Lab Report 1

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Group: 11

Problem Statement:

Consider a countercurrent-flow for the removal of acetone from an air-acetone mixture by means of liquid water. Tray tower for absorption is operating under isothermal and continuous flow conditions. The parameter values and process characteristics are documented below:

System	**Acetone (A)-air (B)-water (C)**
Total number of stages	5
Operating temperature (K)	300
Total pressure (kPa)	101.3
Liquid holdup in each tray (kmol)	3
$y_{0,A}$ (mole fraction)	0.01
$x_{F,A}$ (mole fraction)	0.0
$\bar{G}$ (kmol B/h)	30
$\bar{L}$ (kmol C/h)	90
Equilibrium relationship	$y_A = 2.53x_A$

Investigate the dynamic performance of the representative absorber with a mathematical modelling employing explicit Euler approach to solve the ODE. Consider the integration interval (Δt) as 0.0001h and solve for the following cases:

1. Obtain the start-up profile from start t=0 to t=2 hours for the tray composition in terms of mole ratio of liquid phase (moles of solute/moles of inert liquid). Consider the initial guess for the traywise compositions (mole ratios) as below. Compute the steady state concentration.

Tray composition	Initial guess
$\bar{x}_{1A}$	0.10
$\bar{x}_{2,A}$	0.08
$\bar{x}_{3,A}$	0.06
$\bar{x}_{4,A}$	0.04
$\bar{x}_{5,A}$	0.01

2. In this simulation experiment, the process is initially remained at steady state for 0.2 hours. Subsequently, two consecutive step changes have been introduced in $y_{0,A}$ (changed from 0.01 to 0.02 at time = 0.2 hour and then from 0.02 to 0.01 at time = 0.6 hour). Obtain the tray composition dynamics in all trays in terms of mole ratio (mole ratio of gas phase (moles of solute/moles of inert gas) under this pulse change in gas feed composition.

Algorithm:

The solution to ode dy/dx=f(x,y) given by euler's explicit scheme is y(n+1)=y(n)+dx*f(x(n),y(n)), where dx is unit of discretization.

Here we have five odes in terms of mole ratios of liquid phase x_bar and gas phase y_bar which are related by the equilibrium relation y_bar=2.53*x_bar/(1-1.53*x_bar)

The system of ODEs is solved numerically as follows:-

Part 1:

Program start

Initialize variable

m=3.0; // liquid holdup
L=90.0; // kmol C/h

```
G=30.0;  // kmol B/h
i=20000; // no of iterations = (2-0)/0.0001
NT=5; // no of trays
dt=0.0001; // discrete time unit
```

Initialize Matrix X = zeros(NT, i) , Matrix Y = zeros(NT, i), Vector time = zeroes(i,1) Initialize variable XF = zeros(i), Y0(i) = (0.01/1-0.01)*ones(i) time(1) = 0

Initial guess :-

```
X(1,1) = 0.1;

X(2,1) = 0.08;

X(3,1) = 0.06;

X(4,1) = 0.04;

X(5,1) = 0.01;

Star loop for k=1:i
    XF(k)=0.0;
    Y0(k)=1/99;
   Start loop for n=1:NT
        Y(n,k)=(2.53*X(n,k))/(1-1.53*X(n,k));
    End loop

   Start loop for n=1:NT
        XM(n,k)=X(n,k)/(1+X(n,k));
        YM(n,k)=Y(n,k)/(1+Y(n,k));
    End loop
 // For first tray
    X(1,k+1)=X(1,k)+ (dt/m)* (L*X(2,k)+G*Y0(k)-L*X(1,k)-G*Y(1,k));
//Euler's explicit scheme
    IF(X(1,k+1)>1)
        X(1,k+1)=1;
    End conditional statement
    If(X(1,k+1)<0)
        X(1,k+1)=0;
    End conditional statement
 // For trays 2 to 4
    Start loop for n=2:4
        X(n,k+1)=X(n,k)+(dt/m)*(L*X(n+1,k)+G*Y(n-1,k)-L*X(n,k)-G*Y(n,k));
//Euler's explicit scheme
        If(X(n,k+1)>1)
            X(n,k+1)=1;
        End conditional statement
```

```
        If(X(n,k+1)<0)
            X(n,k+1)=0;
        End conditional statement
    End loop
//  Euler's explicit scheme for final tray
    X(5,k+1)=X(5,k)+(dt/3)*(L*XF(k)+G*Y(4,k)-L*X(5,k)-G*Y(5,k));
    If(X(5,k+1)>1)
        X(5,k+1)=1;
    End conditional statement
    If(X(5,k+1)<0)
        X(5,k+1)=0;
    End conditional statement
    T(k+1)=T(k)+dt;  // updating time value by one discrete unit
End  loop
Start loop for i = 1:NT
 print(string(X(i,20000))) //steady state values
End loop
Plot(X vs  Time)
```

