CBE 450 Chemical Reactor Fundamentals
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Sample Codes
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Non-Isothermal PFRs

There are three input files for modeling Non-Isothermal PFRs

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

1. One irreversible reaction

```
function dydt = sysodeinput(x,y,nvec);
%
%  one reaction in solvent S
%  2A --> B
%
%  example usage:
%  [y,x] = sysode(2,1000,0,20,[10000,0,30000,300]);
%
CA = y(1); % mol/m^3
CB = y(2); % mol/m^3
CS = y(3); % mol/m^3
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-2; % liter/mol/sec
ko = ko/1000; % m^3/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;
%
%  inlet concentrations and temperature
%
CAin = 10000.0; % mol/m^3
CBin = 0.0; % mol/m^3
CSin = 30000.0; % mol/m^3
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;
%
% volumetric flowrate
%
F = 1; % liter/sec
F = F/1000; % cubic meters/sec
%
%  circular pipe
%
Dp = 0.10; % m
Across = 0.25*pi*Dp*Dp; % m^2
%
% velocity
%
v = F/Across; % m/s
%
% residence time
%
l = 20; % m
tr = l/v; % sec
%
%  molar balances
%
% dCAdz = nuA*r/v
dydt(1) = (nuA*r)/v;
```

```
dydt(2) = (nuB*r)/v;
dydt(3) = (nuS*r)/v;
dydt(4) = -DHR*r/v/(CT*Cpmix);

%
%  extra stuff to check that numerical solution matches
%  analytical expression
%
%DHRref = nuA*HfrefA + nuB*HfrefB;
%DCp  = nuA*CpA + nuB*CpB;
%num = (T-Tin)*nuA*CTin/CAin*Cpmixin;
%den = (T-Tref)*DCp+DHRref;
%XA = num/den;
%fprintf('z = %e XA = %e T = %e \n ',x,XA,T);
```

2. One reversible reaction

```
function dydt = sysodeinput(x,y,nvec);
%
%  one reversible reaction in solvent S
%  2A <--> B
%
%  example usage:
%  [y,x] = sysode(2,1000,0,20,[10000,0,30000,300]);
%
CA = y(1); % mol/m^3
CB = y(2); % mol/m^3
CS = y(3); % mol/m^3
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-2; % liter/mol/sec
ko1 = ko1/1000; % m^3/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;
%
%  inlet concentrations and temperature
%
CAin = 10000.0; % mol/m^3
CBin = 0.0; % mol/m^3
CSin = 30000.0; % mol/m^3
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;
%
% volumetric flowrate
%
F = 1; % liter/sec
F = F/1000; % cubic meters/sec
%
%  circular pipe
%
Dp = 0.10; % m
Across = 0.25*pi*Dp*Dp; % m^2
%
% velocity
%
v = F/Across; % m/s
%
% residence time
```

```
%
l = 20; % m
tr = l/v; % sec
%
%  molar balances
%
% dCAdz = nuA*r/v
dydt(1) = (nuA1*r1 + nuA2*r2)/v;
dydt(2) = (nuB1*r1 + nuB2*r2)/v;
dydt(3) = (nuS1*r1 + nuS2*r2)/v;
dydt(4) = -(DHR1*r1 + DHR2*r2)/v/(CT*Cpmix);
```

3. Two simultaneous reactions

```
function dydt = sysodeinput(x,y,nvec);
%
%  two simultaneous reactions in solvent S
%  A + B --> C
%  A + D --> E
%
%  example usage:
%  [y,x] = sysode(2,1000,0,20,[10000,6000,0,5000,0,30000,300]);
%
CA = y(1); % mol/m^3
CB = y(2); % mol/m^3
CC = y(3); % mol/m^3
CD = y(4); % mol/m^3
CE = y(5); % mol/m^3
CS = y(6); % mol/m^3
T = y(7); % K
%
% stoichiometry
%
nuA1 = -1.0;
nuB1 = -1.0;
nuC1 = 1.0;
nuD1 = 0.0;
nuE1 = 0.0;
nuS1 = 0.0;
%
nuA2 = -1.0;
nuB2 = 0.0;
nuC2 = 0.0;
nuD2 = -1.0;
nuE2 = 1.0;
nuS2 = 0.0;
%
% rate law for reaction 1
%
R = 8.314; % J/mol/K
ko1 = 1.0e-2; % liter/mol/sec
ko1 = ko1/1000; % m^3/mol/sec
Ea1 = 2500; % J/mol
k1 = ko1*exp(-Ea1/(R*T));
r1 = k1*CA*CB;
```

```
%
%  pure component heat capacities
%
CpA = 4.0; %J/mol/K
CpB = 5.0; %J/mol/K
CpC = 8.0; %J/mol/K
CpD = 3.0; %J/mol/K
CpE = 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 = -15000; % J/mol
HfrefD = -8000; % J/mol
HfrefE = -6000; % J/mol
HA = CpA*(T-Tref) + HfrefA;
HB = CpB*(T-Tref) + HfrefB;
HC = CpC*(T-Tref) + HfrefC;
HD = CpD*(T-Tref) + HfrefD;
HE = CpE*(T-Tref) + HfrefE;
DHR1 = nuA1*HA + nuB1*HB + nuC1*HC + nuD1*HD + nuE1*HE;
DHR2 = nuA2*HA + nuB2*HB + nuC2*HC + nuD2*HD + nuE2*HE;
%
% rate law for reaction 2
%
ko2 = 1.0e-1; % liter/mol/sec
ko2 = ko2/1000; % m^3/mol/sec
Ea2 = Ea1 - DHR1; % J/mol
k2 = ko2*exp(-Ea2/(R*T));
r2 = k2*CA*CD;
%
%  inlet concentrations and temperature
%
CAin = 10000.0; % mol/m^3
CBin = 6000.0; % mol/m^3
CCin = 0.0; % mol/m^3
CDin = 5000.0; % mol/m^3
CEin = 0.0; % mol/m^3
CSin = 30000.0; % mol/m^3
Tin = 300.0; % 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;
CTin = CAin + CBin + CCin + CDin + CEin + CSin;
xAin = CAin/CTin;
```

```
xBin = CBin/CTin;
xCin = CCin/CTin;
xDin = CDin/CTin;
xEin = CEin/CTin;
xSin = CSin/CTin;
%
% mixture heat capacity
%
Cpmix = xA*CpA + xB*CpB + xC*CpC + xD*CpD + xE*CpE + xS*CpS;
Cpmixin = xAin*CpA + xBin*CpB + xCin*CpC + xDin*CpD + xEin*CpE + xSin*CpS;
%
% volumetric flowrate
%
F = 1; % liter/sec
F = F/1000; % cubic meters/sec
%
%  circular pipe
%
Dp = 0.10; % m
Across = 0.25*pi*Dp*Dp; % m^2
%
% velocity
%
v = F/Across; % m/s
%
% residence time
%
l = 20; % m
tr = l/v; % sec
%
%  molar balances
%
% dCAdz = nuA*r/v
dydt(1) = (nuA1*r1 + nuA2*r2)/v;
dydt(2) = (nuB1*r1 + nuB2*r2)/v;
dydt(3) = (nuC1*r1 + nuC2*r2)/v;
dydt(4) = (nuD1*r1 + nuD2*r2)/v;
dydt(5) = (nuE1*r1 + nuE2*r2)/v;
dydt(6) = (nuS1*r1 + nuS2*r2)/v;
dydt(7) = -(DHR1*r1 + DHR2*r2)/v/(CT*Cpmix);
```