# Custom modelling of packed distillation column using DWSIM and Python


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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. [1,2,9,10]

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 [3,11]

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

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** [4,5]

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

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

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

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

Where,

$\Delta p$ : pressure drop across column

$\alpha,\beta$: packing parameters

$L'$: mass flow rate of liquid ($lb/ft^2s$)

$G'$: mass flow rate of vapor ($lb/ft^2s$)

$L$: molar flow rate of liquid (lbmol/s)

$V$: molar flow rate of vapor (lbmol/s)

$\rho_G$: density of gas ($lb/ft^3$)

**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:**

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

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

Where,

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: bottoms flow rate, x_D given

4: bottoms flow rate, x_B given

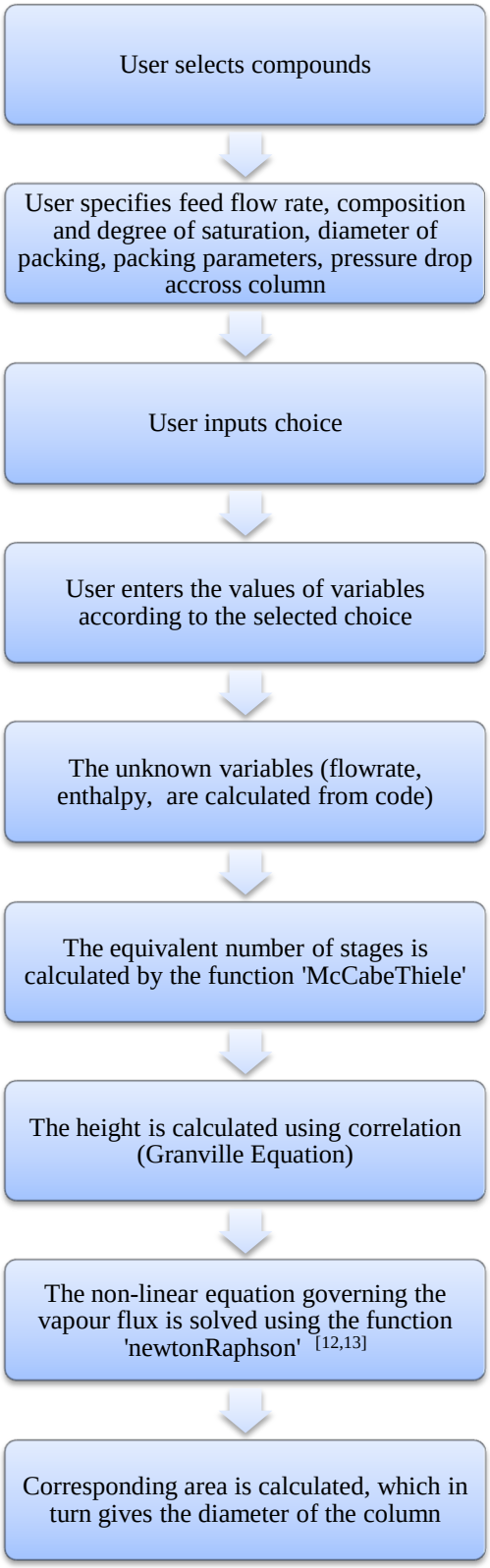
5: flow split_dist, x_D given

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=1000 mol/s, z=0.4

Benzene-Toluene mixture

choice=1

D=405

x_D=0.98

Packing parameters:

$\alpha$=0.52

$\beta$=0.16

$d_p$=25 mm

Solver settings:

Flash algorithm : Nested loops (VLE)

Property package: Soave-Redlich-Kwong (SRK)

Flash specification: Pressure and Enthalpy

Results from simulation:

Equivalent number of stages = 22

Height of column = 7.777 m

Diameter of column = 2.430m

**The code has been run over multiple testcases to validate its results**. Some of the most crucial testcases, which helped to verify the correctness of the code and validate it, are presented here.

The components of distillation for the following testcases are –benzene and toluene. The pressure drop in the column is 0.5 inches of water per foot.

| F (mol/s) | z | Choice | D (mol/s) | B (mol/s) | Flow split-D | Flow split-B | x_D | x_B | α | β | $R_{factor}=\frac{R}{R_{min}}$ | $d_p$ (mm) | Equivalent number of stages | Height (m) | Diameter (m) | Comments |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1000 | 0.4 | 1 | 405 | | | | 0.98 | | 0.52 | 0.16 | 1.2 | 25 | 22 | 7.78 | 2.43 | Shows a general consistency w.r.t to typical values of height and diameter of distillation columns used in a small chemical plant [1,4,5] |
| 1000 | 0.4 | 2 | 405 | | | | | 0.01 | 0.52 | 0.16 | 1.2 | 25 | 20 | 6.72 | 2.41 | |
| 1000 | 0.4 | 3 | | 600 | | | 0.98 | | 0.52 | 0.16 | 1.2 | 25 | 20 | 6.79 | 2.42 | |
| 1000 | 0.4 | 4 | | 600 | | | | 0.01 | 0.52 | 0.16 | 1.2 | 25 | 22 | 7.83 | 2.43 | |
| 1000 | 0.4 | 5 | | | 0.4 | | 0.98 | | 0.52 | 0.16 | 1.2 | 25 | 20 | 6.79 | 2.42 | |
| 1000 | 0.4 | 6 | | | 0.4 | | | 0.01 | 0.52 | 0.16 | 1.2 | 25 | 22 | 7.83 | 2.43 | |
| 1000 | 0.4 | 7 | | | | 0.6 | 0.98 | | 0.52 | 0.16 | 1.2 | 25 | 20 | 6.79 | 2.42 | |
| 1000 | 0.4 | 8 | | | | 0.6 | | 0.01 | 0.52 | 0.16 | 1.2 | 25 | 22 | 7.83 | 2.43 | |
| 3500 | 0.4 | 1 | 1400 | 0.97 | | | | | 0.52 | 0.16 | 1.5 | 17 | 15 | 2.78 | 4.84 | Reference: [5] (motivated from Example problem 12.4-1, pg 368) These two testcases show the consistency of the python code. The input values in the two testcases correspond to the same set of parameters, ie. D=1400, B=2100, x_D=0.97, x_B=0.02 |
| 3500 | 0.4 | 2 | 1400 | | 0.02 | | | | 0.52 | 0.16 | 1.5 | 17 | 15 | 2.78 | 4.84 | |
| 1000 | 0.4 | 1 | 500 | 0.98 | | | | | | | 1.2 | 25 | INVALID INPUT ! | | | Component mole balance not satisfied |
| 1000 | 0.4 | 1 | 400 | 0.62 | | | | | | | 1.2 | 25 | INVALID INPUT ! | | | Slope of operating line of rectification section is negative, hence $R_{min}$ is negative, Hence, this input is not valid. |
| 1000 | 0.5 | 1 | 500 | | | | 0.9999 | | 0.52 | 0.16 | 1.5 | 25.4 | 35 | 15.9 | 2.73 | When a very pure distillate is required, then the number of stages and thus the height if the column is high |

## Detailed explanation of the function 'McCabeThiele' [6,14,15]

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: [6,7,8,16,17]

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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