Liquid Liquid Extraction **Marks-200**

MT2 term project: Submission: 15th March

Digital framework for comparing the cross current operation and countercurrent operation.

Experimental data collection remains expensive and time consuming. Hence it is important to create a ***digital twin of many process systems in industries***. These digital twins can recreate synthetic data that can be useful for making surrogate models using neural network and other methods. Create a software (preferably with a graphic user interface, in python). MATLAB can be used as well.

The software is expected to have the following components that are necessary for ***process parameter optimization.***

1. A simulation framework for solving crosscurrent and countercurrent extraction (either liquid-liquid or solid liquid system) using graphical method using right angled triangle diagram.
   Numerical solver: A simulation framework for solving crosscurrent and countercurrent solid liquid extraction using numerical method/ solvers [example: ***fsolve*** function in MATLAB or python] for solution of a system of non-linear algebraic equation. [More generalized framework for large number of stages]. Initially to test the solutions, you can use the guess values close to the solutions obtained from graphical solution.
2. Also create a graphical user interface so that the user can choose the option of entering various equilibrium data and can opt for crosscurrent or countercurrent operation.
3. The final plot should include the overflow and underflow composition [or raffinate and extract composition] and flow rate for each stage for any number of stages. It should also show the percentage removal at each of the stages.
4. Compare the **degree of separation** between cross current and counter current operation (for 3 stages). Simulate the percentage removal (y axis) as a function of number of stages (x-axis) for cross and counter current operation and plot them on same graph.
5. Generation of response surface and optimization of the process. Create data in the form of input output to construct a surrogate model. **[for example: input 1= number of stage, input 2=solvent amount and input 3= initial feed composition and output 1=percentage removal as the output**]. Fit a neural network model (choose the number of nodes and number of layers) that can predict the percentage removal. Create a response surface of percentage removal as a function of two inputs at a time to create a 3D surface and contour plot. Such plots are necessary for optimization of process parameters.
   *** Use the following data for various groups to use the equilibrium data and solution. However, you need to make a software that can be used to calculate the percentage removal for any number of stages.
   Write the contribution of each member clearly. Each of the group member need to choose various topics and integrate them into making a common software.
   Credit will be given if your algorithm for solving are different from what is provided in class [for tie line interpolation etc] and if you use matlab or python functions that is not discussed in the class 9 other algebraic equation solvers, apart from solve and vpa solve].

DATA for gropup 1 [comparison of crosscurrent and countercurrent operation in terms of number of stages for the same solvent scheme and feed amount/feed composition and raffinate composition]

(*Single stage extraction*)[3] Five hundred kilograms of an aqueous feed containing 50 mass% acetone is contacted with a solvent containing 98% chloroform and 2% acetone. The mass ratio of the feed to the solvent is 1.1. Calculate the mass and composition of the extract and also the fraction of acetone in the feed extracted. The operation is carried out at 25°C and the equilibrium and tie line data are given below (Wankat, 1988).

Aqueous phase (mass fraction)			Chloroform phase (mass fraction)		
Water x_A	Chloroform x_B	Acetone x_C	Water y_A	Chloroform y_B	Acetone y_C
0.8297	0.0123	0.158	0.013	0.70	0.287
0.7311	0.0129	0.256	0.022	0.557	0.421
0.6229	0.0171	0.36	0.044	0.429	0.527
0.456	0.051	0.493	0.103	0.284	0.613
0.345	0.098	0.557	0.186	0.204	0.61

The results in form of figures (with proper axes name and legends) along with the complete code in PowerPoint presentation should be submitted.

Group 2:

[comparison of crosscurrent and countercurrent operation in terms of solvent for a particular raffinate composition and fixed number of stages]

i **(*Number of stages*; *minimum solvent rate*)**[3] An aqueous solution of acetic acid (35% acid; 1000 kg/h) is to be extracted with 'pure' MIBK (*B*) at 25°C supplied at a rate of 1300 kg/h. The raffinate may contain 3% acid (*C*). Determine the number of ideal stages and also the minimum solvent rate required to perform the separation in a countercurrent cascade. The LLE data at 25°C are given below.

Raffinate (Aqueous phase)			Extract (MIBK phase)		
x_A	x_B	x_C	y_A	y_B	y_C
0.9845	0.0155	0.0	0.0212	0.9788	0.0
0.9545	0.017	0.0285	0.028	0.9533	0.0187
0.858	0.025	0.117	0.054	0.857	0.089
0.757	0.038	0.205	0.092	0.735	0.173
0.678	0.06	0.262	0.145	0.609	0.246
0.550	0.122	0.328	0.220	0.472	0.308
0.429	0.225	0.346	0.310	0.354	0.336

Group 3: [Compute the minimum solvent rate that would be required and calculate the stage number as a function of x times that of minimum solvent rate for performing crooscurrent and countercurrent operation).

