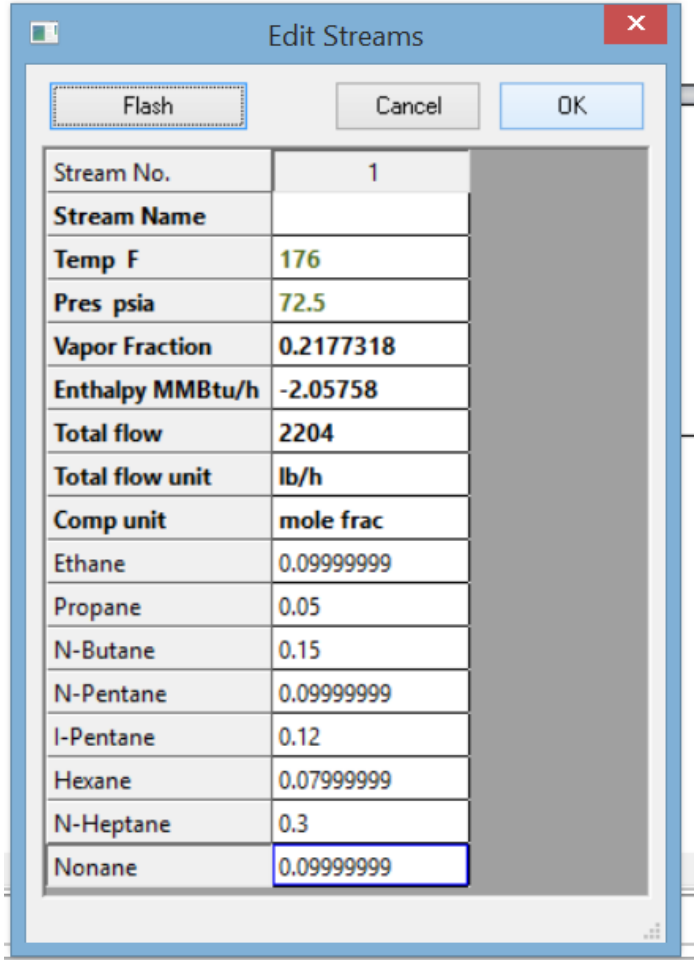
Simple Example 1

- **Step 5: Select K-value and enthalpy options for the process**
  - After pressing OK, the program choose thermodynamic process for your process. Press OK, and the program open a thermodynamic setting
    - If you accept the default thermodynamic model by program press OK, if not change it, from global K values option select the thermodynamic model that you want
    - Here want to change **SRK to Peng-Robinson.**


- Thermodynamic Settings -
K-value Models
Enthalpy Models
Transport Properties
Global K-value Model
Peng-Robinson
The enthalpy model has been updated to reflect your K-model changes.
Ethane/Ethylene, Propane/Propylene:
Regular SRK/PR BIPs
Special SRK/PR BIPs
Vapor Phase Association:
No association
Vapor Fugacity/Poynting Correction:
Correction using
SRK
No Correction
SRK/PR Alpha function:
Standard SRK/PR
Boston-Mathias extrapolation
Special PSRK Gas/Physical Solvent Package
Global Phase Option:
Vapor/Liquid/Solid
Vapor/Liquid/Liquid/Solid
Water/Hydrocarbon Solubility:
Miscible
Immiscible
Wilson model salt
<None>
No. of BIP sets
1
Default BIP set
1
Set Henry components
Set local thermodynamics
Clear all local thermodynamics
Reflash input streams for local H models.
Thermo Acceleration option
Help
Options in gray are not applicable for this K-value option
Cancel
OK

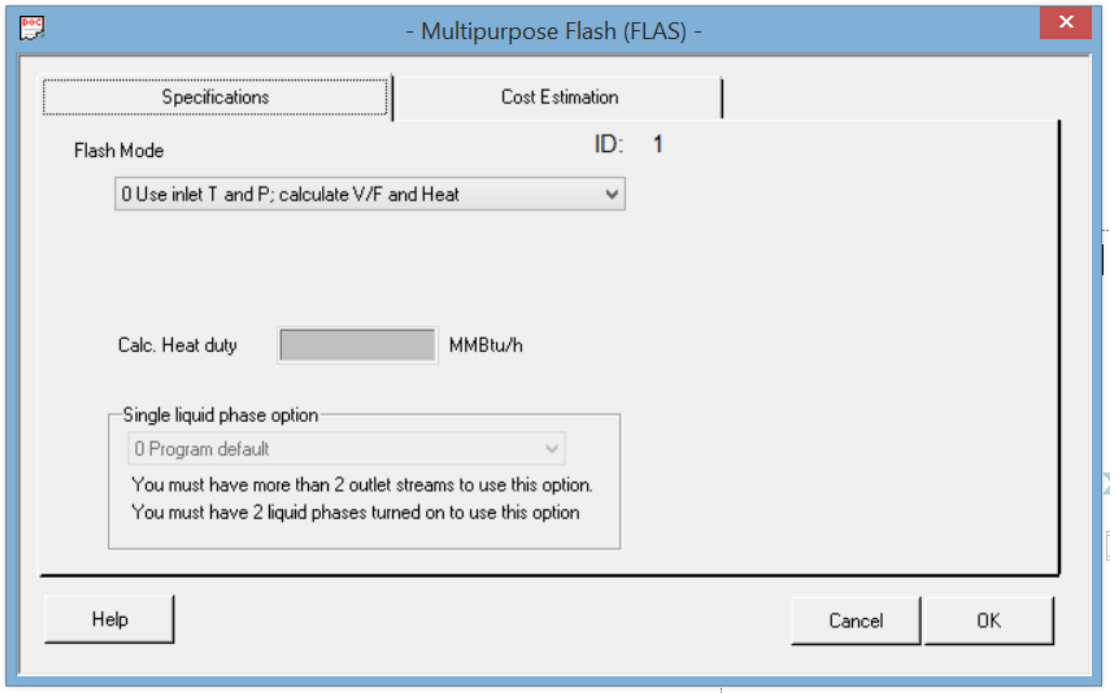
Simple Example 1

- **Step 6: Define the feed streams**
  - Double click on stream 1 entering to the flash separator
  - Enter the name to the stream (optional)
  - Specify temperature and pressure and the enthalpy and vapor fraction calculated automatically
    - OR
  - Specify pressure and vapor fraction and the enthalpy and temperature calculated and so on..
  - After you entered the required data press **flash**, then vapor fraction and enthalpy calculated, after that press OK to transport the next step.



Simple Example 1

- **Step 7: specify the flash**
  - Double click on flash unit operation
  - Since the feed conditions are same as that flash use the 0 mode for flash mode, then press OK.

