USER MANUAL

File: UNIFAC_gamma_1.m

*UNIFAC_gamma_1.m contains the group's attempt to code for a multicomponent system. The group has tried to input the data sample data provided in the lecture presentation 'Local Composition Models', and the code was able to output more or less the same values as the ones indicated in the lecture presentation.

This program computes for the activity coefficients for a multicomponent liquid mixture using the UNIFAC model.

1. Run the program.
2. Enter the temperature of the system in KELVIN.
3. Enter the number of species present in the system.
    a. Example: Binary – 2, Ternary – 3, Quaternary – 4
    b. NOTE: The code only works for multicomponent gas/vapor systems. It will not work for systems with only one species.
4. Enter the number of subgroups present among the species in the mixture.
5. Enter the liquid compositions of each species in the mixture.
6. Enter the UNIFAC Parameters for the system. The program will ask for the following properties:
    a. No. of subgroup (i) present per species (j) (v_k)
    b. Main Group Interaction Parameter values (a_{mn})
    c. Group Volume (R_k) value per subgroup (i) for every species (j)
    d. Area Parameter (Q_k) value per subgroup (i) for every species (j)
7. After all of these are entered, the program automatically computes and shows the values of the activity coefficient per species.

NOTE: Please input NUMBERS only. The code will error if there are non-numerical symbols entered.

File: UNIFAC_gamma_2.m; bPcalcs.m

8. To apply the computed parameters to VLE calculations, simply run the program titled <UNIFAC_gamma_2.m>. The program is a similar version of the <UNIFAC_gamma_1.m>, only tailored for computing activity coefficients for an (1)acetone/(2)cyclohexane system at T = 308.15K
9. Consequently, run the program <bPcalcs.m> to calculate the necessary VLE data of the system. The program is based on the Modified Raoult's Law.
10. To generate the P-x,y and T-x,y diagram, look for the commented codes in the VLE program. Run this code in the command window and the diagram is automatically displayed.

WRITE-UP

The programs <UNIFAC_gamma_1.m> and <UNIFAC_gamma_2.m> both compute for the activity coefficients (γ_i) of a mixture system based a local composition model called the UNIFAC method. The first one is meant for general multicomponent liquid systems while the other one is a tailored version for a particular defined system.

Although different, the programs share the same algorithm in computing the activity coefficients (γ_i). In this write up, the program <UNIFAC_gamma_1.m> will be focused on.

Step 1: Code to Input and Store Parameter Values.

```
clc
clear

% Input the following variables:
temp = input('Enter system temperature (in K): ');
n = input('Enter no. of species in the mixture: ');
m = input('Enter no. of subgroups present in the species of the mixture: ');
% Number assignment of subgroups is based on the UNIFAC-VLE Subgroup Parameter list on SVAS.
% e.g. if the system have species with CH3, CH2, and CH2NH subgroups, CH3 will be assigned with 1, CH2 with 2 and CH2NH with 3.

% Initialize variables
x = zeros(1,n);
vk = zeros(m,n);
a_mn = zeros(m,m);
Rk = zeros(1,m);
Qk = zeros(1,m);

for b = 1 : n
    x(1,b) = input(['Enter liquid composition (x) of species ' num2str(b) ': ']);
end

for i = 1 : m
    for j = 1 : n
        vk(i,j) = input(['Enter no. of subgroup ' num2str(i) ' present in species ' num2str(j) '- '])
    end
end

for f = 1 : m
    for g = 1 : m
        a_mn(f,g) = input(['Enter main group interaction parameter value between subgroup ' num2str(f) ' and subgroup ' num2str(g) '- '])
    end
end

for i = 1 : m
    Rk(1,i) = input(['Enter Rk value for subgroup ' num2str(i) ': ']);
end

for j = 1 : m
    Qk(1,j) = input(['Enter Qk value for subgroup ' num2str(j) ': ']);
end
```

In this section, we define a code that will enable us to input and store the values to be used for the succeeding calculations.

We initialized the variables to make calculations faster. The variables created arrays and matrices from which inputted values can be stored.

In this part, looping was done to prompt user to input necessary property values n/m no of times.