Part 2

Program start

Initialize variable

```
L = 90; // kmol C/h
G=30.0;  // kmol B/h
m = 3;   // liquid holdup
iter = 10000; // total no. of iterations
iter1 = 2000; // iteration for 1st step change to Y0
iter2 = 6000; // iteration for 2nd  step change to Y0
Nt = 5;  // no. of trays
dt = 0.0001; // discrete time unit


Initialize Matrix X = zeros(Nt, iter) , Matrix Y = zeros(Nt, iter),
Vector time = zeroes(iter,1) Initialize variable Xf = 0, Y0 = 0.0101
time(1) = 0
Start loop for i = 1:iter1
Allocate:-
    X(1,i) = 3.0124e-03;
    X(2,i) = 2.1976e-03;
    X(3,i) = 1.5050e-03;
    X(4,i) = 9.1750e-04;
    X(5,i) = 4.2023e-04;
    time(i+1)=time(i)+dt;
```

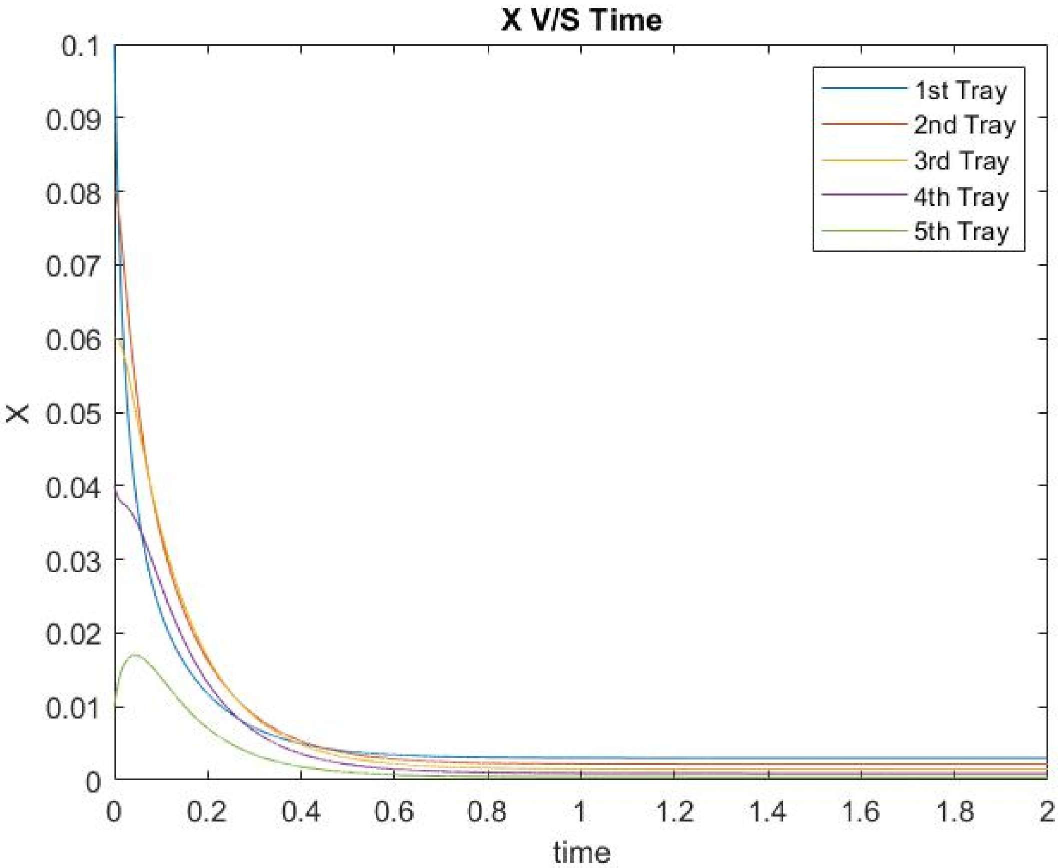
```
    Start loop for a = 1:Nt
      Y(a,i) = (2.53*X(a,i))/(1-(1.53*X(a,i))); // Equilibrium relation
    End loop
End loop

Start loop for i = iter1:iter-1
   IF(i < iter2)
      Y0 = 0.02/(1-0.02);
   Else
       Y0 = 0.01/(1-0.01);
   End conditional statements

 // Euler's explicit scheme
//  1st tray
 X(1,i+1) = X(1,i) + (dt/m)*((L*X(2,i))+(G*Y0)-(L*X(1,i))-(G*Y(1,i)));
// 2nd to 4th  tray
 Start loop for j = 2:Nt-1
    X(j,i+1) = X(j,i) + (dt/m)*((L*X(j+1,i))+(G*Y(j-1,i))-(L*X(j,i))-(G*Y(j,i)));
 End loop
 //5th tray
 X(5,i+1) = X(5,i) + (dt/m)*((L*Xf)+(G*Y(4,i))-(L*X(5,i))-(G*Y(5,i)));
Start loop for k = 1:Nt
 Y(k,i+1) = (2.53*X(k,i+1))/(1-(1.53*X(k,i+1))); // equilibrium  relation
 End loop
 time(i+1)=time(i)+dt; // updating time value by one discrete unit
End loop

Start loop for i = 1:Nt
 print(string(X(i,10000))) //steady state value
End loop
Start loop for i = 1:Nt
 print(string(Y(i,10000))) //steady state value
End loop
Plot(X vs Time);
Plot(Y vs Time); // denotes comments
```

