CBE 450 Chemical Reactor Fundamentals
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Sample Codes

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Non-Isothermal Batch Reactors

There are four input files for modeling Non-Isothermal Batch Reactors

1. One irreversible reaction
2. One reversible reaction
3. Two simultaneous reactions
4. Two sequential reactions

1. One irreversible reaction

```
function dydt = sysodeinput(x,y,nvec);
%
%  one reaction in solvent, S
%  2A --> B
%
%  sample usage:
%  [y,x]=sysode(2,1000,0,10,[10,0,40,300]);
%
CA = y(1); % mol/liter
CB = y(2);
CS = y(3);
T =  y(4); % K
%
%  stoichiometry
%
nuA = -2;
nuB = +1;
nuS = 0;
%
%  rate law
%
ko = 1.0; % liter/mole/sec
Ea = 4000; % J/mol
R = 8.314; %J/mol/K
%DUR =  00000.0; %J/mol
DUR = -10000.0; %J/mol
%DUR =  10000.0; %J/mol

k = ko*exp(-Ea/(R*T)); % liters/mole/sec
r = k*CA*CA; % mole/liter/sec
%
%  pure component heat capacities
%
```

```
CvA = 4.0; %J/mol/K
CvB = 7.0; %J/mol/K
CvS = 3.0; %J/mol/K
%
% mole fractions
%
CT = CA + CB + CS;
xA = CA/CT;
xB = CB/CT;
xS = CS/CT;
%
% mixture heat capacity
%
Cvmix = xA*CvA + xB*CvB + xS*CvS;
%
%  mole and energy balances
%
dydt(1) = nuA*r;
dydt(2) = nuB*r;
dydt(3) = nuS*r;
dydt(4) = -DUR*r/(CT*Cvmix);
```

2. One reversible reaction

```
function dydt = sysodeinput(x,y,nvec);
%
%  one reversible reaction in solvent, S
%  2A <--> B
%
%  sample usage:
%  [y,x]=sysode(2,1000,0,10,[10,0,40,300]);
%
CA = y(1); % mol/liter
CB = y(2);
CS = y(3);
T =  y(4); % K
%
%  stoichiometry
%
nuA1 = -2;
nuB1 = 1;
nuS1 = 0;
nuA2 = 2;
nuB2 = -1;
nuS2 = 0;

%
%  rate law
%
ko1 = 1.0; % liter/mole/sec
Ea1 = 4000; % J/mol
R = 8.314; %J/mol/K
DUR1 =  00000.0; %J/mol
%DUR1 = -10000.0; %J/mol
%DUR1 =  10000.0; %J/mol
```

```
k1 = ko1*exp(-Ea1/(R*T)); % liters/mole/sec
r1 = k1*CA*CA; % mole/liter/sec
%
ko2 = 1.0; % 1/sec
Ea2 = Ea1 - DUR1; % J/mol
R = 8.314; %J/mol/K
DUR2 = -DUR1;
k2 = ko2*exp(-Ea2/(R*T)); % 1/sec
r2 = k2*CB; % mole/liter/sec
%
%  pure component heat capacities
%
CvA = 4.0; %J/mol/K
CvB = 7.0; %J/mol/K
CvS = 3.0; %J/mol/K
%
% mole fractions
%
CT = CA + CB + CS;
xA = CA/CT;
xB = CB/CT;
xS = CS/CT;
%
% mixture heat capacity
%
Cvmix = xA*CvA + xB*CvB + xS*CvS;
%
%  mole and energy balances
%
dydt(1) = nuA1*r1 + nuA2*r2;
dydt(2) = nuB1*r1 + nuB2*r2;
dydt(3) = nuS1*r1 + nuS2*r2;
dydt(4) = -(DUR1*r1 + DUR2*r2)/(CT*Cvmix);
```