Step 2: Code to calculate r_i and q_i

```
%Calculate r and q
for i = 1 : n
    r(i) = 0;    %Initialize
    q(i) = 0;    %Initialize
    for k = 1 : m
        r(i) = r(i) + vk(k,i)*Rk(k);
        q(i) = q(i) + vk(k,i)*Qk(k);
    end
end
```

r_i and q_i was calculated from the values of v_k, R_k, and Q_k. Nested looping was done since the values depend on the two indices, n and m.

Step 3: Code to calculate J_i and L_i

```
%Calculate J and L
denomJ = 0;     %Initialize
denomL = 0;     %Initialize
for a = 1 : n
    denomJ = denomJ + r(a)*x(a);
    denomL = denomL + q(a)*x(a);
end

for b = 1 : n
    J(b) = r(b)/denomJ;
    L(b) = q(b)/denomL;
end
```

In this part, we first calculated the denominators, <denom> and <denomL>. J_i and L_i was then computed from these values along with their numerator terms.

Step 4: Code to calculate e_{ki}

```
%Calculate e
for k = 1 : m
    for j = 1 : n
        e(k,j) = vk(k,j)*Qk(k)/q(j);
    end
end
```

Similar with the first step, nested loops were used to calculate e_{ki}. v_k, Q_k and q_i depend on two dimensions, n and m respectively.

Step 5: Code to calculate τ_{mn}

```
%Calculate tau
for c = 1 : m
    for d = 1 : m
        tau(c,d) = exp(-(a_mn(c,d))/temp);
    end
end
```

In calculating τ_{mn}, one of the important elements is the main group interaction parameter matrix a_{mn}. Since it is a matrix, whose values depend on m and n, we loop the calculation inside of the other.

Step 6: Code to calculate β_{ik}

```
%Calculate beta
for a = 1 : n
    for b = 1 : m
        beta(a,b) = 0;
        for l = 1 : m
            beta(a,b) = beta(a,b) + e(l,a)*tau(l,b);
        end
    end
end
```

In this matrix, we perform looping three times. β_{ik} depends on the computed e_{ki} and τ_{mn}. Since we are multiplying vectors, order was an important consideration in laying down the code.

Step 7: Code to calculate θ_k

```
%Calculate theta
for y = 1 : m
    theta(y) = 0;
    for z = 1 : n
        theta(y) = theta(y) + (x(z)*q(z)*e(y,z));
    end
    theta(y) = theta(y)/denomL;
end
```

This part is similar with the other steps. We used looping and interpreted the calculation procedure according to the formula.

Step 8: Code to calculate s_k

```
%Calculate s
for t = 1 : m
    s(t) = 0;
    for u = 1 : m
        s(t) = s(t) + (theta(u)*tau(u,t));
    end
end
```

This part is similar with the last step. Again, since we multiplied vectors, we paid attention to the order of factors in the operations.

Step 9: Code to calculate $\ln(\gamma_i)$ and γ_i

```
%Calculate gamma
for i = 1 : n
    lngammaC(i) = 1 - J(i) + log(J(i)) - 5*q(i)*((1 - (J(i)/L(i)) + (log(J(i)/L(i)))));
    lngammaR(i) = 0;
    for j = 1 : m
        lngammaR(i) = lngammaR(i) + (theta(j)*(beta(i,j)/s(j))) - (e(j,i)*(log(beta(i,j)/s(j))));
    end
    lngammaR(i) = q(i)*(1 - lngammaR(i));
    gamma(i) = exp(lngammaC(i) + lngammaR(i));
end

fprintf(['The activity coefficients of the mixture are: ']);
fprintf('\n');
for a = 1 : n
    fprintf('gamma%d:   %.4f\n', a, gamma(1,a));
end
```

In this part, we calculated for the combinatorial and residual $\ln(\gamma_i)$ then γ_i. Again, nested looping was observed because the parameter is dependent on n and m. The last set of codes instructs how to display the values obtained from the calculation.

