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 PFR. 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

Note: All concentrations are given in moles/m^3, rather than moles/liter in order to maintain consistency of units with velocities expressed in m/s and pipe lengths in m.

Example 1.

```
function dydt = sysodeinput(x,y,nvec);
%
%  one reaction
%  2A --> B
%
%  sample command
% [y,x] = sysode(2,1000,0,20,[10000,0]);
%
CA = y(1);
CB = y(2);
%
%  define the stoichiometry
%
nuA = -2.0;
nuB = 1.0;
%
%  define the rate law
%
R = 8.314; % J/mol/K
T = 300; % 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));
rate = k*CA*CA;
%
%  define mole balance
%
```

```
% 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
%
%  molar balances
%
% dCAdz = nuA*r/v
dydt(1) = (nuA*rate)/v;
dydt(2) = (nuB*rate)/v;
```