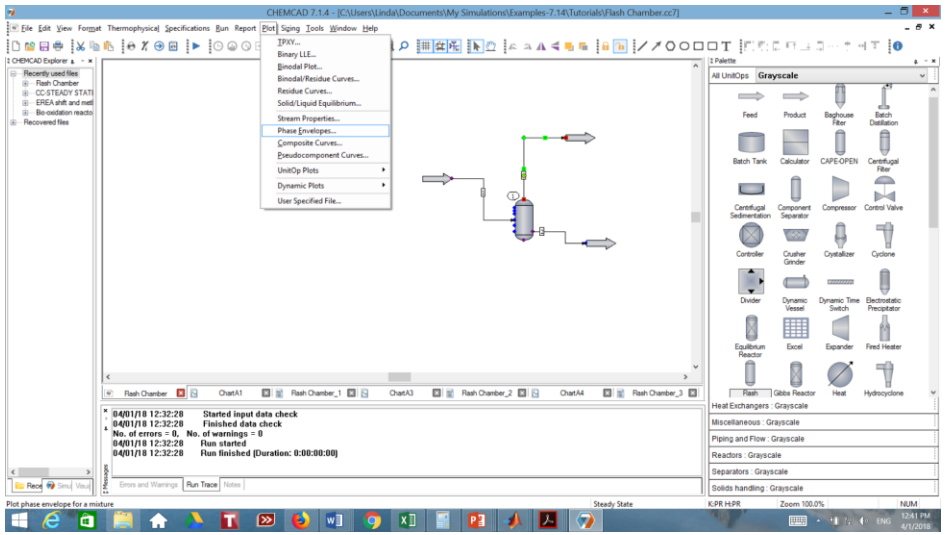


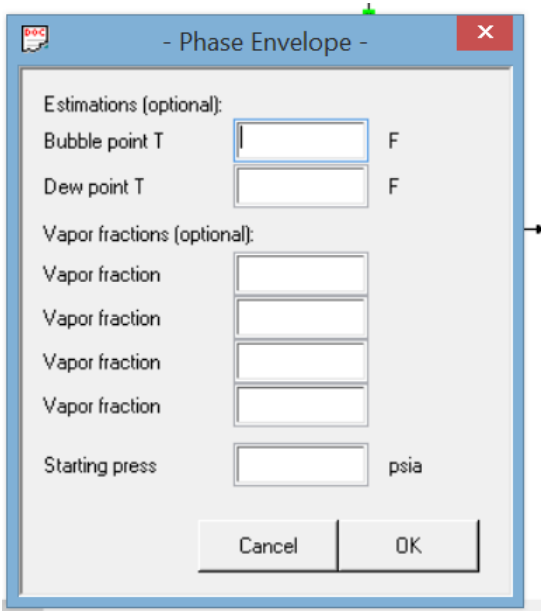
Simple Example 1

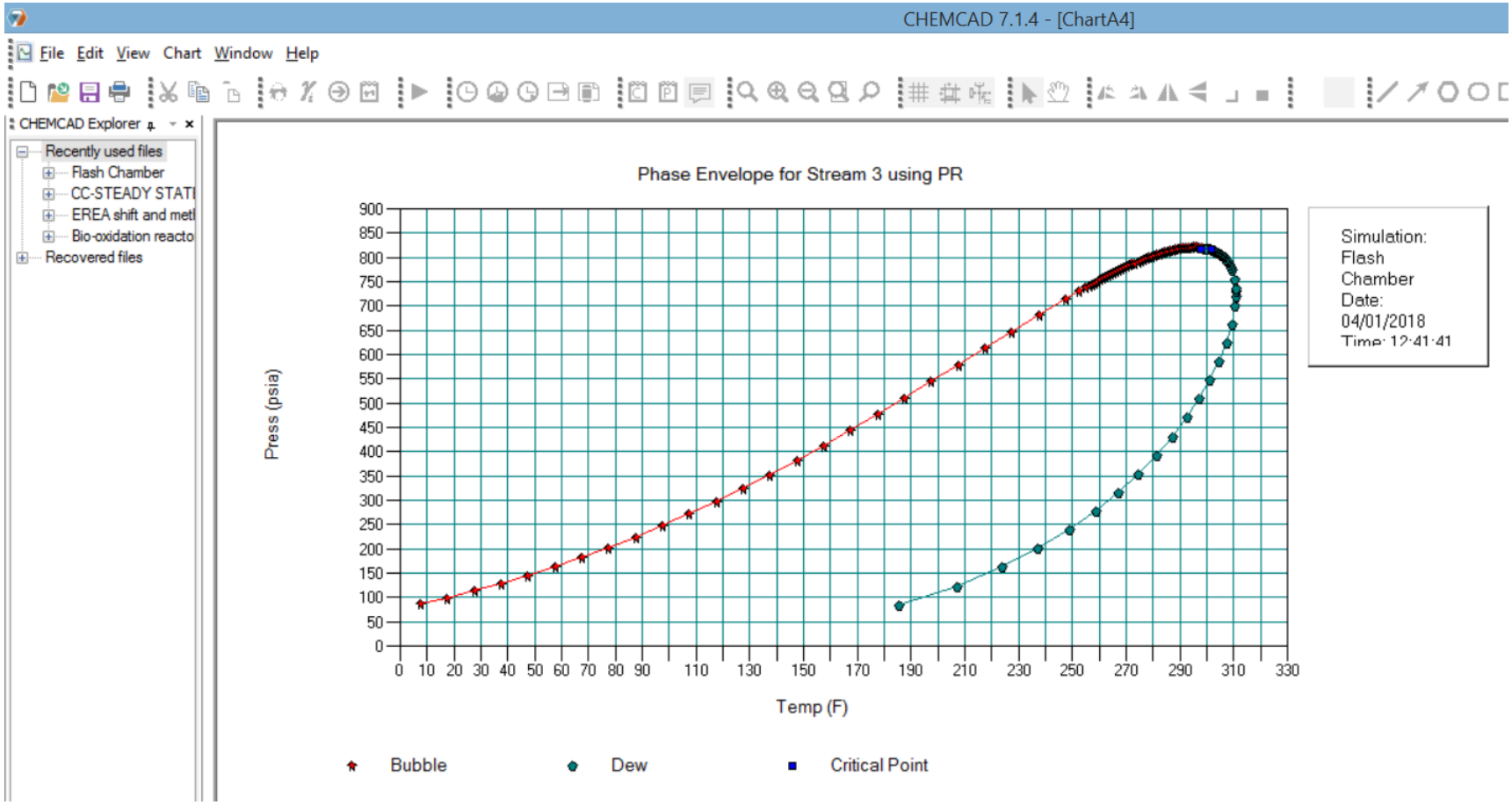
- **Step 8:**
  - from run list choose Run>>Run all, or from toolbar press  to run the simulation.
  - After running simulation check the outputs by:
    1. Double click on stream 2 & 3
    2. go to specifications >> select streams >> write the number of streams or click on them one by one.

Simple Example 1

- **Plot Results:**
  - For example to check the dew and bubble points for the vapor (stream 3):
    1. Select stream 3
       >> Plot
       >> Phase Envelop
       >> select streams
    2. All information in this window is optional
    3. press OK