These are the formulas used to calculate γ_i

$$r_i = \sum_k v_k^{(i)} R_k \qquad q_i = \sum_k v_k^{(i)} Q_k \qquad \ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R$$

$$J_i = \frac{r_i}{\sum_j r_j x_j};\ L_i = \frac{q_i}{\sum_j q_j x_j} \qquad e_{ki} = \frac{v_k^{(i)} Q_k}{q_i} \qquad \psi_{mn} = \exp\left(\frac{-a_{mk}}{T}\right)$$

$$\beta_{ik} = \sum_m e_{mi}\tau_{mk} \qquad \theta_k = \frac{\sum_i x_i q_i e_{ki}}{\sum_j x_j q_j} \qquad s_k = \sum_m \theta_m \tau_{mk}$$

$$\ln \gamma_i^R = q_i\left[1 - \sum_k \left(\theta_k \frac{\beta_{ik}}{s_k} - e_{ki} \ln\left(\frac{\beta_{ik}}{s_k}\right)\right)\right] \qquad \ln \gamma_i^C = 1 - J_i + \ln J_i - 5q_i\left(1 - \frac{J_i}{L_i} + \ln\left(\frac{J_i}{L_i}\right)\right)$$

TEST:
System A: n-butane(1), n-pentane(2), n-heptane (3), and isobutane(4) at 368.15K (x_1 = 0.25, x_2 = 0.30, x_3 = 0.25, x_4 = 0.20)
file: UNIFAC_gamma_1.m

```
Enter system temperature (in K):
368.15
Enter no. of species in the mixture:
4
Enter no. of subgroups present in the species of the mixture:
3
Enter liquid composition (x) of species 1:
0.25
Enter liquid composition (x) of species 2:
0.30
Enter liquid composition (x) of species 3:
0.25
Enter liquid composition (x) of species 4:
0.20
Enter no. of subgroup 1 present in species 1-
2

vk =

     2     0     0     0
     0     0     0     0
     0     0     0     0

Enter no. of subgroup 1 present in species 2-
2

vk =

     2     2     0     0
     0     0     0     0
     0     0     0     0

Enter no. of subgroup 1 present in species 3-
2
```

```
vk =

     2     2     2     0
     0     0     0     0
     0     0     0     0

Enter no. of subgroup 1 present in species 4-
3

vk =

     2     2     2     3
     0     0     0     0
     0     0     0     0

Enter no. of subgroup 2 present in species 1-
2

vk =

     2     2     2     3
     2     0     0     0
     0     0     0     0

Enter no. of subgroup 2 present in species 2-
3

vk =

     2     2     2     3
     2     3     0     0
     0     0     0     0

Enter no. of subgroup 2 present in species 3-
5

vk =

     2     2     2     3
```

```
     2     3     5     0
     0     0     0     0

Enter no. of subgroup 2 present in species 4-
0

vk =

     2     2     2     3
     2     3     5     0
     0     0     0     0

Enter no. of subgroup 3 present in species 1-
0

vk =

     2     2     2     3
     2     3     5     0
     0     0     0     0

Enter no. of subgroup 3 present in species 2-
0

vk =

     2     2     2     3
     2     3     5     0
     0     0     0     0

Enter no. of subgroup 3 present in species 3-
0

vk =

     2     2     2     3
     2     3     5     0
     0     0     0     0

Enter no. of subgroup 3 present in species 4-
```

```
1

vk =

     2     2     2     3
     2     3     5     0
     0     0     0     1

Enter main group interaction parameter value between subgroup 1 and subgroup 1-
0

a_mn =

     0     0     0
     0     0     0
     0     0     0

Enter main group interaction parameter value between subgroup 1 and subgroup 2-
0

a_mn =

     0     0     0
     0     0     0
     0     0     0

Enter main group interaction parameter value between subgroup 1 and subgroup 3-
0

a_mn =

     0     0     0
     0     0     0
     0     0     0

Enter main group interaction parameter value between subgroup 2 and subgroup 1-
0

a_mn =
```

```
     0     0     0
     0     0     0
     0     0     0

Enter main group interaction parameter value between subgroup 2 and subgroup 2-
0

a_mn =

     0     0     0
     0     0     0
     0     0     0

Enter main group interaction parameter value between subgroup 2 and subgroup 3-
0

a_mn =

     0     0     0
     0     0     0
     0     0     0

Enter main group interaction parameter value between subgroup 3 and subgroup 1-
0

a_mn =

     0     0     0
     0     0     0
     0     0     0

Enter main group interaction parameter value between subgroup 3 and subgroup 2-
0

a_mn =

     0     0     0
     0     0     0
     0     0     0
```

```
Enter main group interaction parameter value between subgroup 3 and subgroup 3-
0

a_mn =

     0     0     0
     0     0     0
     0     0     0

Enter Rk value for subgroup 1:
0.9011
Enter Rk value for subgroup 2:
0.6744
Enter Rk value for subgroup 3:
0.4469
Enter Qk value for subgroup 1:
0.848
Enter Qk value for subgroup 2:
0.540
Enter Qk value for subgroup 3:
0.228
The activity coefficients of the mixture are:
gamma1:   0.9829
gamma2:   1.0000
gamma3:   0.9575
gamma4:   0.9826
```