(*Multistage countercurrent extraction*)[3] A feed of one thousand kilograms aqueous solution of pyridine per hour (50% by mass) is to be extracted with pure benzene to reduce the solute content in the raffinate to 2%. Determine the number of ideal stages required if the solvent rate is 1.3 times the minimum.

Equilibrium data

Water layer		Benzene layer	
Pyridine, mass%	Benzene, mass%	Pyridine, mass%	Benzene, mass%
1.17	0.0	3.28	94.54
3.55	0.0	9.75	87.46
7.39	0.0	18.35	79.49
13.46	0.15	26.99	71.31
22.78	0.25	31.42	66.46
32.15	0.44	34.32	64.48
42.47	2.38	36.85	59.35
48.87	3.99	39.45	56.43
49.82	4.28	39.27	55.72
56.05	19.56	48.39	40.05

Group 4: Composition for raffinate composition and extraction composition for various number of stages for counter and crosscurrent extraction.

(*Janecke diagram*)[3] The mutual solubility and the tie-line data for the MEK(A)–ethylene glycol(C)–water(B) system at 30°C are given below:

Extract (MEK phase)			Raffinate (water)		
y_A	y_B	y_C	x_A	x_B	x_C
0.884	0.111	0.005	0.208	0.697	0.095
0.871	0.112	0.017	0.21	0.656	0.134
0.849	0.113	0.038	0.221	0.583	0.196
0.827	0.116	0.057	0.236	0.524	0.240
0.806	0.118	0.076	0.261	0.461	0.278
0.50	0.205	0.295		Plait point	

Group 5: Comparison of crosscurrent and countercurrent operation in terms of number of stages for the same solvent scheme and feed amount/feed composition and raffinate composition

9.4 (*Countercurrent liquid–solid contact*)[3] Experimental 'equilibrium data' on extraction of oil from a meal by using benzene are given below:

Mass fraction of oil (C) in solution	*Mass fractions in the underflow*		
y_C	x_C	x_A	x_B
0	0	0.67	0.33
0.1	0.0336	0.664	0.302
0.2	0.0682	0.660	0.272
0.3	0.1039	0.6541	0.242
0.4	0.1419	0.6451	0.213
0.5	0.1817	0.6366	0.1817
0.6	0.224	0.6268	0.1492
0.7	0.268	0.6172	0.1148

Two thousand kilograms per hour of the meal containing 26 mass% oil is extracted with 2100 kg/h of benzene. The underflow leaving the countercurrent cascade must not contain more than 0.015 mass fraction of oil. The feed benzene has 0.005 mass fraction oil in it. The overflow is essentially solid-free. Calculate the mass fraction in the rich extract leaving the cascade and the number of ideal stages required.

Group 5: Comparison of crosscurrent and countercurrent operation in terms of solvent required for fixed feed amount/feed composition and raffinate composition. Comparison of various solvent schemes. And calculation of minimum solvent required.

EXAMPLE 9.1 (*Solid–liquid extraction equilibrium data*) A set of experimental test data on solid–liquid extraction 'equilibrium' for the system *oil seed meal(A)–hexane(B)–oil(C)* is reported below. Mixtures of the 'components' at various overall composition are stirred in a laboratory vessel and then allowed to settle. Samples of the *overflow* (oil + solvent hexane + traces of the inert meal) and the *underflow* (inert meal + entrained solution) were drawn and analyzed. The following data were collected.

Overflow (100 kg), *solution*			*Underflow* (100 kg), *slurry*		
w_A (kg)	w_B (kg)	w_C (kg)	w'_A (kg)	w'_B (kg)	w'_C (kg)
0.3	99.7	0.0	67.2	32.8	0.0
0.45	90.6	8.95	67.1	29.94	2.96
0.54	84.54	14.92	66.93	28.11	4.96
0.70	74.47	24.83	66.58	25.06	8.36
0.77	69.46	29.77	66.26	23.62	10.12
0.91	60.44	38.65	65.75	20.9	13.35
0.99	54.45	44.56	65.33	19.07	15.6
1.19	44.46	54.35	64.39	16.02	19.59
1.28	38.50	60.22	63.77	14.13	22.10
1.28	34.55	64.17	63.23	12.87	23.90
1.48	24.63	73.89	61.54	9.61	28.85

Plot the 'equilibrium data' (a) as the right-triangular plot, and (b) as the 'Ponchon-Savarit' diagram.

EXAMPLE 9.2 (*Solid–liquid extraction in a single-stage batch contactor*) One thousand kilograms of crushed oil seeds (19.5% oil, 80.5% meal) is extracted with 1500 kg of 'pure' hexane in a batch extraction vessel. Calculate the fraction of the oil extracted using (a) the right-triangular diagram and (b) the 'Ponchon–Savarit diagram'. The equilibrium data given in Example 9.1 are applicable.