Results:

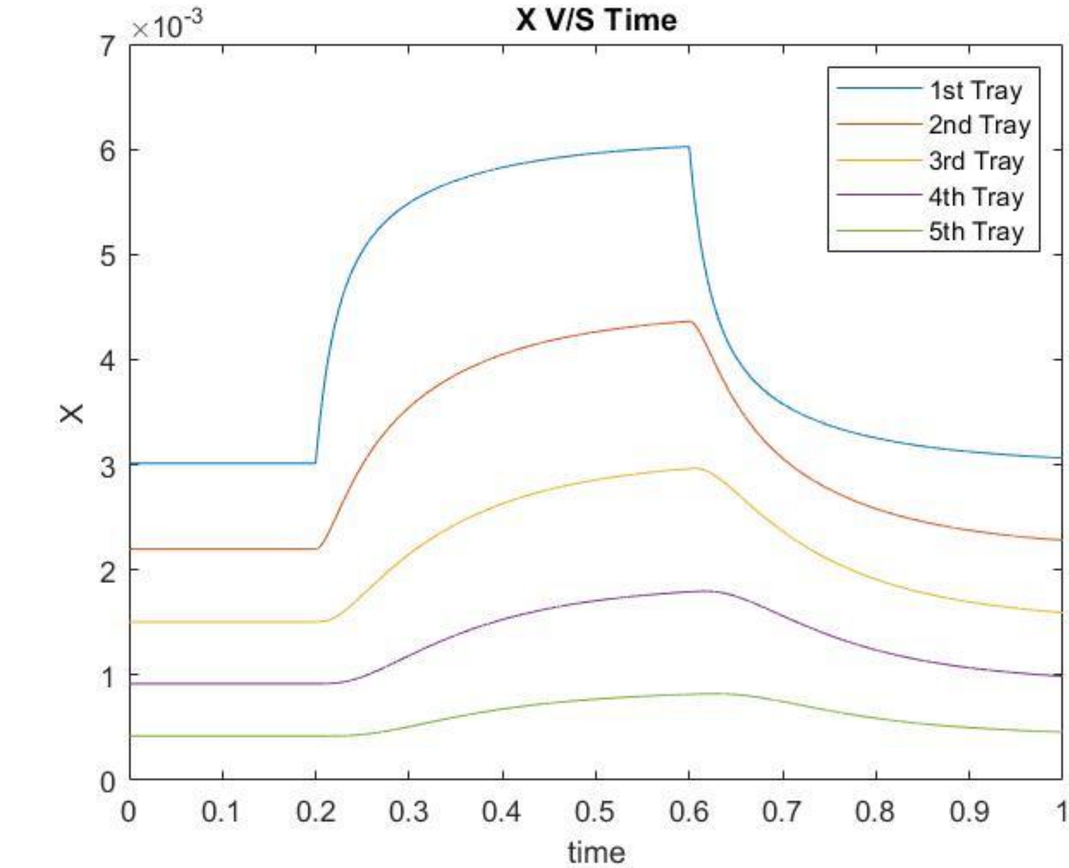
Part 1:

