1. Liquid-liquid extraction: Single stage operation

EXAMPLE 8.2 (*Single-stage extraction*) One thousand kilograms of an aqueous solution containing 50% acetone is contacted with 800 kg of chlorobenzene containing 0.5 mass% acetone in a mixer-settler unit, followed by separation of the extract and the raffinate phases. (a) Determine the composition of the extract and the raffinate phases and the fraction of acetone extracted. (b) Also calculate the amount of solvent required if 90% of the acetone is to be removed. Equilibrium and tie line data are given below.

Aqueous phase (*Raffinate*)			Organic phase (*Extract*)		
Water	Chlorobenzene	Acetone	Water	Chlorobenzene	Acetone
x_A	x_B	x_C	y_A	y_B	y_C
0.9989	0.0011	0.0	0.0018	0.9982	0.0
0.8979	0.0021	0.1	0.0049	0.8872	0.1079
0.7969	0.0031	0.2	0.0079	0.7698	0.2223
0.6942	0.0058	0.3	0.0172	0.608	0.3748
0.5864	0.0136	0.4	0.0305	0.4751	0.4944
0.4628	0.0372	0.5	0.0724	0.3357	0.5919
0.2741	0.1259	0.6	0.2285	0.1508	0.6107
0.2566	0.1376	0.6058	0.2566	0.1376	0.6058

Ude MATLAB/ Python to answer the questions.

The data is given in the code to draw the ternary equilibrium curve (liquid-liquid equilibrium curve) on the right-angled triangle co-ordinate.
Also we provide the approach to store the information for drawing the ties lines.
Question 1: Based on above data points, draw the four tie lines using MATLAB/python. Suppose for a particular extraction process you find that $x_{c,M}$ =0.17 , $x_{B,\ M}$ =0. 43 (M point). Construct a code to automate the drawing of tie line through any point M, Draw a tie line [1st, 3rd, 5th and 7th points from experimental data)] through M point. If , $x_{c,\ M}$=0.5, $x_{B,\ M}$ =0.2, draw the tie line in the LLE diagram on right-angles triangle co-ordinate.

Hints on interpolation of slope:
tie_slope(i) + (My - xc_int(i)) * (tie_slope(i+1) - tie_slope(i)) / (xc_int(i+1) – xc_int(i));

Question 2: Fit two polynomials [in the form, $y = ax^n + bx^{n-1} + \ldots\ldots + c$], one with the raffinate phase (order n= 5) and one with the extract phase data (order 3) using polyfit function. Check the goodness of fit using the plot of experimental data in x axis and simulated data in y axis. Calculate the RMSE for the two cases. Plot the actual points in blue circles and predicted points in red circles and show them on LLE curve. [Adsorption revision].

