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%converting volume percentage of ethanol to mole fraction:
liters_gin=10;
percent_ethanol_gin=0.4;
percent_water_gin=1-percent_ethanol_gin;

%using density (in g/L) and molar mass (in g/mol) to calculate moles:
mol_ethanol=liters_gin*percent_ethanol_gin*789/46.07;
mol_water=liters_gin*percent_water_gin*1000/18.016;
mol_total=mol_ethanol+mol_water;

%dividing the calculated moles by the mol total to get mol fraction:
ethanol_mol_fraction=mol_ethanol/mol_total;
water_mol_fraction=mol_water/mol_total;
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SAMPLE OUTPUT w/ 10L input feed:

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mol_ethanol =
    68.5044
mol_water =
    333.0373
mol_total =
    401.5417
ethanol_mol_fraction =
    0.1706
water_mol_fraction =
    0.8294
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%calculating mole fraction in liquid and vapor phase, looping for the 5
%runs
%setting initial z (mol composition of feed) values:
z1=ethanol_mol_fraction; z2=water_mol_fraction;
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for i=1:5
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%using antoine equation and vapor pressure values from Poling,
Prausnitz, and O'Connell (2001),
%antoine eqn:  $\ln P_{sat}[kPa] = A - B/(C+T[degC])$ 
A1=16.8958; B1=3795.17; C1=230.918; %for ethanol (1)
A2=16.3872; B2=3885.70; C2=230.170; %for water (2)
pressure=101.325; %pressure at which the VLE apparatus operates
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%finding the bubble and dew temp to determine the appropriate temp
%range for the runs:
bubble_temp=fzero(@(bubble_temp) pressure-z1*exp(A1-
B1/(bubble_temp+C1))-z2*exp(A2-B2/(bubble_temp+C2)), 75);
dew_temp=fzero(@(dew_temp) 1/pressure-z1/exp(A1-B1/(dew_temp+C1))-
z2/exp(A2-B2/(dew_temp+C2)), 75);
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%getting the temp input for each run
temp=input(['Input temperature of run ' num2str(i) ' (in Celsius,
between ' num2str(bubble_temp) ' and ' num2str(dew_temp) '): ']);
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%using Raoult's law,  $y_i P = x_i P_i^{sat}$  and Rachford-Rice eqn,  $\sum \frac{z_i(K_i-1)}{1+\frac{V}{F}(K_i-1)} = 0$ 
sat_pressure_ethanol=exp(A1- (B1/(temp+C1)));
sat_pressure_water=exp(A2- (B2/(temp+C2)));
%solving Rachford-Rice equation numerically to find a=V/F:
K_ethanol=sat_pressure_ethanol/pressure;
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K_water=sat_pressure_water/pressure;
k_ethanol=1/(K_ethanol-1); k_water=1/(K_water-1);
a=fzero(@(a) z1/(k_ethanol+a) + z2/(k_water+a), 1);
%solving the molar composition of the liquid (x1 and x2) and vapor (y1
and y2) phases from a
x1=z1/(1+a*(K_ethanol-1)); x2=z2/(1+a*(K_water-1));
y1=K_ethanol*x1; y2=K_water*x2;

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SAMPLE OUTPUT w/ 10L input feed:

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Input temperature of run 5 (in Celsius, between 94.6344 and 97.2262): 96.5

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x1 =
    0.1072
x2 =
    0.8928
y1 =
    0.2129
y2 =
    0.7871

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%performing mass balance on the system
%where eqn1 is the overall mass balance, L+V=total moles
%and eqn2 is the ethanol mass balance, x1L+y1V=z1*total moles
eqn1=[1, 1; x1, y1]; eqn2=[mol_total; z1*mol_total];
sol=linsolve(eqn1,eqn2);
mol_total=sol(2); %new total moles is the vapor output

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%converting moles and mol fraction to volume and volume percent using
density (in g/L) and molar mass (in g/mol)
volume_ethanol=mol_total*y1*46.07/789;
volume_water=mol_total*y2*18.016/1000;
volume_total=volume_ethanol+volume_water;
fprintf('Total volume (liters): %.3f\n%%v/v ethanol: %.2f%%\n%%v/v
water: %.2f%%\n', volume_total, volume_ethanol/volume_total*100,
volume_water/volume_total*100);

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z1=y1; z2=y2; %new feed composition is the resulting liquid composition
end

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FINAL OUTPUT W/ THE CHOSEN TEMPERATURES

Input temperature of run 1 (in Celsius, between 94.6344 and 97.2262): 96.7
Total volume (liters): 7.294
Volume of ethanol (liters): 3.280, %v/v ethanol: 44.97%
Volume of water (liters): 4.014, %v/v water: 55.03%
Input temperature of run 2 (in Celsius, between 93.7777 and 96.7): 95.7
Total volume (liters): 4.303
Volume of ethanol (liters): 2.282, %v/v ethanol: 53.03%
Volume of water (liters): 2.021, %v/v water: 46.97%
Input temperature of run 3 (in Celsius, between 92.2623 and 95.7): 94.7
Total volume (liters): 2.877
Volume of ethanol (liters): 1.717, %v/v ethanol: 59.68%
Volume of water (liters): 1.160, %v/v water: 40.32%
Input temperature of run 4 (in Celsius, between 90.8782 and 94.7): 93.7
Total volume (liters): 2.069
Volume of ethanol (liters): 1.350, %v/v ethanol: 65.26%
Volume of water (liters): 0.719, %v/v water: 34.74%
Input temperature of run 5 (in Celsius, between 89.6087 and 93.7): 92.7
Total volume (liters): 1.558
Volume of ethanol (liters): 1.091, %v/v ethanol: 70.01%
Volume of water (liters): 0.467, %v/v water: 29.99%
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