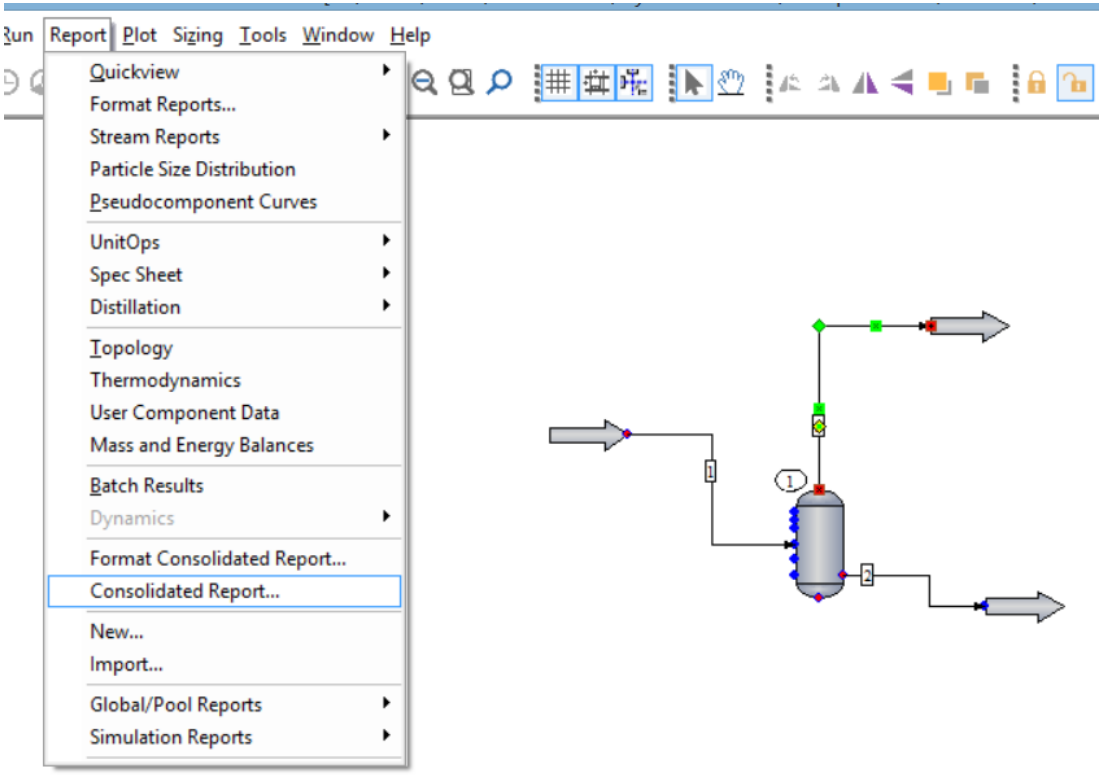


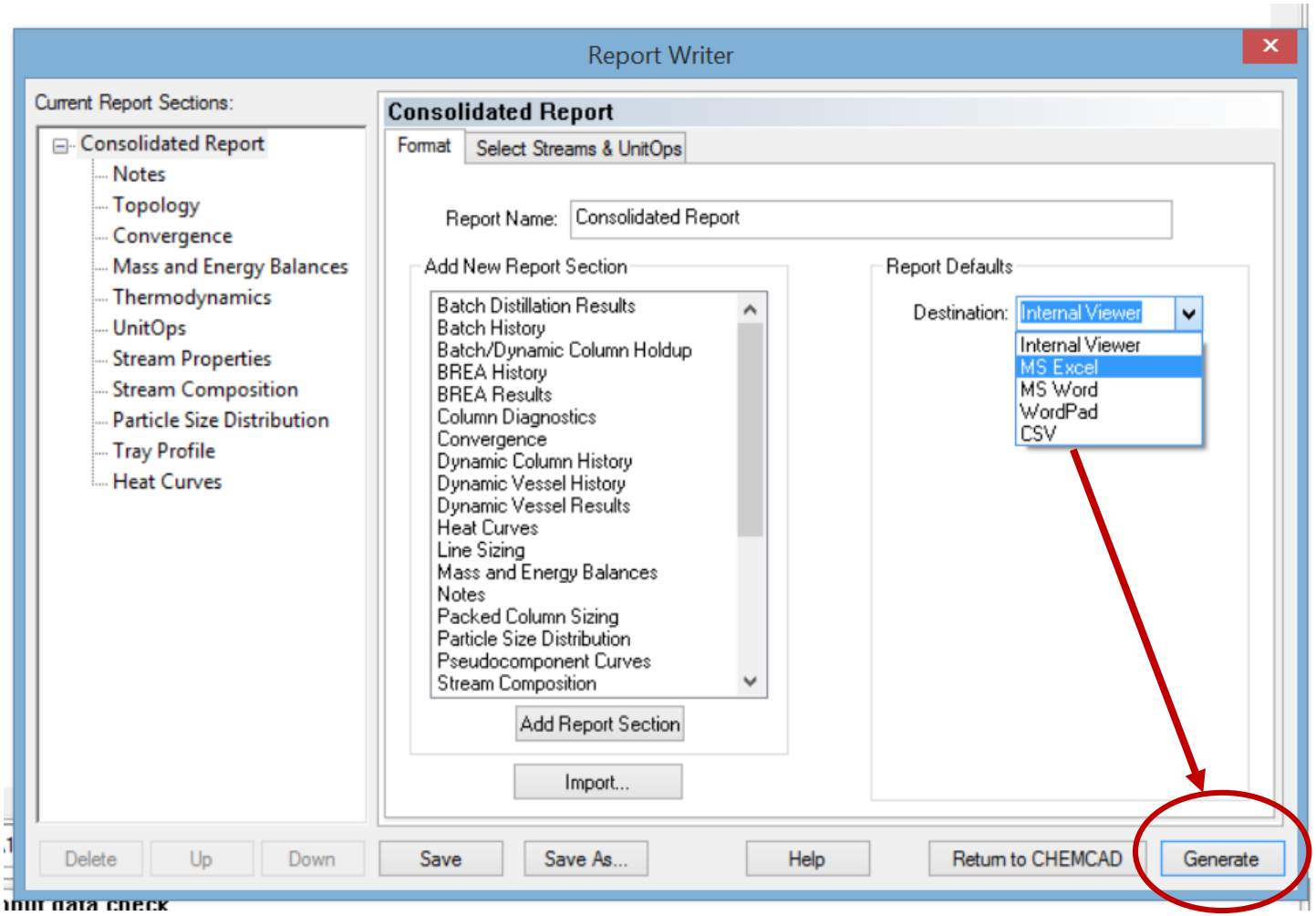



CHEMCAD 7.1.4 - [ChartA4]
File Edit View Chart Window Help
CHEMCAD Explorer
Recently used files
Flash Chamber
CC-STEADY STATI
EREA shift and metl
Bio-oxidation reacto
Recovered files
Phase Envelope for Stream 3 using PR
Press (psia)
900
850
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
0 10 20 30 40 50 60 70 80 90 110 130 150 170 190 210 230 250 270 290 310 330
Temp (F)
Simulation:
Flash
Chamber
Date:
04/01/2018
Time: 12:41:41
Bubble
Dew
Critical Point

Simple Example 1

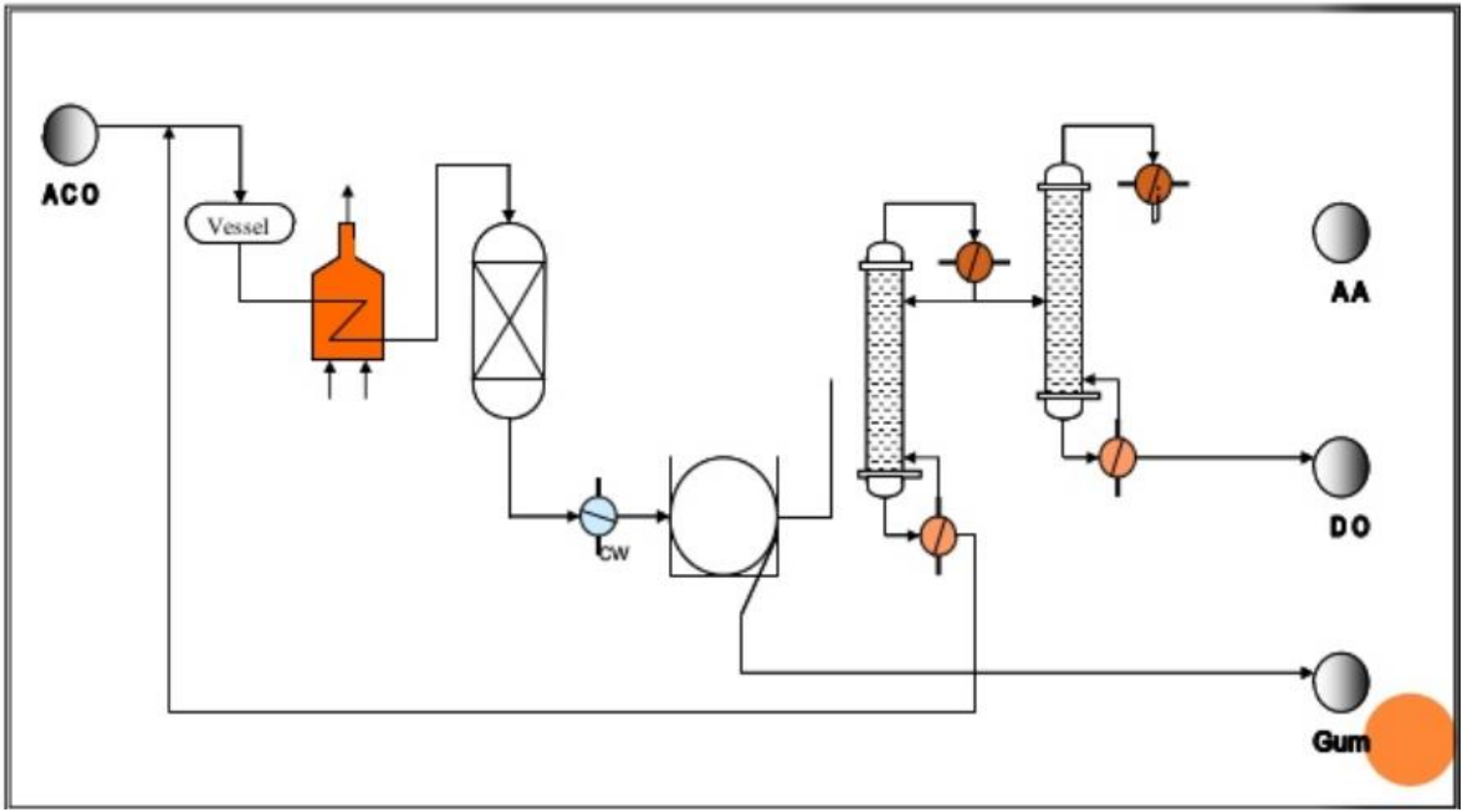
- **Producing Report**
  - Report
    >> Consolidated Report
    >> Report Format
    >> Choose output for report
    (Word or Excel)
  - We will choose Excel
    >> Generate
    >> calculate and Give Result




