%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;

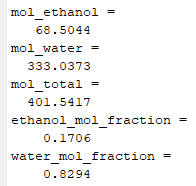
mol\_total=mol\_ethanol+mol\_water;

%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;

SAMPLE OUTPUT w/ 10L input feed:



%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;

for i=1:5

%using antoine equation and vapor pressure values from Poling, Prausnitz, and O’Connell (2001),

%antoine eqn: ln Psat[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

%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);

%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) '): ']);

%using Raoult's law, and Rachford-Rice eqn,

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;

K\_water=sat\_pressure\_water/pressure;

k\_ethanol=1/(K\_ethanol-1); k\_water=1/(K\_water-1);

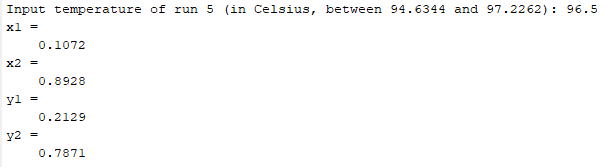
a=fzero(@(a) z1/(k\_ethanol+a) + z2/(k\_water+a), 1);

%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;

SAMPLE OUTPUT w/ 10L input feed:



%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

%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);

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

end

FINAL OUTPUT W/ THE CHOSEN TEMPERATURES