TEST:
System B: acetone(1)/n pentane(2) at 307 K
(x_1 = 0.047, x_2 = 0.953)
file: UNIFAC_gamma_1.m

```
Enter system temperature (in K):
307
Enter no. of species in the mixture:
2
Enter no. of subgroups present in the species of the mixture:
3
Enter liquid composition (x) of species 1:
0.047
Enter liquid composition (x) of species 2:
0.953
Enter no. of subgroup 1 present in species 1-
1

vk =

     1     0
     0     0
     0     0

Enter no. of subgroup 1 present in species 2-
2

vk =

     1     2
     0     0
     0     0

Enter no. of subgroup 2 present in species 1-
0

vk =

     1     2
```

```
     0     0
     0     0

Enter no. of subgroup 2 present in species 2-
3

vk =

     1     2
     0     3
     0     0

Enter no. of subgroup 3 present in species 1-
1

vk =

     1     2
     0     3
     1     0

Enter no. of subgroup 3 present in species 2-
0

vk =

     1     2
     0     3
     1     0

Enter main group interaction parameter value between subgroup 1 and subgroup 1-
0

a_mn =

     0     0     0
     0     0     0
     0     0     0

Enter main group interaction parameter value between subgroup 1 and subgroup 2-
```

```
0

a_mn =

     0     0     0
     0     0     0
     0     0     0

Enter main group interaction parameter value between subgroup 1 and subgroup 3-
476.40

a_mn =

         0         0  476.4000
         0         0         0
         0         0         0

Enter main group interaction parameter value between subgroup 2 and subgroup 1-
0

a_mn =

         0         0  476.4000
         0         0         0
         0         0         0

Enter main group interaction parameter value between subgroup 2 and subgroup 2-
0

a_mn =

         0         0  476.4000
         0         0         0
         0         0         0

Enter main group interaction parameter value between subgroup 2 and subgroup 3-
476.40

a_mn =
```

```
         0         0  476.4000
         0         0  476.4000
         0         0         0

Enter main group interaction parameter value between subgroup 3 and subgroup 1-
26.76

a_mn =

         0         0  476.4000
         0         0  476.4000
   26.7600         0         0

Enter main group interaction parameter value between subgroup 3 and subgroup 2-
26.76

a_mn =

         0         0  476.4000
         0         0  476.4000
   26.7600   26.7600         0

Enter main group interaction parameter value between subgroup 3 and subgroup 3-
0

a_mn =

         0         0  476.4000
         0         0  476.4000
   26.7600   26.7600         0

Enter Rk value for subgroup 1:
0.9011
Enter Rk value for subgroup 2:
0.6744
Enter Rk value for subgroup 3:
1.6724
Enter Qk value for subgroup 1:
0.848
```

```
Enter Qk value for subgroup 2:
0.540
Enter Qk value for subgroup 3:
1.488
The activity coefficients of the mixture are:
gamma1:   4.9920
gamma2:   1.0053
```

