Custom model of packed column using Python and DWSIM

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Description:

This project aims to model a packed distillation column using Python and DWSIM. Given certain combinations of necessary input parameters, the column height and diameter is predicted.

Model equations:

1. Determination of the column height

The theoretical stage method (Concept of HETP) is used for calculating the height of column.

The height of the packing is calculated by

H=HETP*n

where,

N=number of theoretical stages (determined by the McCabe-Thiele method)

HETP=height Equivalent of a Theoretical Plate

H=height of the packing

The value of the HETP can be determined by the modified Granville equation

$$HETP = 28 \cdot d_p \cdot m_a \cdot \frac{V}{L} \cdot \left(\frac{H}{2.4} \right)^{1/3}$$

Where,

d_p= diameter of the packing [m]

m_a= average slope of the equilibrium curve

V= molar vapor flow rate (mol/s)

L= molar liquid flow rate (mol/s)

$$m_a = \frac{\sum_{i=1}^{n} m_i}{n}$$

where m_i is the local slope of the equilibrium curve at theoretical plate i

2. Determination of column diameter

$$\Delta p = \alpha(10^{\beta L'})(\frac{G'^2}{\rho_G})$$

$$\frac{L'}{G'}\frac{lb/(s-ft^2)}{lb/(s-ft^2)} = \frac{L}{V}\frac{\frac{mol}{s}}{\frac{mol}{s}}\frac{(MW\ liquid\ \frac{lb}{mol})}{(MW\ vapor\ \frac{lb}{mol})}$$

$$Area = \frac{(V\ \frac{lbmol}{s})(M.W.\ vapor\ \frac{lb}{lbmol})}{G'\ \frac{lb}{sft^2}}$$

$$Diameter = (\frac{4\ Area}{\pi})^{1/2}$$

Where,

Δp : pressure drop across column

α,β: packing parameters

L′: mass flow rate of liquid

G′: mass flow rate of vapor

L: molar flow rate of liquid

V: molar flow rate of vapor

3. Mole balance:

F=D+B

$Fz=D*x_D+B*x_B$

where,

F: molar feed flow rate

D: molar distillate flow rate

B: molar bottoms flow rate

D: molar distillate flow rate

x_D: mole fraction in distillate

x_B: mole fraction in bottoms

z: mole fraction in feed

4. Energy balance:

$H_{D0}=D_0*(x_{D0}*Cp_0+x_{D1}*Cp_1)*(T_{D0}-T_{F0})+H_{F0}$

$H_{B0}=B_0*(x_{B0}*C_{p0}+x_{B1}*Cp_1)*(T_{B0}-T_{F0})+H_{F0}$

H: enthalpy

x: mole fraction

Cp: specific enthalpy

T: temperature

Subscript 0 indicates component 1

Subscript 1 indicates component 2

5. Equilibrium equations:

$y = \frac{\alpha x}{1+(\alpha-1)x}$

where α: relative volatility

6. Input choices:

1: distillate flow, x_D rate given

2: distillate flow rate, x_B given

3: distillate flow rate, x_B given

4: bottoms flow rate, x_B given

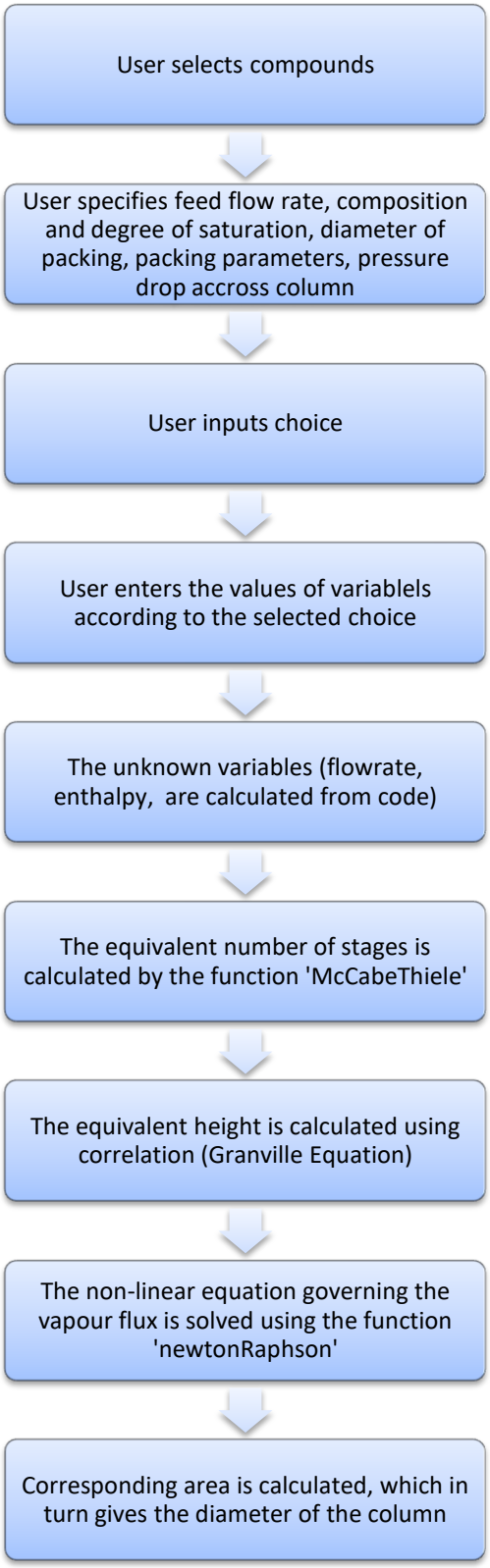
5: flow split_dist, x_D given

6: flow split_dist, x_B given

7: flow split_bottom, x_D given

8: flow split_bottom, x_B given

Basic flow scheme of code:



Results:

Distillation parameters:

F=500 mol/s, z=0.4

Benzene-Toluene mixture

choice=1

D=200

x_D=0.98

Packing parameters:

α=0.52

β=0.16

d_p=25 mm

Solver settings:

Flash algorithm :Nested loops (VLE)

Flash specification:Temperature and pressure

Results from simulation:

Equivalent number of stages=16

Height of column = 4.93733 m

Diameter of column = 1.8248 m

Detailed explanation of the function 'McCabeThiele'

This is the master function used for calculating the theoretical number of stages

It performs the McCabe-Thiele construction in order to calculate the number of stages

INPUTS:

PaVap :Vapour pressure of component a (more volatile)

PbVap :Vapour pressure of component b (less volatile)

R_factor :Amount Rmin is scaled by to obtain the actual reflux ratio

xf :Feed composition

xd :Distillate composition

xb :Bottoms composition

q :Liquid fraction of feed

OUTPUTS:

Equivalent number of stages actual reflux ratio

Basic flow-scheme:

1. Getting equilibrium data
2. Finding where the q-line intersects the equilibrium curve (by solving quadratic)
3. Find out where q line intersects the operating line
4. Step down the stages through the rectification section, update the number of steps as soon as one step is complete
5. Step down the stages through the stripping section
6. Note: steps 4 and 5 get reversed if the bottoms composition is specified
7. Continue stepping until the desired concentration is achieved

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