**CBE 450 Chemical Reactor Fundamentals**
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**Sample Codes**
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## Non-Isothermal CSTRs

There are four input files for modeling Non-Isothermal CSTRs

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
%
%  example usage:
%  [y,x] = sysode(2,1000,0,100,[10,0,30,300]);
%
CA = y(1); % mol/liter
CB = y(2); % mol/liter
CS = y(3); % mol/liter
T = y(4); % K
%
% stoichiometry
%
nuA = -2.0;
nuB = 1.0;
nuS = 0.0;
%
% rate law
%
R = 8.314; % J/mol/K
ko = 1.0e-1; % liter/mol/sec
Ea = 2500; % J/mol
k = ko*exp(-Ea/(R*T));
r = k*CA*CA;
%
%  pure component heat capacities
%
CpA = 4.0; %J/mol/K
CpB = 7.0; %J/mol/K
CpS = 3.0; %J/mol/K
%
```

```
%  enthalpies of formation
%
Tref = 298.15; % K
pref = 101325; % Pa
HfrefA = -1000; %J/mol
HfrefB = -10000; % J/mol
HA = CpA*(T-Tref) + HfrefA;
HB = CpB*(T-Tref) + HfrefB;
DHR = nuA*HA + nuB*HB;
%
% constant volume
%
V = 1000.0; % liter
F = 1; % liter/sec
Fin = F;
Fout = F;
%
%  inlet concentrations
%
CAin = 10.0; % mol/liter
CBin = 0.0; % mol/liter
CSin = 30.0; % mol/liter
Tin = 300.0; % K
%
% mole fractions
%
CT = CA + CB + CS;
xA = CA/CT;
xB = CB/CT;
xS = CS/CT;
CTin = CAin + CBin + CSin;
xAin = CAin/CTin;
xBin = CBin/CTin;
xSin = CSin/CTin;
%
% mixture heat capacity
%
Cpmix = xA*CpA + xB*CpB + xS*CpS;
Cpmixin = xAin*CpA + xBin*CpB + xSin*CpS;
%
%  molar balances
%
dydt(1) = Fin/V*CAin - Fout/V*CA + nuA*r;
dydt(2) = Fin/V*CBin - Fout/V*CB + nuB*r;
dydt(3) = Fin/V*CSin - Fout/V*CS + nuS*r;
dydt(4) = ( Fin/V*CTin*Cpmixin*(Tin - T) - DHR*r )/(CT*Cpmix);
```

## 2. One reversible reaction

```
function dydt = sysodeinput(x,y,nvec);
%
%  one reversible reaction in solvent S
%  2A <--> B
%
```

```
%  example usage:
%  [y,x] = sysode(2,1000,0,100,[10,0,30,300]);
%
CA = y(1); % mol/liter
CB = y(2); % mol/liter
CS = y(3); % mol/liter
T = y(4); % K
%
% stoichiometry
%
nuA1 = -2.0;
nuB1 = 1.0;
nuS1 = 0.0;
%
nuA2 = 2.0;
nuB2 = -1.0;
nuS2 = 0.0;
%
% rate law for reaction 1
%
R = 8.314; % J/mol/K
ko1 = 1.0e-1; % liter/mol/sec
Ea1 = 2500; % J/mol
k1 = ko1*exp(-Ea1/(R*T));
r1 = k1*CA*CA;
%
%  pure component heat capacities
%
CpA = 4.0; %J/mol/K
CpB = 7.0; %J/mol/K
CpS = 3.0; %J/mol/K
%
%  enthalpies of formation
%
Tref = 298.15; % K
pref = 101325; % Pa
HfrefA = -1000; %J/mol
HfrefB = -10000; % J/mol
HA = CpA*(T-Tref) + HfrefA;
HB = CpB*(T-Tref) + HfrefB;
DHR1 = nuA1*HA + nuB1*HB;
DHR2 = nuA2*HA + nuB2*HB;
%
% rate law for reaction 2
%
ko2 = 1.0e-1; % 1/sec
Ea2 = Ea1 - DHR1; % J/mol
k2 = ko2*exp(-Ea2/(R*T));
r2 = k2*CB;
%
% constant volume
%
V = 1000.0; % liter
F = 1; % liter/sec
Fin = F;
Fout = F;
```