TEST:
Generate a P-x,y diagram at 308.15K
(1)acetone/(2)n-hexane system at x = 0:0.5:1
files: UNIFAC_gamma_2.m/bPcalcs.m

```
h = figure;
set(h,'Color',[1 1 1]);
plot(xA,b_P,'b',y(:,1),b_P,'r')
xlabel('x1, y1')
ylabel('P(in kPa)')
title('P-x,y diagram of (1)Acetone/(2)Cyclohexane system at T = 308.15K')
xlim([0 1])
hold on
scatter(x1, Pb)
scatter(y1, Pb)
hold off
```

```
h = figure;
set(h,'Color',[1 1 1]);
plot(xA,b_P,'b',y(:,1),b_P,'r')
xlabel('x1, y1')
ylabel('P(in kPa)')
title('P-x,y diagram of (1)Acetone/(2)Cyclohexane system at T = 308.15K')
xlim([0 1])
```

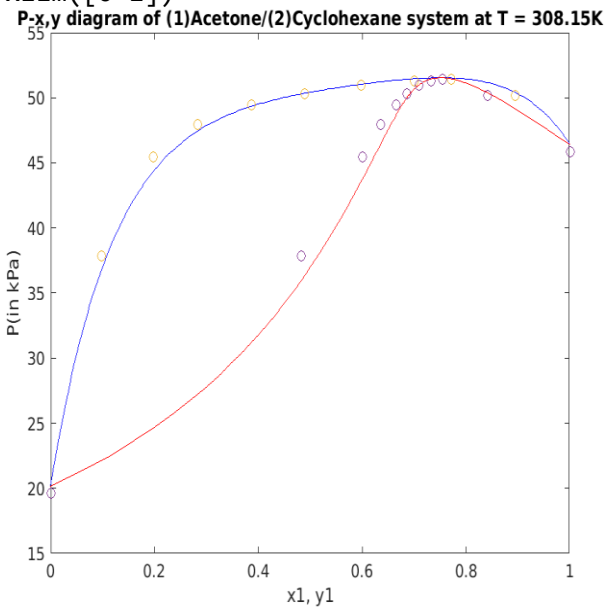


Fig. 1: P-x,y diagram of the system at T = 308.15K overlapped with the data points from Table 1 in LPA2

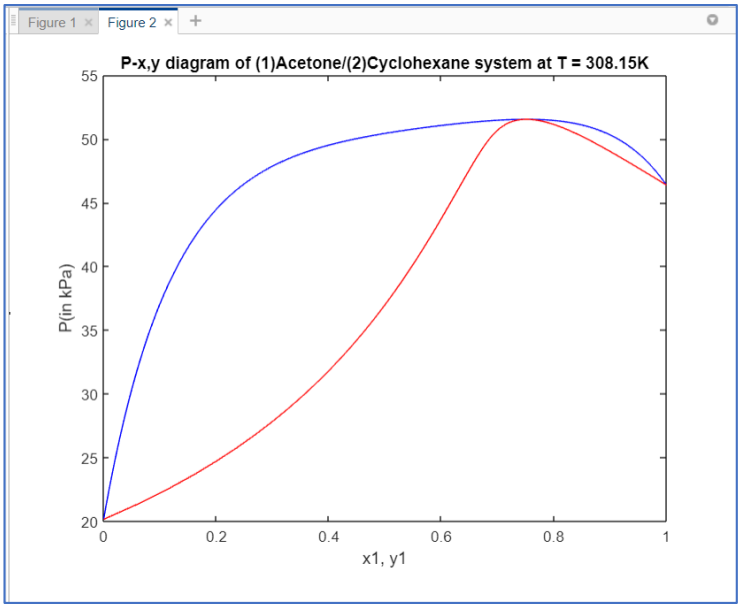
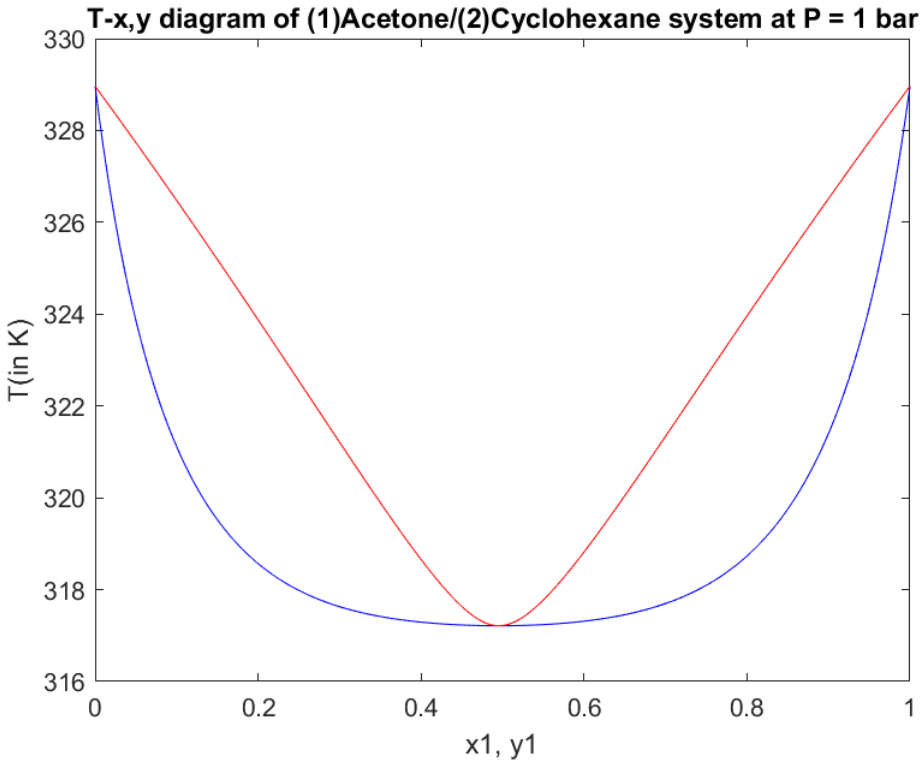