Report Writer
Current Report Sections:
Consolidated Report
Notes
Topology
Convergence
Mass and Energy Balances
Thermodynamics
UnitOps
Stream Properties
Stream Composition
Particle Size Distribution
Tray Profile
Heat Curves
Consolidated Report
Format
Select Streams & UnitOps
Report Name:
Consolidated Report
Add New Report Section
Batch Distillation Results
Batch History
Batch/Dynamic Column Holdup
BREA History
BREA Results
Column Diagnostics
Convergence
Dynamic Column History
Dynamic Vessel History
Dynamic Vessel Results
Heat Curves
Line Sizing
Mass and Energy Balances
Notes
Packed Column Sizing
Particle Size Distribution
Pseudocomponent Curves
Stream Composition
Add Report Section
Import...
Report Defaults
Destination:
Internal Viewer
Internal Viewer
MS Excel
MS Word
WordPad
CSV
Delete
Up
Down
Save
Save As...
Help
Return to CHEMCAD
Generate

Example 2

1-TETRADECENE PLANT PROCESS FLOWSHEET



MATERIAL BALANCE

$$C_{16}H_{32}O_2 \rightarrow CH_3COOH + C_{14}H_{28}$$

(Acetylated castor oil) **(acetic acid)** **(1-tetradecene)**

$$2C_{14}H_{28} \rightarrow C_{28}H_{56}$$

(1-tetradecene) **(1-octadecene)**

Production rate = 100tonne/yr of 1-Tetradecene

= 12.6264 kg/hr

Feed required = 148.2228 tonne/yr (ACO)

= 18.715 kg/hr

MIXING VESSEL:

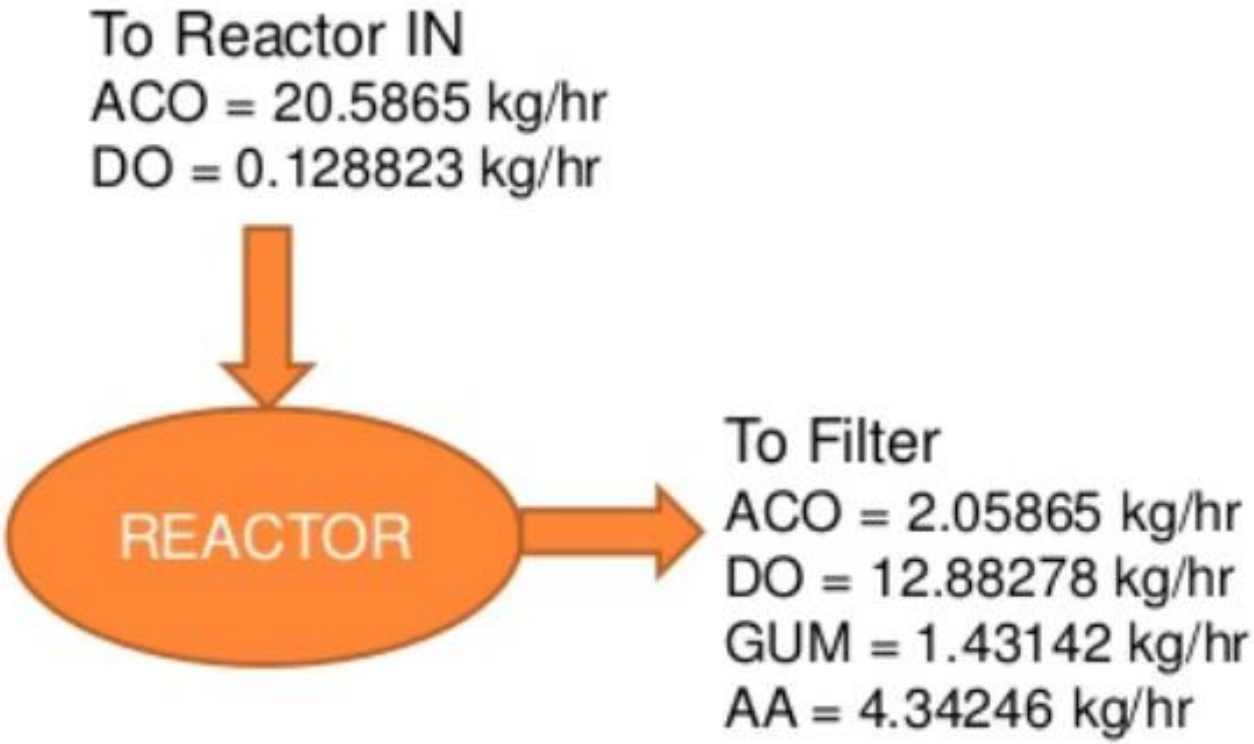
Feed IN
ACO=18.52685 kg/hr

Recycle IN
ACO=2.05865 kg/hr
DO=0.128823 kg/hr

To Reactor OUT
ACO = 20.5865 kg/hr
DO = 0.128823

Total IN = Total OUT = 20.715323 kg/hr

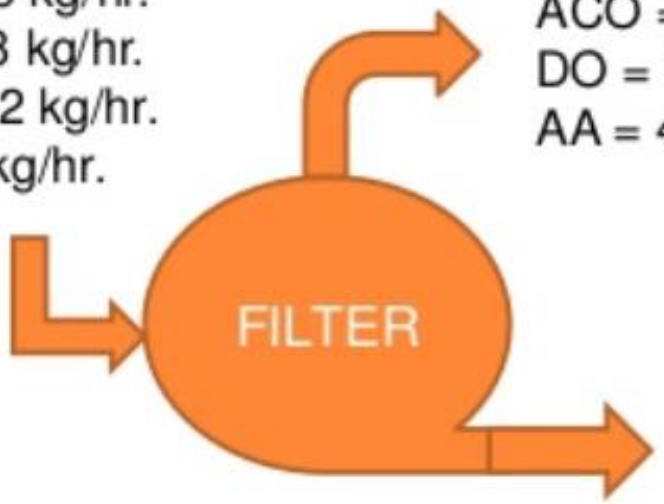
REACTOR:



Total IN = Total OUT = 20.71531 kg/hr

FILTER:

To Filter IN
ACO = 2.05865 kg/hr.
DO = 12.88278 kg/hr.
GUM = 1.43142 kg/hr.
AA = 4.34246 kg/hr.