3. Two simultaneous reactions

```
function dydt = sysodeinput(x,y,nvec);
%
%  two simultaneous reactions in solvent, S
%  A + B --> D
%  A + C --> E
%
%  sample usage:
%  [y,x]=sysode(2,1000,0,10,[10,8,8,0,0,40,300]);
%
CA = y(1); % mol/liter
CB = y(2);
CC = y(3);
CD = y(4);
CE = y(5);
CS = y(6);
T =  y(7); % K
%
%  stoichiometry
%
```

```
nuA1 = -1;
nuB1 = -1;
nuC1 = 0;
nuD1 = 1;
nuE1 = 0;
nuS1 = 0;
%
nuA2 = -1;
nuB2 = 0;
nuC2 = -1;
nuD2 = 0;
nuE2 = 1;
nuS2 = 0;
%
%  rate law
%
ko1 = 1.0; % liter/mole/sec
Ea1 = 4000; % J/mol
R = 8.314; %J/mol/K
DUR1 = -10000.0; %J/mol
k1 = ko1*exp(-Ea1/(R*T)); % liters/mole/sec
r1 = k1*CA*CB; % mole/liter/sec
%
ko2 = 1.0; % 1/sec
Ea2 = 3000; % J/mol
R = 8.314; %J/mol/K
DUR2 = 10000;
k2 = ko2*exp(-Ea2/(R*T)); % 1/sec
r2 = k2*CA*CC; % mole/liter/sec
%
%  pure component heat capacities
%
CvA = 4.0; %J/mol/K
CvB = 3.0; %J/mol/K
CvC = 5.0; %J/mol/K
CvD = 6.0; %J/mol/K
CvE = 7.0; %J/mol/K
CvS = 4.0; %J/mol/K
%
% mole fractions
%
CT = CA + CB + CC + CD + CE + CS;
xA = CA/CT;
xB = CB/CT;
xC = CC/CT;
xD = CD/CT;
xE = CE/CT;
xS = CS/CT;
%
% mixture heat capacity
%
Cvmix = xA*CvA + xB*CvB + xD*CvC + xD*CvD + xE*CvE + xS*CvS;
%
%  mole and energy balances
%
dydt(1) = nuA1*r1 + nuA2*r2;
```

```
dydt(2) = nuB1*r1 + nuB2*r2;
dydt(3) = nuC1*r1 + nuC2*r2;
dydt(4) = nuD1*r1 + nuD2*r2;
dydt(5) = nuE1*r1 + nuE2*r2;
dydt(6) = nuS1*r1 + nuS2*r2;
dydt(7) = -(DUR1*r1 + DUR2*r2)/(CT*Cvmix);
```

4. Two sequential reactions

```
function dydt = sysodeinput(x,y,nvec);
%
%  two sequential reactions in solvent, S
%  A + B --> C
%  A + C --> D
%
%  sample usage:
%  [y,x]=sysode(2,1000,0,10,[10,4,0,0,40,300]);
%
CA = y(1); % mol/liter
CB = y(2);
CC = y(3);
CD = y(4);
CS = y(5);
T =  y(6); % K
%
%  stoichiometry
%
nuA1 = -1;
nuB1 = -1;
nuC1 = 1;
nuD1 = 0;
nuS1 = 0;
%
nuA2 = -1;
nuB2 = 0;
nuC2 = -1;
nuD2 = 1;
nuS2 = 0;
%
%  rate law
%
ko1 = 1.0; % liter/mole/sec
Ea1 = 4000; % J/mol
R = 8.314; %J/mol/K
DUR1 = -10000.0; %J/mol
k1 = ko1*exp(-Ea1/(R*T)); % liters/mole/sec
r1 = k1*CA*CB; % mole/liter/sec
%
ko2 = 1.0; % 1/sec
Ea2 = 3000; % J/mol
R = 8.314; %J/mol/K
DUR2 = -10000;
k2 = ko2*exp(-Ea2/(R*T)); % 1/sec
r2 = k2*CA*CC; % mole/liter/sec
%
```

```
%  pure component heat capacities
%
CvA = 4.0; %J/mol/K
CvB = 3.0; %J/mol/K
CvC = 6.0; %J/mol/K
CvD = 9.0; %J/mol/K
CvS = 4.0; %J/mol/K
%
% mole fractions
%
CT = CA + CB + CC + CD  + CS;
xA = CA/CT;
xB = CB/CT;
xC = CC/CT;
xD = CD/CT;
xS = CS/CT;
%
% mixture heat capacity
%
Cvmix = xA*CvA + xB*CvB + xD*CvC + xD*CvD  + xS*CvS;
%
%  mole and energy balances
%
dydt(1) = nuA1*r1 + nuA2*r2;
dydt(2) = nuB1*r1 + nuB2*r2;
dydt(3) = nuC1*r1 + nuC2*r2;
dydt(4) = nuD1*r1 + nuD2*r2;
dydt(5) = nuS1*r1 + nuS2*r2;
dydt(6) = -(DUR1*r1 + DUR2*r2)/(CT*Cvmix);
```