Fig. 2: P-x,y diagram of the system at T = 308.15K

TEST:
Generate a T-x,y diagram at 308.15K
(1)acetone/(2)n-hexane system at x = 0:0.5:1
files: UNIFAC_gamma_2.m/bPcalcs.m

```
T-xy plot
h = figure;
set(h,'Color',[1 1 1]);
plot(xA,b_T,'b',y_t(:,1),b_T,'r')
xlabel('x1, y1')
ylabel('T(in K)')
title('T-x,y diagram of (1)Acetone/(2)Cyclohexane system at P = 1 bar')
xlim([0 1])
```



Program File Name: UNIFAC_gamma_1.m

```
clc
clear

% Input the following variables:
temp = input('Enter system temperature (in K): ');
n = input('Enter no. of species in the mixture: ');
m = input('Enter no. of subgroups present in the species of the mixture: ');
% Number assignment of subgroups is based on the UNIFAC-VLE Subgroup Parameter list
on SVAS.
% e.g. if the system have species with CH3, CH2, and CH2NH subgroups, CH3 will be
assigned with 1, CH2 with 2 and CH2NH with 3.

% Initialize variables
x = zeros(1,n);
vk = zeros(m,n);
a_mn = zeros(m,m);
Rk = zeros(1,m);
Qk = zeros(1,m);

for b = 1 : n
    x(1,b) = input(['Enter liquid composition (x) of species ' num2str(b) ': ']);
end

for i = 1 : m
    for j = 1 : n
        vk(i,j) = input(['Enter no. of subgroup ' num2str(i) ' present in species '
num2str(j) '- '])
    end
end

for f = 1 : m
    for g = 1 : m
        a_mn(f,g) = input(['Enter main group interaction parameter value between
subgroup ' num2str(f) ' and subgroup ' num2str(g) '- '])
    end
end

for i = 1 : m
    Rk(1,i) = input(['Enter Rk value for subgroup ' num2str(i) ': ']);
end

for j = 1 : m
    Qk(1,j) = input(['Enter Qk value for subgroup ' num2str(j) ': ']);
end

%Calculate r and q
for i = 1 : n
    r(i) = 0;    %Initialize
    q(i) = 0;    %Initialize
    for k = 1 : m
        r(i) = r(i) + vk(k,i)*Rk(k);
        q(i) = q(i) + vk(k,i)*Qk(k);
    end
```

```
end

%Calculate J and L
denomJ = 0;     %Initialize
denomL = 0;     %Initialize
for a = 1 : n
    denomJ = denomJ + r(a)*x(a);
    denomL = denomL + q(a)*x(a);
end

for b = 1 : n
    J(b) = r(b)/denomJ;
    L(b) = q(b)/denomL;
end

%Calculate e
for k = 1 : m
    for j = 1 : n
        e(k,j) = vk(k,j)*Qk(k)/q(j);
    end
end

%Calculate tau
for c = 1 : m
    for d = 1 : m
        tau(c,d) = exp(-(a_mn(c,d))/temp);
    end
end

%Calculate beta
for a = 1 : n
    for b = 1 : m
        beta(a,b) = 0;
        for l = 1 : m
            beta(a,b) = beta(a,b) + e(l,a)*tau(l,b);
        end
    end
end

%Calculate theta
for y = 1 : m
    theta(y) = 0;
    for z = 1 : n
        theta(y) = theta(y) + (x(z)*q(z)*e(y,z));
    end
    theta(y) = theta(y)/denomL;
end

%Calculate s
for t = 1 : m
    s(t) = 0;
    for u = 1 : m
        s(t) = s(t) + (theta(u)*tau(u,t));
    end
end
```

```
%Calculate gamma
for i = 1 : n
    lngammaC(i) = 1 - J(i) + log(J(i)) - 5*q(i)*((1 - (J(i)/L(i)) +
(log(J(i)/L(i)))));
    lngammaR(i) = 0;
    for j = 1 : m
