Simulation of CSTR by ODE's

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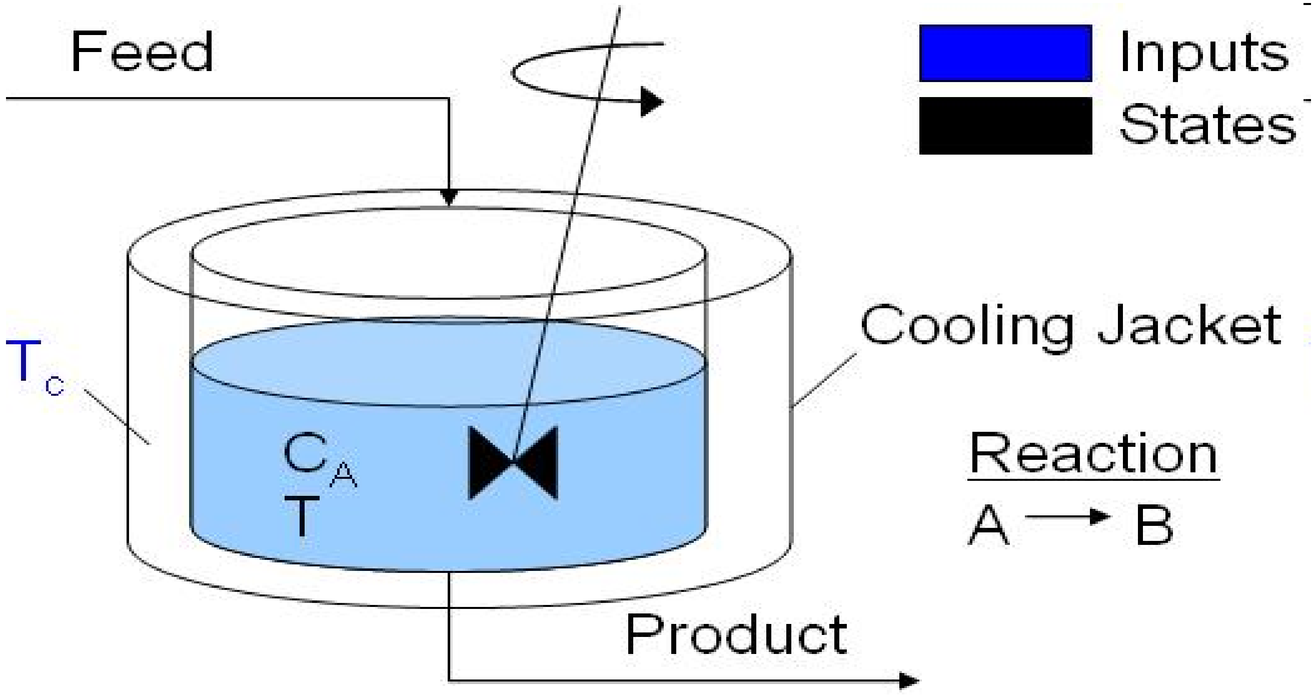
Models



Feed
Inputs
States
T_c
Cooling Jacket
C_A
T
Reaction
A → B
Product

Variables in CSTR Model

T_c	Cooling water temperature (K)
c_a	Concentration of species A (mol/m^3)
T	Reactor temperature
q	Volumetric flowrate (m^3/sec)
V	Reactor volume (m^3)
ρ	Density of A-B mixture (kg/m^3)
C_p	Heat capacity of A-B mixture (J/kg-K)
ΔH	Heat of reaction for A->B (J/mol)

E/R	Activation energy in the Arrhenius Equation (J/mol) / Universal Gas Constant (8.31451 J/mol-K)
k_0	Pre-exponential factor (1/sec)
UA	Overall Heat Transfer Coefficient (W/m^2-K) * Area (m^2)
C_{af}	Feed Concentration (mol/m^3)
T_f	Feed Temperature (K)

ODEs for concentration and temperature

- Equations in CSTR Model

Species balance for component A:

$$V\frac{\partial c_a}{\partial t} = q\left(C_{af} - C_a\right) - k_0 \exp\left(-\frac{E}{RT}\right)VC_a$$

Energy balance:

$$A = \Delta H k_0 \exp\left(-\frac{E}{RT}\right)VC_a$$

$$B = UA\left(T_c - T\right)$$

$$\rho C_p V\frac{\partial T}{\partial t} = \rho C_p q\left(T_f - T\right) + A + B$$