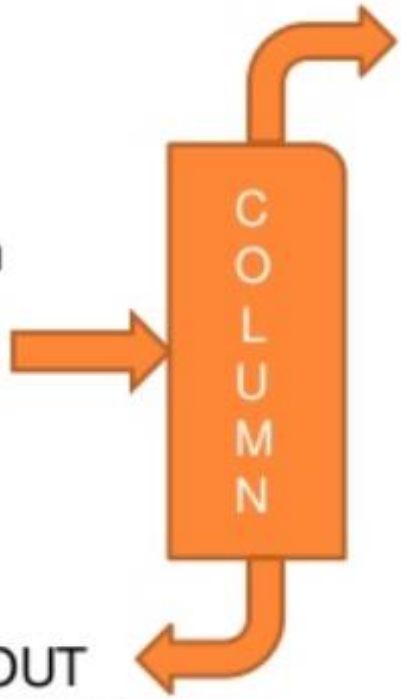


OUT To Recycle Column
ACO = 2.05865 kg/hr.
DO = 12.88278 kg/hr.
AA = 4.34246 kg/hr.

Gum OUT = 1.43142 kg/hr.

Total IN = Total OUT = 20.71531 kg/hr.

ACO RECYCLE COLUMN:



OUT To Purification Column 2
AA = 4.34246 kg/hr.
DO = 12.75395 kg/hr.

IN To Recycle Column
ACO = 2.05865 kg/hr.
DO = 12.88278 kg/hr.
AA = 4.34246 kg/hr.

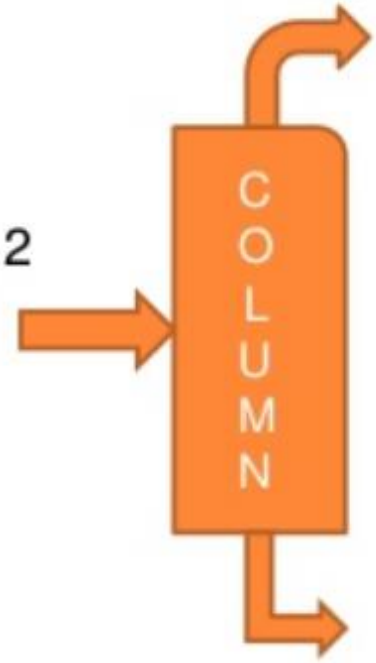
Recycle OUT
ACO = 2.05865 kg/hr.
DO = 0.1288278 kg/hr.

Total IN = Total OUT = 19.28389 kg/hr.

DO Purification Column:

Product OUT
AA = 4.2990 kg/hr.
DO = 0.127539 kg/hr.

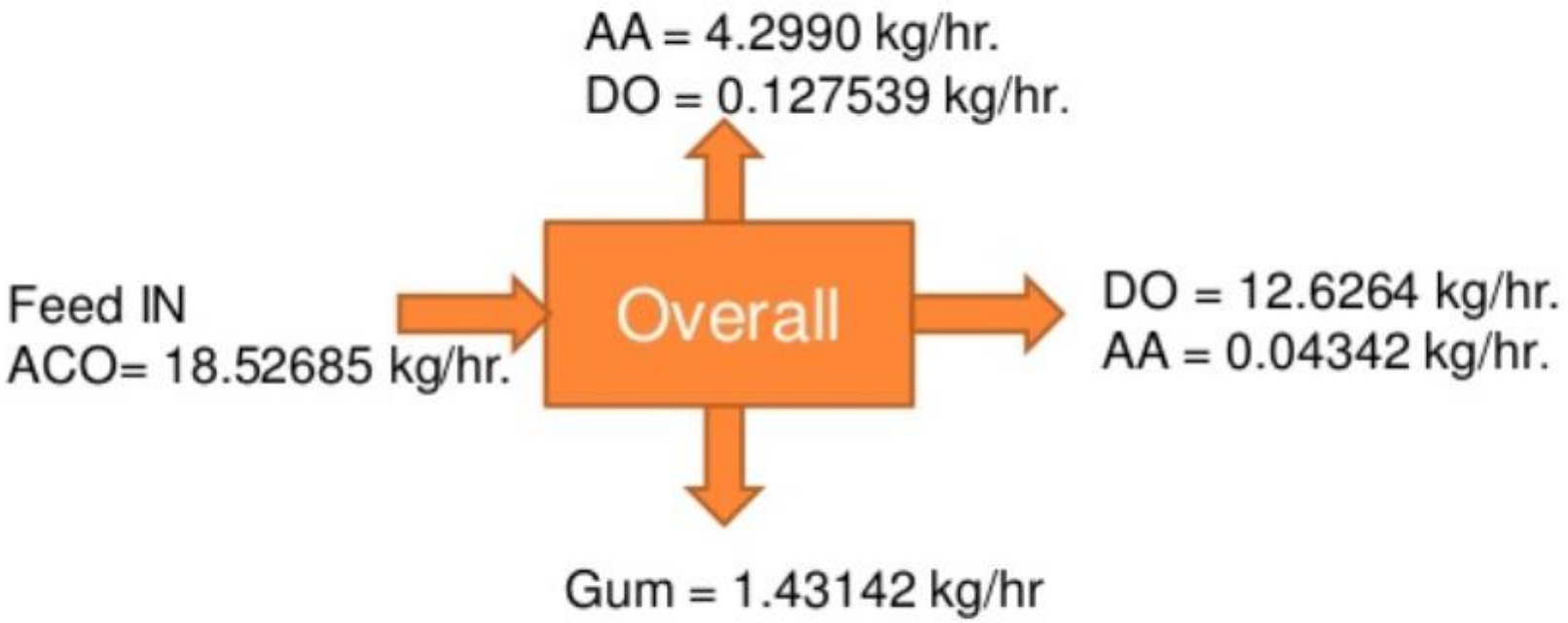
IN To Distillation column 2
AA = 4.34246 kg/hr.
DO = 12.75395 kg/hr.



Product OUT
DO = 12.6264 kg/hr.
AA = 0.04342 kg/hr.

Total IN = Total OUT = 17.09641 kg/hr.

OVERALL MASS BALANCE:



