COUNTER CURRENT STAGEWISE ADSORPTION TOWER

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1. INTRODUCTION & THEORY

This custom model implements a Counter current stagewise Adsorption tower compatible with DWSIM. A schematic for the same is given for reference in Figure 1. The code uses Freundlich isotherm as the equilibrium relation at each level.

Freundlich isotherm is given by,

$$Y^* = mX^n$$

where,

Y = mass solute/ mass solvent at equilibrium

X = mass solute/ mass adsorbent

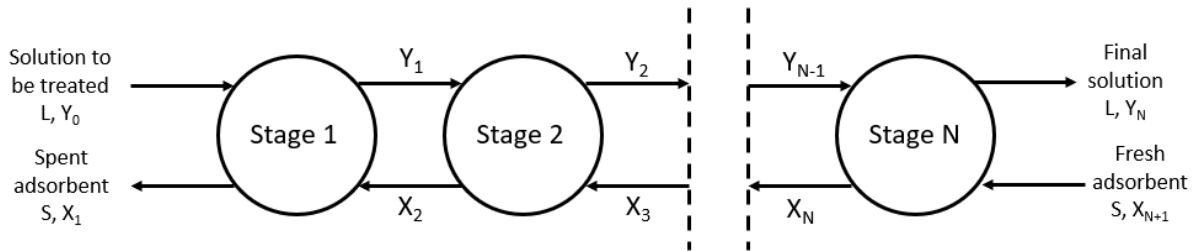'm' and 'n' are the Freundlich parameters which are dimensionless.

Figure 1: Counter current Adsorption Tower

2. ASSUMPTIONS

   a. Isothermal process is assumed. (Explanation: Introducing temperature changes across stages may lead to varying Freundlich parameters as the Freundlich isotherm is usually valid for a particular temperature.)
   b. The code does not differentiate between vapor and liquid phases. For example, if the feed stream has 90% liquid and 10% vapor phases, then this custom model will apply the adsorption process to 100% of the feed stream. This assumption may limit the thermodynamic property packages you can use.
   c. The solvent and adsorbent are assumed to be non-interactive.

3. NECESSARY INPUTS

   a. Both the input streams (Feed and Fresh Adsorbent) have to be defined completely (i.e., compositions, flow rates and thermodynamic properties)
   b. Number of stages in the adsorption tower N.
   c. Freundlich parameters m, n. (NOTE: Both are dimensionless)

4. OUTPUT
The custom model outputs the compositions and flow rates of output streams (Final solution and Spent Adsorbent)

5. DEFAULT SETTINGS
Default custom model contains the following three components:
  i.   Water (solvent)
  ii.   Benzene (solute)
  iii. Carbon (adsorbent)

Obviously, one is free to change these components, but be sure to keep the order (solvent-solute-adsorbent) the same. If this order is changed, the code WILL NOT work properly.

NOTE 1: Depending on the Property package you choose, energy balance may not converge to less than 0.01.
NOTE 2: Most adsorption processes involve a solid adsorbent. So be sure to use the corresponding .json file for that solid.
NOTE 3: The .json file for the carbon used in the default settings is available here.

6. TESTING WITH VARIOUS COMPONENT SYSTEMS AND THERMODYNAMICS

  a. Example problem 6 from Chapter 12 of Mass Transfer Theory and Practices [2]
      Components: Air, Water, Silica gel
      Property package: Raoult's Law or NRTL or Chao-Seeder or UNIFAC
      Mass flow rate of FEED stream = 505 kg/min
      Mass flow rate of FRESH ADSORBENT stream = 25 kg/min
      Number of stages in the tower = 4
      Freundlich isotherm parameters: m = 0.027 and n = 0.897 (Calculated by fitting the given experimental values to the Freundlich isotherm)

Mass fractions of input streams:

Name of component	AIR	WATER	CARBON
Mass fraction in FEED	0.9901	0.0099	0
Mass fraction in FRESH ADSORBENT	0	0	1

Mass fractions of output streams:

Name of component	AIR	WATER	CARBON
Mass fraction in FINAL SOLUTION	0.9992	0.0008	0
Mass fraction in SPENT ADSORBENT	0	0.1547	0.8453

Mass flow rate of FINAL SOLUTION stream = 500.4 kg/min
Mass flow rate of FRESH ADSORBENT stream = 29.6 kg/min

In the solved example, the required concentration of water in air is 0.001 kg of water/ kg of air. Result obtained using the custom model is 0.0008 kg of water/ 0.9992 kg of air = 0.0008006 kg of water/ kg of air.
The value of X_1 in the solved example is 0.18 and the result obtained using the custom model is 0.183.

