CBE 450 Chemical Reactor Fundamentals
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Sample Codes

David Keffer
Department of Chemical and Biomolecular Engineering
University of Tennessee
dkeffer@utk.edu

Sample input files for modeling the CSTR. The codes are run at the command line prompt using

```
[y,x] = sysode(m,n,xo,xf,yo);
   m = 2 for Classical Runge-Kutta 4rth order method
   n = number of steps
   xo = starting value of x
   xf = ending value of x
   yo = initial condition at xo
```

Example 1.

```
function dydt = sysodeinput(x,y,nvec);
%
%  one reaction
%  2A --> B
%
CA = y(1);
CB = y(2);
nuA = -2.0;
nuB = 1.0;
k = 1.0e-0 ; % 1/sec
% constant volume;
F = 1; % liter/sec
Fin = F;
Fout = F;
CAin = 10.0; % mol/liter
CBin = 0.0; % mol/liter
V = 10; % liter
R = 8.314; % J/mol/K
T = 300; % K
ko = 1.0e-1; % liter/mol/sec
Ea = 2500; % J/mol
k = ko*exp(-Ea/(R*T));
rate = k*CA*CA;
%
%  molar balance on A - concentration
%
dydt(1) = Fin/V*CAin - Fout/V*CA + nuA*rate;
%
%  molar balance on B - concentration
%
dydt(2) = Fin/V*CBin - Fout/V*CB + nuB*rate;
```

Sample 2.

```
function dydt = sysodeinput(x,y,nvec);
%
%  reversible reaction
%  2A --> B
%  B --> 2A
%
CA = y(1);
CB = y(2);
nuA1 = -2.0;
nuB1 = 1.0;
nuA2 = 2.0;
nuB2 = -1.0;
% constant volume;
F = 1; % liter/sec
Fin = F;
Fout = F;
CAin = 10.0; % mol/liter
CBin = 0.0; % mol/liter
V = 10; % liter
R = 8.314; % J/mol/K
T = 300; % K
ko1 = 1.0e-1; % liter/mol/sec
Ea1 = 2500; % J/mol
k1 = ko1*exp(-Ea1/(R*T));
rate1 = k1*CA*CA;
ko2 = 1.0e-1; % liter/mol/sec
Ea2 = 3500; % J/mol
k2 = ko2*exp(-Ea2/(R*T));
rate2 = k2*CB;%
%  molar balance on A - concentration
%
dydt(1) = Fin/V*CAin - Fout/V*CA + nuA1*rate1 + nuA2*rate2;
%
%  molar balance on B - concentration
%
dydt(2) = Fin/V*CBin - Fout/V*CB + nuB1*rate1 + nuB2*rate2;
```

Sample 3.

```
function dydt = sysodeinput(x,y,nvec);
%
%  polymerization reactions
%  A + A --> B
%  B + A --> C
%  C + A --> D
%  D + A --> E
%  E + A --> F
%
CA = y(1);
CB = y(2);
CC = y(3);
```

```
CD = y(4);
CE = y(5);
CF = y(6);
%
nuA1 = -2.0;
nuB1 = 1.0;
nuC1 = 0.0;
nuD1 = 0.0;
nuE1 = 0.0;
nuF1 = 0.0;
%
nuA2 = -1.0;
nuB2 = -1.0;
nuC2 = 1.0;
nuD2 = 0.0;
nuE2 = 0.0;
nuF2 = 0.0;
%
nuA3 = -1.0;
nuB3 = 0.0;
nuC3 = -1.0;
nuD3 = 1.0;
nuE3 = 0.0;
nuF3 = 0.0;
%
nuA4 = -1.0;
nuB4 = 0.0;
nuC4 = 0.0;
nuD4 = -1.0;
nuE4 = 1.0;
nuF4 = 0.0;
%
nuA5 = -1.0;
nuB5 = 0.0;
nuC5 = 0.0;
nuD5 = 0.0;
nuE5 = -1.0;
nuF5 = 1.0;
% constant volume;
F = 1; % liter/sec
Fin = F;
Fout = F;
CAin = 10.0; % mol/liter
CBin = 0.0; % mol/liter
CCin = 0.0; % mol/liter
CDin = 0.0; % mol/liter
CEin = 0.0; % mol/liter
CFin = 0.0; % mol/liter
V = 10; % liter
R = 8.314; % J/mol/K
T = 300; % K
%
ko(1:5) = 1.0e-1; % liter/mol/sec
%
Ea(1:5) = 2500; % J/mol
%
```

```
for i = 1:1:5
   k(i) = ko(i)*exp(-Ea(i)/(R*T));
end
rate1 = k(1)*CA*CA;
rate2 = k(2)*CA*CB;
rate3 = k(3)*CA*CC;
rate4 = k(4)*CA*CD;
rate5 = k(5)*CA*CE;
%
%  molar balances
%
dydt(1) = Fin/V*CAin - Fout/V*CA + nuA1*rate1 + nuA2*rate2 + nuA3*rate3 + nuA4*rate4 + nuA5*rate5;
dydt(2) = Fin/V*CBin - Fout/V*CB + nuB1*rate1 + nuB2*rate2 + nuB3*rate3 + nuB4*rate4 + nuB5*rate5;
dydt(3) = Fin/V*CCin - Fout/V*CC + nuC1*rate1 + nuC2*rate2 + nuC3*rate3 + nuC4*rate4 + nuC5*rate5;
dydt(4) = Fin/V*CDin - Fout/V*CD + nuD1*rate1 + nuD2*rate2 + nuD3*rate3 + nuD4*rate4 + nuD5*rate5;
dydt(5) = Fin/V*CEin - Fout/V*CE + nuE1*rate1 + nuE2*rate2 + nuE3*rate3 + nuE4*rate4 + nuE5*rate5;
dydt(6) = Fin/V*CFin - Fout/V*CF + nuF1*rate1 + nuF2*rate2 + nuF3*rate3 + nuF4*rate4 + nuF5*rate5;
```