Q1 Hints:

```
%clear all;
% clc; close all;
%%%% Data %%%%%

B = [0 0.0011 0.0021 0.0031 0.0058 0.0136 0.0372 0.11 0.1259 0.1376 0.1508 0.16 0.3357
0.4751 0.608 0.7698 0.8872 0.9982 1];

C = [0 0 0.1 0.2 0.3 0.4 0.5 0.5821 0.6 0.6058 0.6107 0.6093 0.5819 0.4944 0.3748 0.2223
0.1079 0 0];
figure(1)
plot(B,C,'bo-');grid on;
hold on;
%% Plotting the right triangle (0,0), (1,0),(0,1) and (0,0)

plot([0    ],[0     ],'k-.','linewidth',1.25)
xlabel('');ylabel('');
title('raw data');
%%% Example tie lines (You can change this according to the mixture point)
tiexc = [.   ];
tieyc = [.      ];
tiexb = [0.0021 0.0136];
tieyb = [0.8872 0.4751];

for i = 1:length(tiexc)
   plot([tiexb(i) tieyb(i)], [tiexc(i) tieyc(i)], 'mo:', 'linewidth', 1.25);
end
%% calculate the slope of the picked tielines
tie_slope = zeros(1,length(tiexc));
for i =  1:length(tiexc);
   tie_slope(i) = (tieyc(i) - tiexc(i))/(tieyb(i) - tiexb(i));
end

% Calculating slope through interpolation
if (0 < My) && (My <= 0.1)
   slope = 0 + (My - 0) * tie_slope(1) / 0.1;
elseif (0.1 < My) && (My <= 0.4)
   slope = tie_slope(1) + ( ---- - ----) * (tie_slope(2) - tie_slope(1)) / (0. - 0.  );
elseif (My > 0.4)
   slope = tie_slope(2) + (My - 0.4) * 0.25 / (----- - 0.4);
end
% Draw the line with the calculated slope through the point (Mx, My)

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x_vals = linspace(0, 1, 10);
```
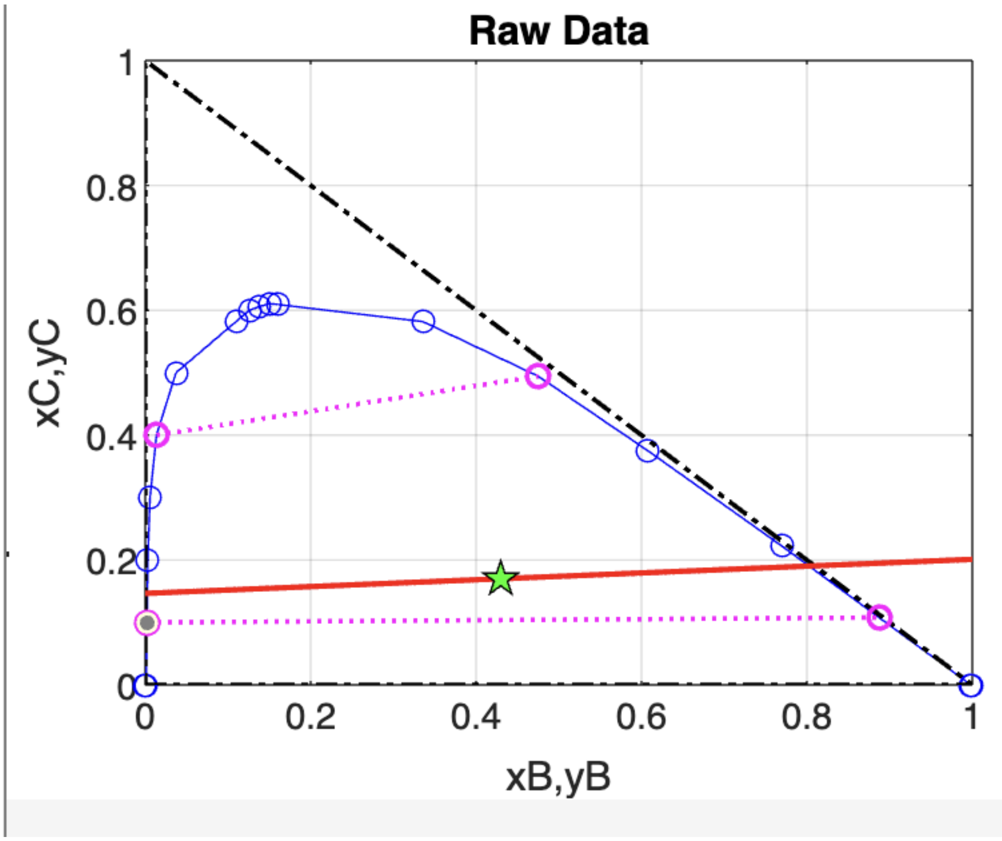
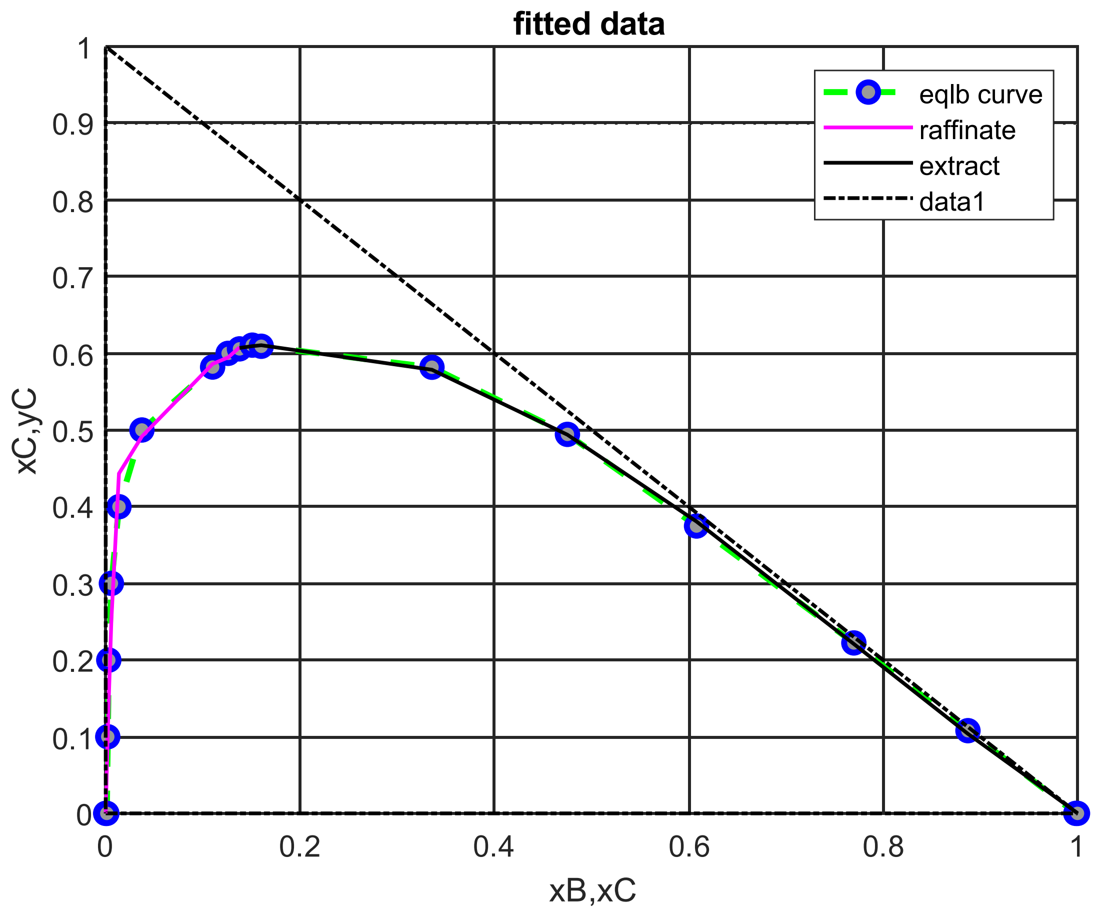

```
y_vals = slope * (x_vals - Mx) + My
```

```
plot(x_vals, y_vals, 'r-', 'linewidth', 1.5);
plot(Mx, My, 'kp', 'MarkerSize', 10, 'MarkerFaceColor', 'g');
```



Q2 Hints:

```
% Curve fitting

p1 = polyfit(____, ____, ____);      %%%%Extract phase
f1 = polyval(p1, ____);
plot(B(1:10),f1,'m','linewidth',1.25);grid on;
```



fitted data
eqlb curve
raffinate
extract
data1
xC,yC
xB,xC
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
0.2
0.4
0.6
0.8
1