        lngammaR(i) = lngammaR(i) + (theta(j)*(beta(i,j)/s(j))) -
(e(j,i)*(log(beta(i,j)/s(j))));
    end
    lngammaR(i) = q(i)*(1 - lngammaR(i));
    gamma(i) = exp(lngammaC(i) + lngammaR(i));
end

fprintf(['The activity coefficients of the mixture are: ']);
fprintf('\n');
for a = 1 : n
    fprintf('gamma%d:   %.4f\n', a, gamma(1,a));
end
```

Program File Name: UNIFAC_gamma_2.m

```
clc;
clear;

%input
xA = [0:0.005:1];
xB = 1 - xA;
x = cat(1,xA,xB);
x(:,1) = [];
x(:,200) = [];
x;
temp = 308.15;

%activity coefficient calculations
global gamma;
for row1 = 1 : numel(x(1,:))
    gammafinal(row1,:) = gamma_unifac(temp, x(:,row1));
end
gamma01 = [0 1];
gamma02 = [1 0];
gamma = [gamma01; gammafinal; gamma02];

function gamma = gamma_unifac(temp, x)
%This function computes for the activity coefficients for an (1)Acetone
%/(2)Cyclohexane system at temperature temp(K) at various liquid fractions
%of Acetone based on the UNIFAC model.
    %precalculations
    n = 2;
    m = 3;
    vk = [1 2; 0 4; 1 0];
    a_mn = [0 0 476.4; 0 0 476.4; 26.7 26.7 0];
    Rk = [0.9011 0.6744 1.6724];
    Qk = [0.8480 0.5400 1.4880];

    %Calculate r and q
    for i = 1 : n
        r(i) = 0;    %Initialize
        q(i) = 0;    %Initialize
        for k = 1 : m
            r(i) = r(i) + vk(k,i)*Rk(k);
            q(i) = q(i) + vk(k,i)*Qk(k);
        end
    end

    %Calculate J and L
    denomJ = 0;     %Initialize
    denomL = 0;     %Initialize
    for a = 1 : n
        denomJ = denomJ + r(a)*x(a);
        denomL = denomL + q(a)*x(a);
    end

    for b = 1 : n
        J(b) = r(b)/denomJ;
```

```
        L(b) = q(b)/denomL;
    end

    %Calculate e
    for k = 1 : m
        for j = 1 : n
            e(k,j) = vk(k,j)*Qk(k)/q(j);
        end
    end

    %Calculate tau
    for c = 1 : m
        for d = 1 : m
            tau(c,d) = exp(-(a_mn(c,d))/temp);
        end
    end

    %Calculate beta
    for a = 1 : n
        for b = 1 : m
            beta(a,b) = 0;
            for l = 1 : m
                beta(a,b) = beta(a,b) + e(l,a)*tau(l,b);
            end
        end
    end

    %Calculate theta
    for y = 1 : m
        theta(y) = 0;
        for z = 1 : n
            theta(y) = theta(y) + (x(z)*q(z)*e(y,z));
        end
        theta(y) = theta(y)/denomL;
    end

    %Calculate s
    for t = 1 : m
        s(t) = 0;
        for u = 1 : m
            s(t) = s(t) + (theta(u)*tau(u,t));
        end
    end

    %Calculate gamma
    for i = 1 : n
        lngammaC(i) = 1 - J(i) + log(J(i)) - 5*q(i)*((1 - (J(i)/L(i)) +
(log(J(i)/L(i)))));
        lngammaR(i) = 0;
        for j = 1 : m
            lngammaR(i) = lngammaR(i) + (theta(j)*(beta(i,j)/s(j))) -
(e(j,i)*(log(beta(i,j)/s(j))));
        end
        lngammaR(i) = q(i)*(1 - lngammaR(i));
        gamma(i) = exp(lngammaC(i) + lngammaR(i));

        end
    end
```