Feed IN = Feed OUT

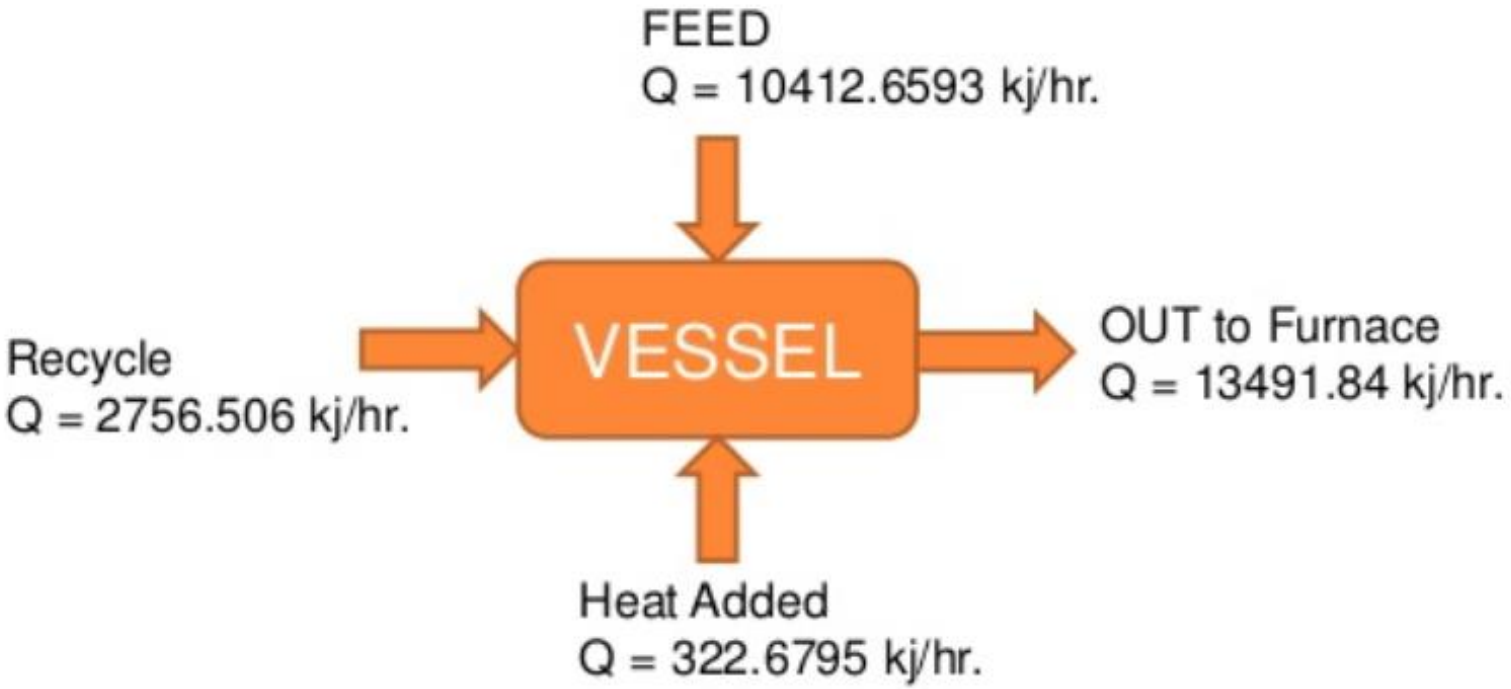
ACO = AA + DO + GUM

18.52685 kg/hr. = 17.528 kg/hr.

BALANCED

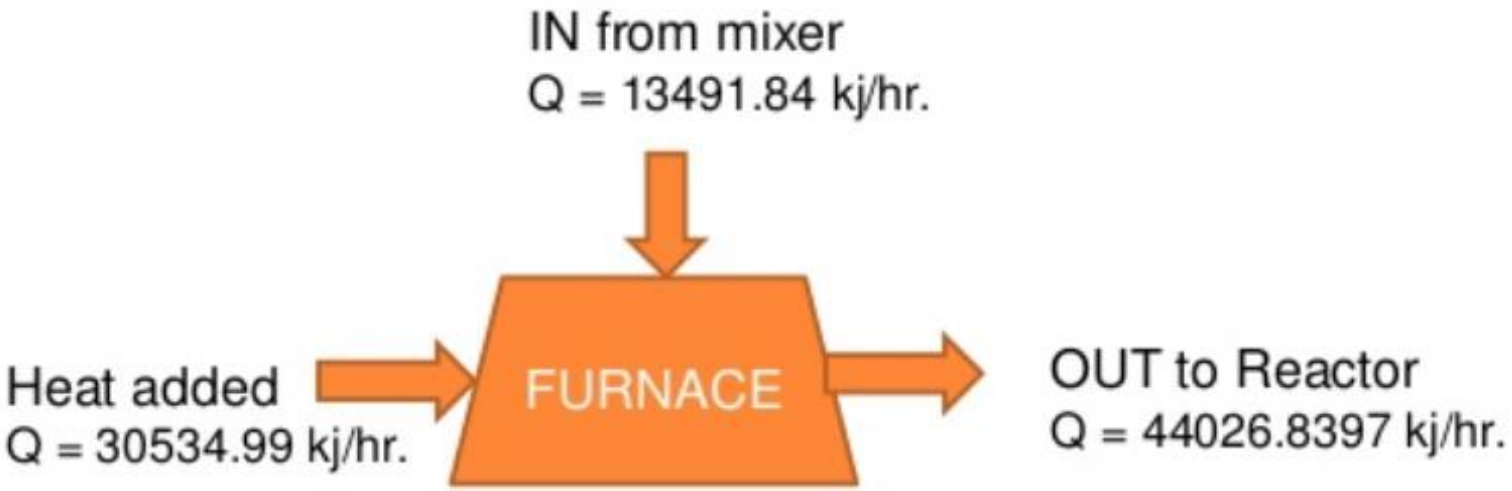
ENERGY BALANCE

MIXING VESSEL:



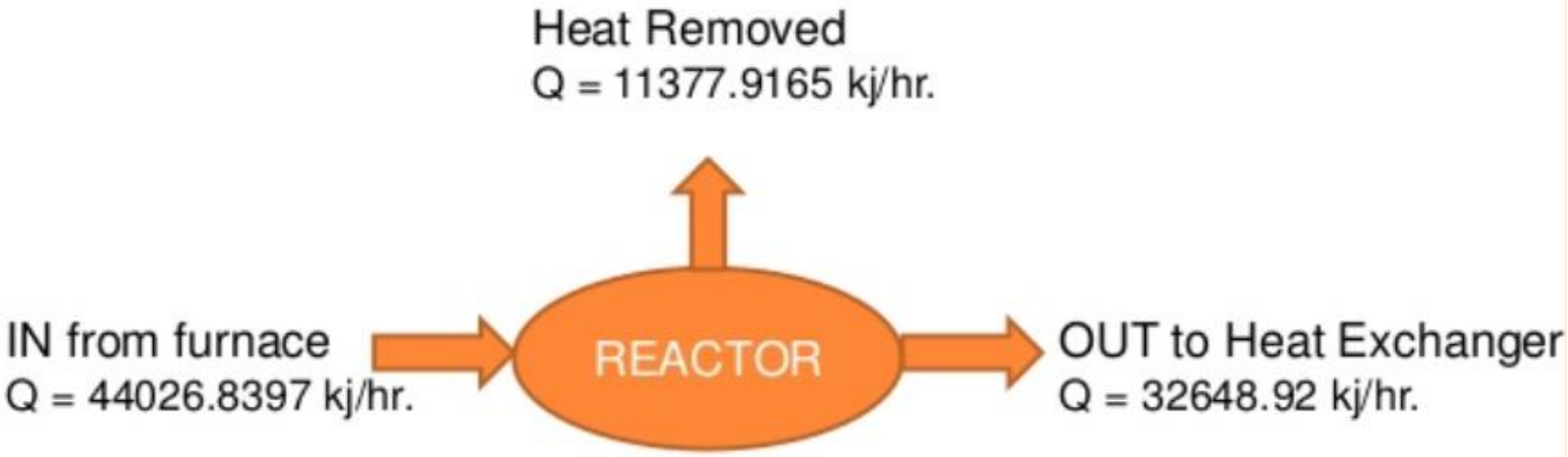
Total IN = Total OUT = 3491.84 kj/hr.