```
%
%  inlet concentrations
%
CAin = 10.0; % mol/liter
CBin = 0.0; % mol/liter
CSin = 30.0; % mol/liter
Tin = 300.0; % K
%
% mole fractions
%
CT = CA + CB + CS;
xA = CA/CT;
xB = CB/CT;
xS = CS/CT;
CTin = CAin + CBin + CSin;
xAin = CAin/CTin;
xBin = CBin/CTin;
xSin = CSin/CTin;
%
% mixture heat capacity
%
Cpmix = xA*CpA + xB*CpB + xS*CpS;
Cpmixin = xAin*CpA + xBin*CpB + xSin*CpS;
%
%  molar balances
%
dydt(1) = Fin/V*CAin - Fout/V*CA + nuA1*r1 + nuA2*r2;
dydt(2) = Fin/V*CBin - Fout/V*CB + nuB1*r1 + nuB2*r2;
dydt(3) = Fin/V*CSin - Fout/V*CS + nuS1*r1 + nuS2*r2;
dydt(4) = ( Fin/V*CTin*Cpmixin*(Tin - T) - DHR1*r1 - DHR2*r2 )/(CT*Cpmix);
```

## 3. Two simultaneous reactions

```
function dydt = sysodeinput(x,y,nvec);
%
%  two simultaneous irreversible reactions in solvent S
%  2A --> B
%  A + C --> D
%
%  example usage:
%  [y,x] = sysode(2,1000,0,1000,[10,0,10,0,30,300]);
%
CA = y(1); % mol/liter
CB = y(2); % mol/liter
CC = y(3); % mol/liter
CD = y(4); % mol/liter
CS = y(5); % mol/liter
T = y(6); % K
%
% stoichiometry
%
nuA1 = -2.0;
nuB1 = 1.0;
nuC1 = 0.0;
```

```
nuD1 = 0.0;
nuS1 = 0.0;
%
nuA2 = -1.0;
nuB2 = 0.0;
nuC2 = -1.0;
nuD2 = 1.0;
nuS2 = 0.0;
%
% rate law for reaction 1
%
R = 8.314; % J/mol/K
ko1 = 1.0e-1; % liter/mol/sec
Ea1 = 2500; % J/mol
k1 = ko1*exp(-Ea1/(R*T));
r1 = k1*CA*CA;
%
%  pure component heat capacities
%
CpA = 4.0; %J/mol/K
CpB = 7.0; %J/mol/K
CpC = 3.0; %J/mol/K
CpD = 6.0; %J/mol/K
CpS = 3.0; %J/mol/K
%
%  enthalpies of formation
%
Tref = 298.15; % K
pref = 101325; % Pa
HfrefA = -1000; %J/mol
HfrefB = -10000; % J/mol
HfrefC = -2000; % J/mol
HfrefD = -4000; % J/mol
HA = CpA*(T-Tref) + HfrefA;
HB = CpB*(T-Tref) + HfrefB;
HC = CpC*(T-Tref) + HfrefC;
HD = CpD*(T-Tref) + HfrefD;
DHR1 = nuA1*HA + nuB1*HB + nuC1*HC  + nuD1*HD;
DHR2 = nuA2*HA + nuB2*HB + nuC2*HC  + nuD2*HD;
%
% rate law for reaction 2
%
ko2 = 1.0e-1; % liter/mole/sec
Ea2 = Ea1 - DHR1; % J/mol
k2 = ko2*exp(-Ea2/(R*T));
r2 = k2*CA*CC;
%
% constant volume
%
V = 1000.0; % liter
F = 1; % liter/sec
Fin = F;
Fout = F;
%
%  inlet concentrations
%
```

```
CAin = 10.0; % mol/liter
CBin = 0.0; % mol/liter
CCin = 10.0; % mol/liter
CDin = 0.0; % mol/liter
CSin = 30.0; % mol/liter
Tin = 300.0; % K
%
% mole fractions
%
CT = CA + CB + CC + CD + CS;
xA = CA/CT;
xB = CB/CT;
xC = CC/CT;
xD = CD/CT;
xS = CS/CT;
CTin = CAin + CBin + CCin + CDin + CSin;
xAin = CAin/CTin;
xBin = CBin/CTin;
xCin = CCin/CTin;
xDin = CDin/CTin;
xSin = CSin/CTin;
%
% mixture heat capacity
%
Cpmix = xA*CpA + xB*CpB + xC*CpC + xD*CpD + xS*CpS;
Cpmixin = xAin*CpA + xBin*CpB + xCin*CpC + xDin*CpD + xSin*CpS;
%
%  molar balances
%
dydt(1) = Fin/V*CAin - Fout/V*CA + nuA1*r1 + nuA2*r2;
dydt(2) = Fin/V*CBin - Fout/V*CB + nuB1*r1 + nuB2*r2;
dydt(3) = Fin/V*CCin - Fout/V*CC + nuC1*r1 + nuC2*r2;
dydt(4) = Fin/V*CDin - Fout/V*CD + nuD1*r1 + nuD2*r2;
dydt(5) = Fin/V*CSin - Fout/V*CS + nuS1*r1 + nuS2*r2;
dydt(6) = ( Fin/V*CTin*Cpmixin*(Tin - T) - DHR1*r1 - DHR2*r2 )/(CT*Cpmix);
```