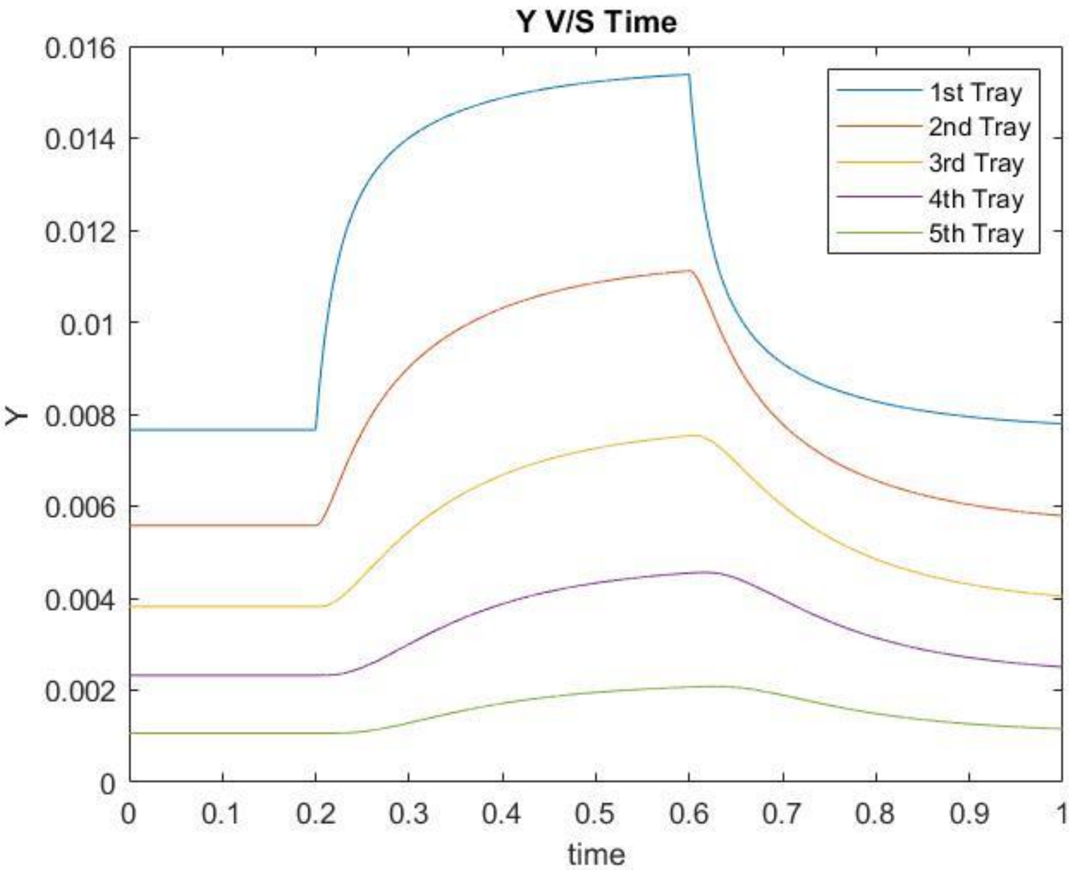
Tray Composition	Initial Guess	Steady state value
X1,A	0.10	0.00301240
X2,A	0.08	0.00219760
X3,A	0.06	0.0015050

X4,A	0.04	0.00091750
X5,A	0.01	0.00042023



Part 2:


X V/S Time
$\times 10^{-3}$
7
6
5
4
3
2
1
0
X
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
time
1st Tray
2nd Tray
3rd Tray
4th Tray
5th Tray


Y V/S Time
0.016
0.014
0.012
0.01
0.008
0.006
0.004
0.002
0
Y
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
time
1st Tray
2nd Tray
3rd Tray
4th Tray
5th Tray