FURNACE:



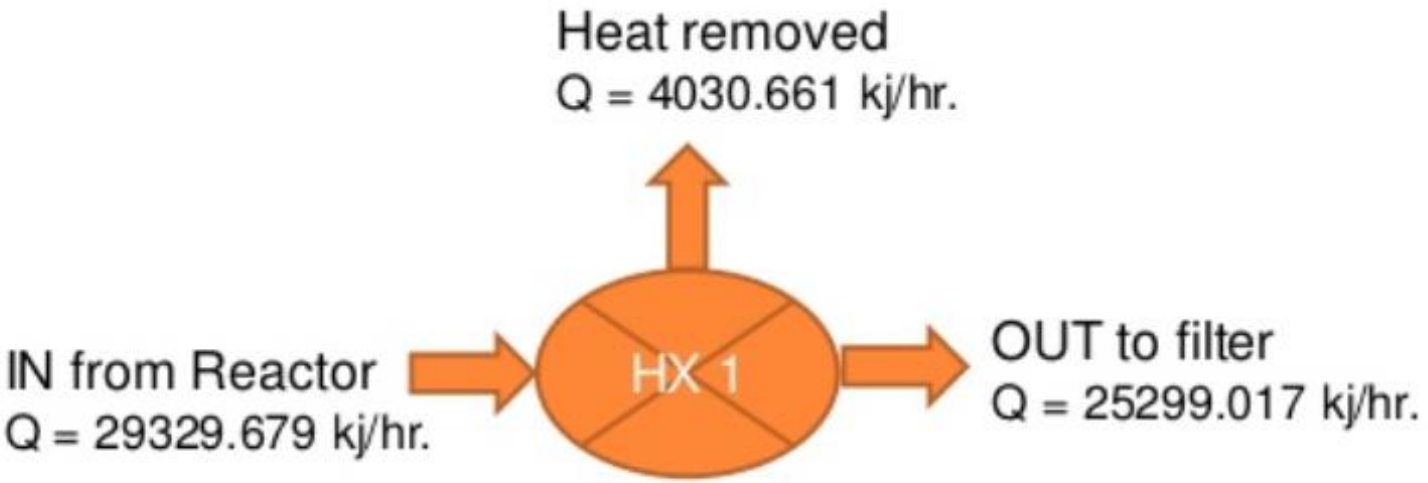
Total IN = Total OUT = 44026.8397 kj/hr.

REACTOR:



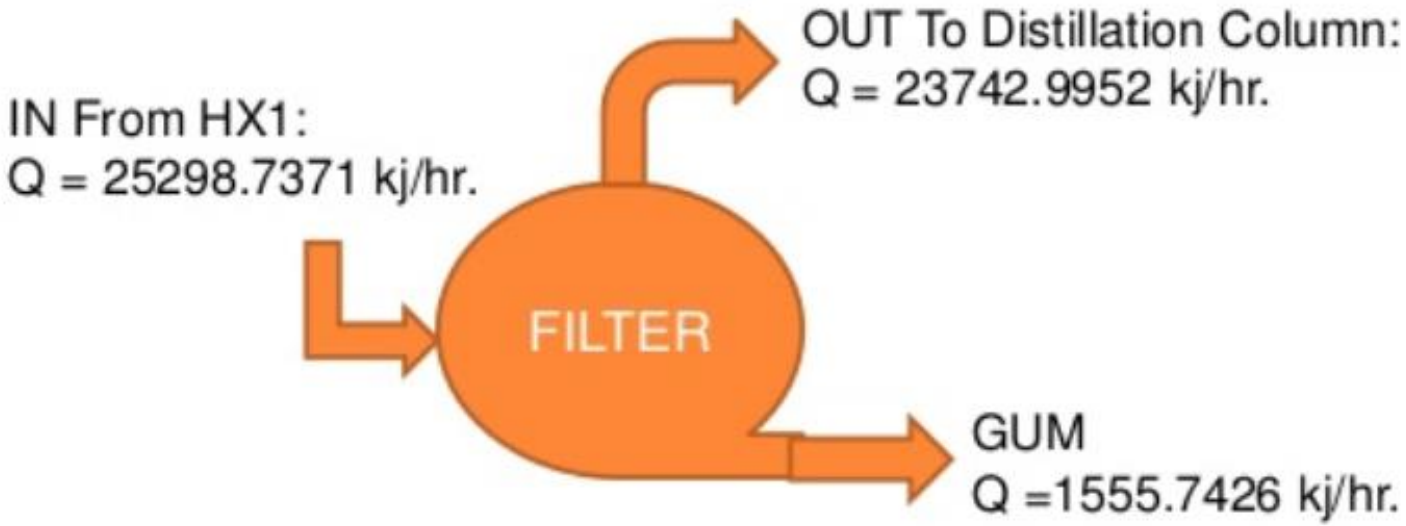
Total IN = Total OUT = 44026.8397 kj/hr.

HEAT EXCHANGER



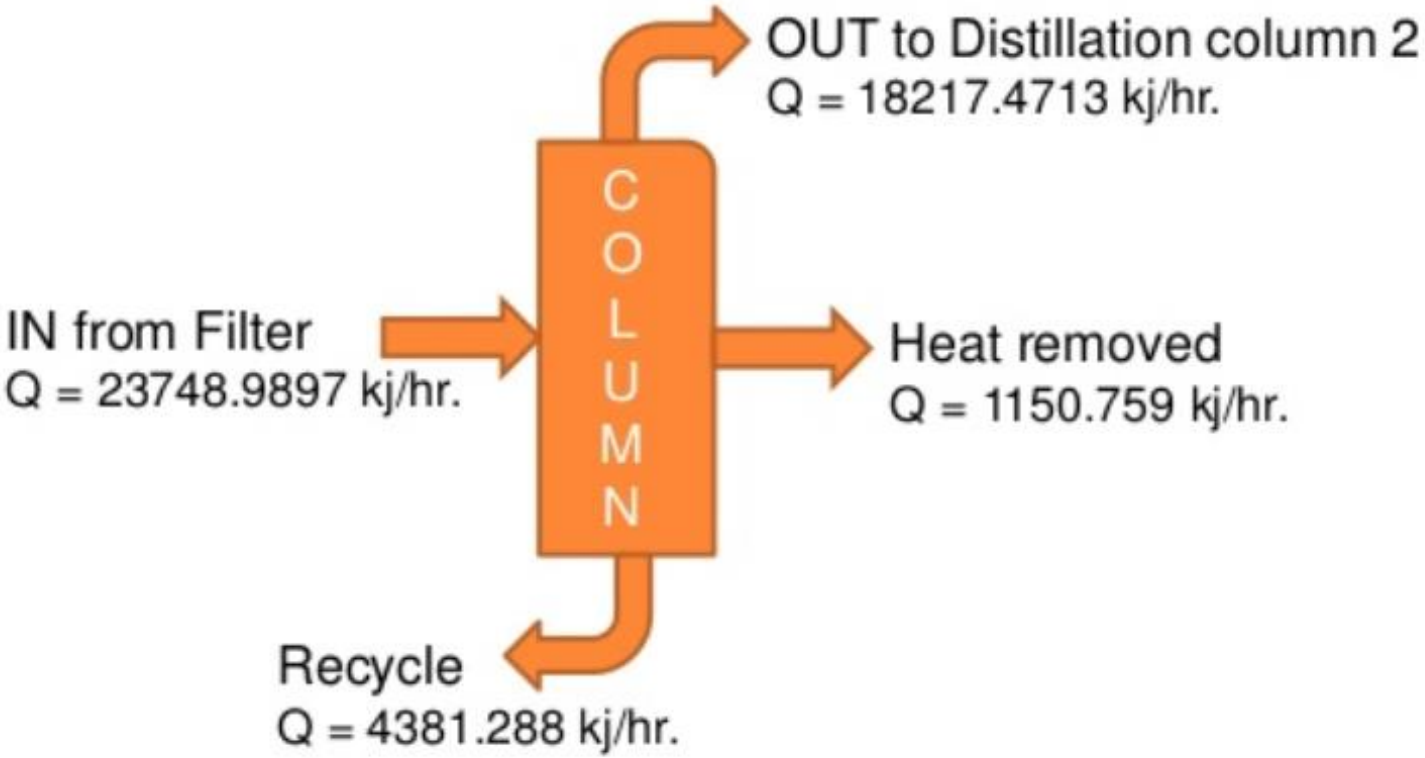
Total IN = Total OUT = 29329.679 kj/hr.