Program File Name: bPcalcs.m

```
clc
clear

%input
xA = [0:0.005:1];
xB = 1 - xA;
xC = cat(1,xA,xB);
xD = xC.';
global gamma;
temp = 308.15;  %in K

%P-xy data calculations
global b_P;
global y;
[b_P, y] = bubblePcalcs(temp, xD, gamma);

%P-xy data from Part 2 of LPA 2
Pb = [19.625; 37.877; 45.476; 47.969; 49.489; 50.316; 50.969; 51.302; 51.409; 50.196;
45.863];
xl = [0; 0.098; 0.198; 0.283; 0.387; 0.489; 0.598; 0.7; 0.771; 0.895; 1];
yl = [0; 0.482; 0.601; 0.635; 0.665; 0.686; 0.709; 0.732; 0.754; 0.841; 1];

%P-xy plot
%to plot the P-x,y data, enter the following in the command window.
%h = figure;
%set(h,'Color',[1 1 1]);
%plot(xA,b_P,'b',y(:,1),b_P,'r')
%xlabel('x1, y1')
%ylabel('P(in kPa)')
%title('P-x,y diagram of (1)Acetone/(2)Cyclohexane system at T = 308.15K')
%xlim([0 1])
%to overlap the given P-x,y data, enter the succeeding command therafter.
%hold on
%scatter(x1, Pb)
%scatter(y1, Pb)
%hold off

function [b_P,y] = bubblePcalcs(temp, xD, gamma)
%This function computes for the bubble pressure and vapor compositions
%for an (1)Acetone /(2)Cyclohexane system at temperature temp(K) at
%various liquid fractions of Acetone based on the Modified Raoult's Law.
    %initialize variable and matrix holders
    P1sat = 0;
    P2sat = 0;
    Pbub = zeros(1,numel(xD(:,1)));
    y = zeros(numel(xD(:,1)),2);
    %precalculations
    A1 = 14.3145;
    A2 = 13.6568;
    B1 = 2756.22;
    B2 = 2723.44;
    C1 = 228.060;
    C2 = 220.618;
```

```
    %calculate the saturated pressure (Psat(kPa)) of each species at the given
    %temp. using the Antoine Equation
    P1sat = exp(A1-(B1/((temp-273.15)+C1)));
    P2sat = exp(A2-(B2/((temp-273.15)+C2)));
    %calculate bubble pressure and vapor composition of the mixture
        %calculate the bubble pressure, Pbub
        Pbub = gamma(:,1).*xD(:,1).*P1sat + gamma(:,2).*xD(:,2).*P2sat;
        %calculate the vapor phase composition of each species, y(i)
        y1 = (gamma(:,1).*xD(:,1).*P1sat)./(Pbub);
        y2 = (gamma(:,2).*xD(:,2).*P2sat)./(Pbub);
        y = [y1 y2];
        b_P = Pbub;
end
```