Matlab Function Program

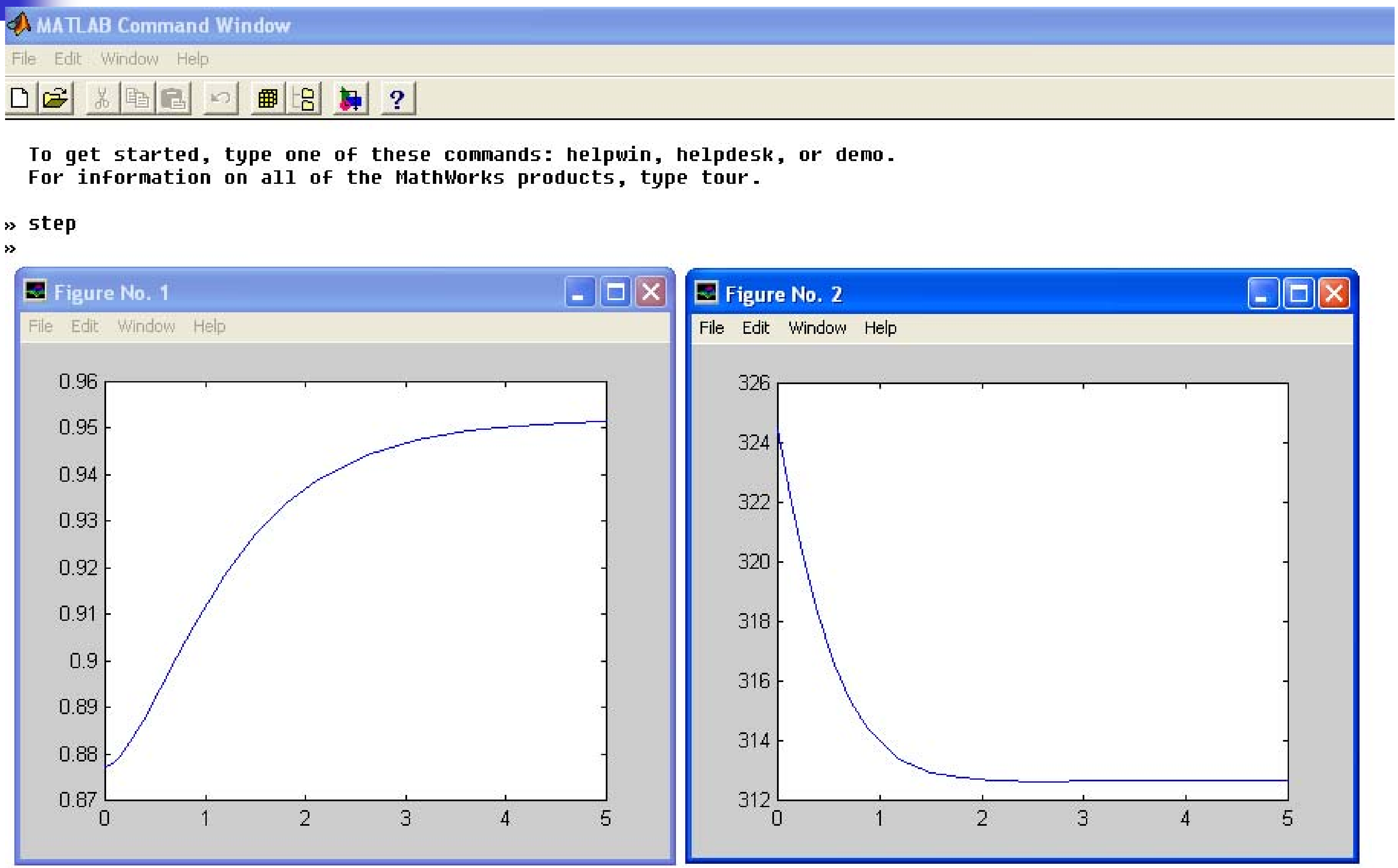
```
function xdot=cstr1(t,x)
global u

% T of cooling jacket (K)
Tc = u;
% Conc in CSTR (mol/m^3)
Ca = x(1,1);
% Temperature in CSTR (K)
T = x(2,1);
% Flowrate (m^3/sec)
q = 100;
% Volume of CSTR (m^3)
V = 100;
% Density (kg/m^3)
rho = 1000;
 % Heat capacity of A-B
 Mixture (J/kg-K)
 Cp = .239;
 % Heat of reaction for A->B
 (J/mol)
mdelH = 5e4;
% E = Arrhenius Equation
(J/mol)
% R = Univ Gas Constant
EoverR = 8750;
% Pre-exponential factor
(1/sec)
k0 = 7.2e10;
% U - Heat Trans Coeff
(W/m^2-K)
% A - Area (m^2)
UA = 5e4;
% Feed Conc (mol/m^3)
Caf = 1;
% Feed Temperature (K)
Tf = 350;

% Compute xdot:
xdot(1,1) = (q/V*(Caf - Ca)
- k0*exp(-EoverR/T)*Ca);

xdot(2,1) = (q/V*(Tf - T) +
mdelH/(rho*Cp)*k0*exp(-
EoverR/T)*Ca +
UA/V/rho/Cp*(Tc-T));
```

Matlab Main Program

```
% Step test for Model 1
CSTR
global u
% Initial Conditions-States
Ca_ss = 0.87725294608097;
T_ss = 324.475443431599;
x_ss = [Ca_ss;T_ss];

% Initial Condition-Control
u_ss = 300;

% Open Loop Step Change
u = 290;
```

```
% Final Time (sec)
tf = 5;

[t,x] = ode15s('cstr1',[0
tf],x_ss);

% Parse out the state
values
Ca = x(:,1);
T = x(:,2);

% Plot the results
figure(1);
plot(t,Ca);

figure(2)
plot(t,T);
```

Results and Discussion



Summary

- These model equations were solved by MATLAB numerical integrator. In this case ODE15s was used to solve the differential equations over a 5 second period. The jacket temperature was dropped from 300 K to 290 K. The cooling of the reactor jacket results in a decrease in reactor temperature and an increase in the concentration of species A.
- The results are displayed in two plots of the temperature and reactor concentration calculated by the program of step.m.