In the example problem solved in the book, the minimum number of theoretical stages required were calculated. The output stream will have a lesser concentration than desired at the end of all the stages due to the 'minimum' requirement. This explains the slight discrepancy in the results.

b. Components: Air, Benzene, Carbon
Property package: Raoult's Law or NRTL or Chao-Seeder or UNIFAC
Mass flow rate of FEED stream = 1 kg/s
Mass flow rate of FRESH ADSORBENT stream = 1 kg/s
Number of stages in the tower = 3
Freundlich isotherm parameters: m = 1.33 and n = 1/0.44

Mass fractions of input streams:

Name of component	AIR	BENZENE	CARBON
Mass fraction in FEED	0.6	0.4	0
Mass fraction in FRESH ADSORBENT	0	0	1

Mass fractions of output streams:

Name of component	AIR	BENZENE	CARBON
Mass fraction in FINAL SOLUTION	0.999	5.284×10^{-6}	0
Mass fraction in SPENT ADSORBENT	0	0.286	0.714

Mass flow rate of FINAL SOLUTION stream = 0.600 kg/s
Mass flow rate of SPENT ADSORBENT stream = 1.400 kg/s

Verification:
Mass balance: Mass conservation on solute
Mass of solute in inlet stream = 0.4 kg/s
Mass of solute in output streams = 0.00(0.600 kg/s) + 0.286(1.400 kg/s) = 0.400 kg/s

Mass balance on solute for k stages is given by,
$$L(Y_0 - Y_k) = S(X_1 - X_{k+1})$$
$$X_{k+1} = X_1 - \frac{L}{S}(Y_0 - Y_k)$$
In this example,
$X_1 = 0.4$, $Y_0 = 0.667$, $X_4 = 0$, $Y_3 = 5.289 \times 10^{-6}$, L = 0.6 kg/s and S = 1 kg/s
Therefore,
$$X_{k+1} = 0.4 - 0.6(0.667 - Y_k)$$
Equilibrium curve is given by,
$$Y_k = 1.33\, X_k^{2.273}$$
Solving the problem stage by stage,
$$Y_1 = 1.33\,(0.4)^{2.273} = 0.166$$
$$X_2 = 0.4 - 0.6(0.667 - 0.166) = 0.099$$
$$Y_2 = 1.33(0.099)^{2.273} = 0.007$$
$$X_3 = 0.4 - 0.6(0.667 - 0.007) = 0.004$$
$$Y_3 = 1.33(0.002)^{2.273} = 5.28 \times 10^{-6}$$
$$X_4 = 8.28 \times 10^{-6} \text{ (for tolerance set to } 1 \times 10^{-5})$$
Both the results match.

7. THE ALGORITHM

Brief ideas about the algorithm are given here for better understanding of the Custom Model. The idea for calculations in a counter current adsorption tower can be represented by the following graph.
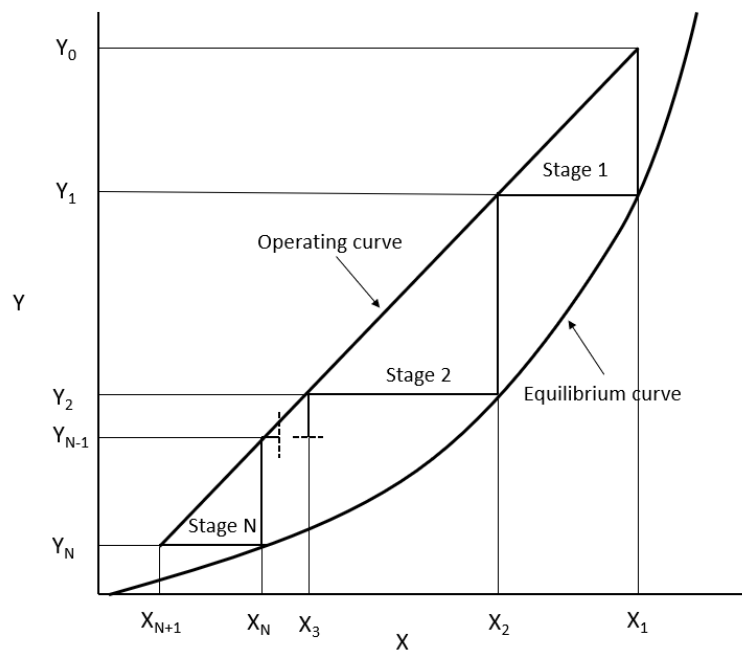

Figure 2

Here, we know the equilibrium curve parameters (Freundlich parameters), slope of the line (L, S), the input conditions (Y_0, X_{N+1}) and the number of stages (N).

However, with this information we cannot find out the operating line exactly. So, we make a guess for the output adsorbent stream (X_1) and find out the corresponding X_{N+1} value and use this as a feedback to better our guess. This is the basic idea behind this custom model.