FILTER:



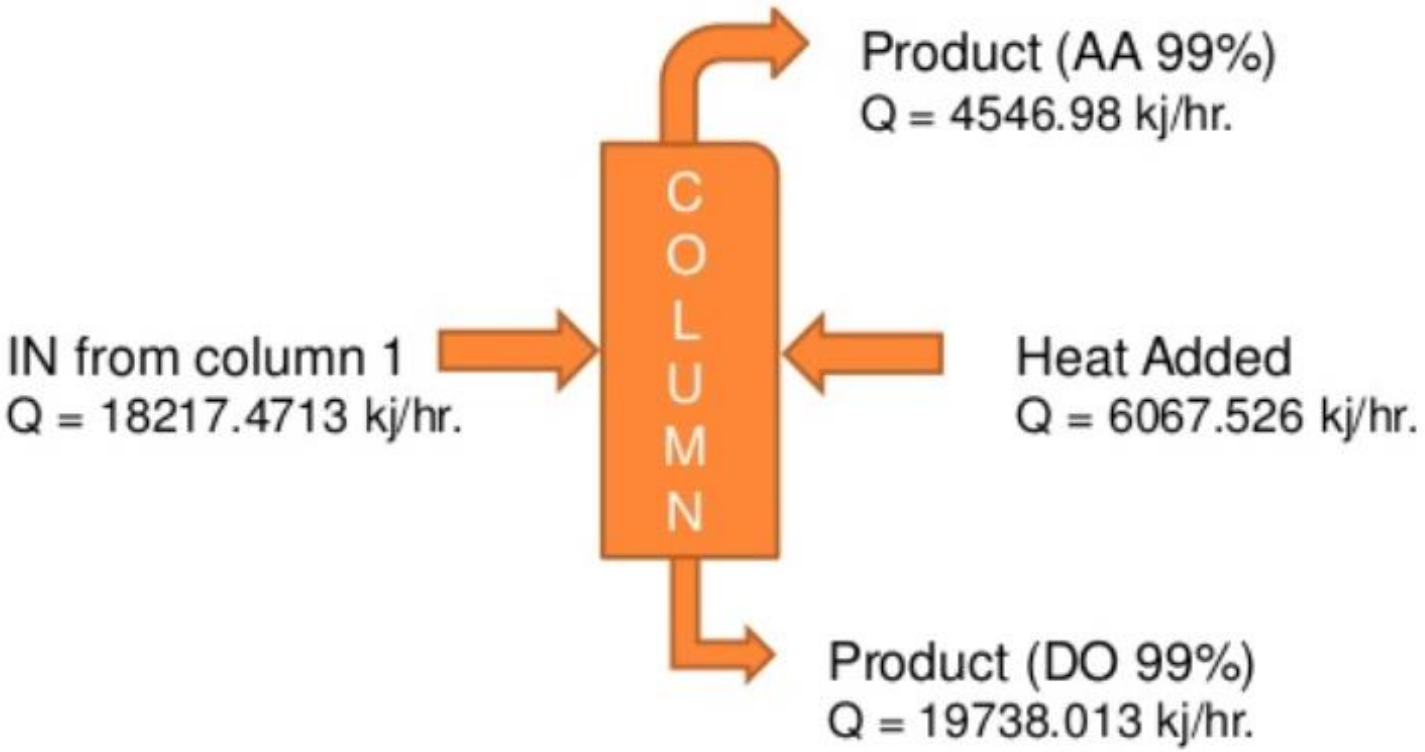
Total IN = Total OUT = 2598.7371 kj/hr.

ACO RECYCLE COLUMN:



Total IN = Total OUT = 23748.9897 kj/hr.

D.O. PURIFICATION COLUMN:



Total IN = Total OUT = 24284.998 kj/hr.

Heat exchanger 2:

Heat Removed
Q=-1624.7752 kj/hr.

Heat exchanger 3:

Heat removed
Q = -11599.6613 kj/hr.

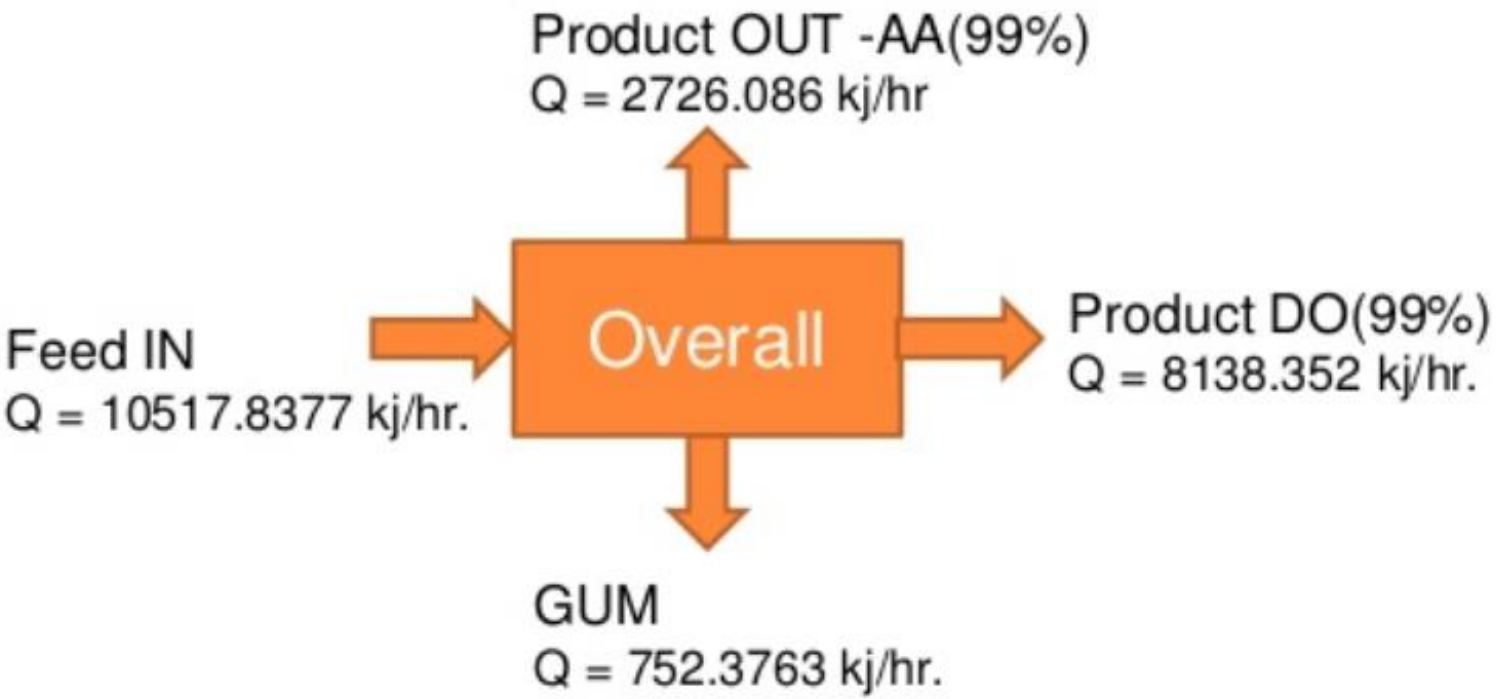
Heat exchanger 4:

Heat Removed
Q = -1820.8976 kj/hr.

Heat exchanger 5:

Heat Removed
Q = -803.3663 kj/hr.

OVERALL energy BALANCE:



Total IN = Total OUT = 10517.8377 kj/hr.
BALANCED