CBE 450 Chemical Reactor Fundamentals
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Sample Codes
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Jacketed Reactors

There are three input files for modeling jacketed reactors

1. batch reactor
2. CSTR
3. PFR

1. batch reactor

```
function dydt = sysodeinput(x,y,nvec);
%
%  one reaction in solvent, S
%  2A --> B
%
%  sample usage:
%  [y,x]=sysode(2,1000,0,10,[10,0,40,300,273.15]);
%
CA = y(1); % mol/liter
CB = y(2);
CS = y(3);
T =  y(4); % K
Tj = y(5); % 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;
%
%  heat loss information
%
As = 3.0; % m^2
U = 1500.0; % J/s/m^2/K
Qdot = As*U*(Tj-T);
V = 1000.0; % liters
Vj = 500; % liters
Cpj = 4.184; % J/mol/K
Cj = 55.6; % mol/liter
Fj = 10.0; % liters/sec
Tjin = 273.15; % K
%
%  mole and energy balances
%
dydt(1) = nuA*r;
dydt(2) = nuB*r;
dydt(3) = nuS*r;
dydt(4) = (-V*DUR*r+Qdot)/(CT*Cvmix*V);
dydt(5) = Fj/Vj*(Tjin-Tj) - Qdot/(Cj*Cpj*Vj);
```

2. CSTR

```
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,[10,0,10,0,30,300,273.15]);
%
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
Tj = y(7); % 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;
%
%  heat loss information
%
As = 3.0; % m^2
U = 1500.0; % J/s/m^2/K
Qdot = As*U*(Tj-T);
Vj = 500; % liters
Cpj = 4.184; % J/mol/K
Cj = 55.6; % mol/liter
Fj = 10.0; % liters/sec
Tjin = 273.15; % K
%
%  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 + Qdot/V )/(CT*Cpmix);
dydt(7) = Fj/Vj*(Tjin-Tj) - Qdot/(Cj*Cpj*Vj);
```

3. PFRs

```
function dydt = sysodeinput(x,y,nvec);
%
%  two simultaneous reactions in solvent S
%  A + B --> C
%  A + D --> E
%
%  example usage:
%  [y,x] = sysode(2,1000,0,10,[10000,6000,0,5000,0,30000,500,273.15]);
%
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
Tj = y(8); % 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 = -100000; % 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;
%
% 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
%
Cpmix = xA*CpA + xB*CpB + xC*CpC + xD*CpD + xE*CpE + xS*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
l = 5; % m
V = Across*l; % m^3
%
% axial velocity
%
vz = F/Across; % m/s
%
% residence time
%
```

```
tr = l/vz; % sec
%
%  heat loss information
%
As = 3.0; % m^2
U = 1500.0; % J/s/m^2/K
Qdot = As*U*(Tj-T);
Cpj = 4.184; % J/mol/K
Cj = 55.6; % mol/liter
Cj = Cj*1000; % mol/cubic meter
Fj = 10.0; % liters/sec
Fj = Fj/1000; % cubic meters/sec
Dpj = 0.30; % m
Acrossj = 0.25*pi*Dpj*Dpj - 0.25*pi*Dp*Dp; % m^2
Vj = Acrossj*l; % m^3
vzj = Fj/Acrossj; % m/s
%
%  molar balances
%
% dCAdz = nuA*r/v
dydt(1) = (nuA1*r1 + nuA2*r2)/vz;
dydt(2) = (nuB1*r1 + nuB2*r2)/vz;
dydt(3) = (nuC1*r1 + nuC2*r2)/vz;
dydt(4) = (nuD1*r1 + nuD2*r2)/vz;
dydt(5) = (nuE1*r1 + nuE2*r2)/vz;
dydt(6) = (nuS1*r1 + nuS2*r2)/vz;
dydt(7) = (-DHR1*r1 - DHR2*r2 + Qdot/V)/(vz*CT*Cpmix);
dydt(8) = -Qdot/(vzj*Vj*Cj*Cpj);
```