8. FLOW SHEET

Nomenclature:

Y_0 = (Input) mass of solute/mass of solvent in the solution to be treated

X_1 = (Output) mass of solute/mass of adsorbent in the adsorbent spent
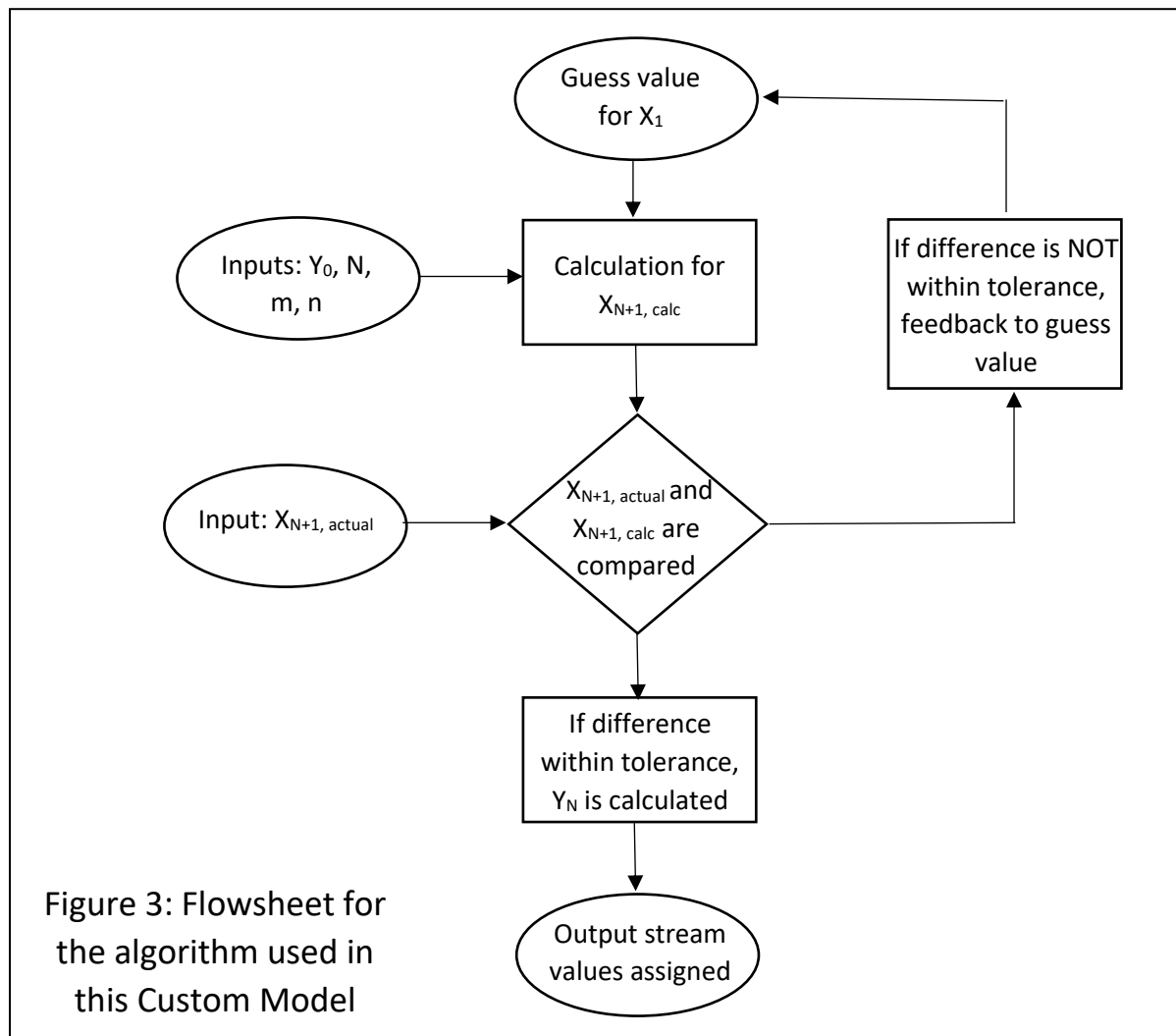
Y_N = (Output) mass of solute/mass of solvent in the final solution

X_{N+1} = (Input) mass of solute/mass of adsorbent in the fresh adsorbent

N = (Input) Number of stages

m = (Input) Freundlich parameter

n = (Input) Freundlich parameter

Figure 3: Flowsheet for the algorithm used in this Custom Model

Guess value for X_1

Inputs: Y_0, N, m, n

Calculation for $X_{N+1, \text{calc}}$

If difference is NOT within tolerance, feedback to guess value

Input: $X_{N+1, \text{actual}}$

$X_{N+1, \text{actual}}$ and $X_{N+1, \text{calc}}$ are compared

If difference within tolerance, Y_N is calculated

Output stream values assigned

9. ACKNOWLEDGEMENTS

10. REFERENCES

[1] Chapter 11, Mass-Transfer Operations by Robert E. Treybal, Third Edition, McGraw Hill Education India

[2] Page 413, Example 6, Chapter 12, Mass Transfer Theory and Practice by N. Anantharaman and K.M. Meera Sheriffa Begum, PHI Learning Private Limited