Exothermic Continuous Stirred-Tank Reactor

```
File: Ch02 E05 CSTR.m
```

Nonlinear dynamics of an exothermic continuous stirred-tank reactor (CSTR). This is example 2.05 from Seborg, et al.

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Model Equations

```
dCa
--- = q*(Cai - Ca) - V*k*Ca
dt

dT
-- = (w*Cp*(Tin - T) + U*A*(Tc - T) + (-delta_H)*V*k*Ca)/(V*rho*Cp)
dt

Arrhenius law:
k = ko * exp(-E/(R*T))
```

Nominal Operating Conditions (Table 2.3)

```
q = 100; % Flowrate [L/min]
cAi = 1; % Inlet feed concentration [mol/L]
Ti = 350; % Inlet feed temperature [K]
V = 100; % Volume [L]
rho = 1000; % Density [g/L]
C = 0.239; % Heat capacity [J/g/K]
dHr = -5e4; % Heat of reaction [J/mol]

ER = 8750; % Ea/R [K]
k0 = 7.2e10; % Arrhenius rate constant
UA = 5e4; % Heat transfer [J/min/K]
Tc = 300; % Coolant temperature [K]

cA0 = 0.5; % Initial concentration [mol/L]
T0 = 350; % Initial temperature [K]
```

Arrhenius Rate (Equation 2-63)

```
k = @(T) k0*exp(-ER/T);
```

Dynamic Mass and Energy Balances (Equations 2-66 and 2-68)

```
deriv = @(cA,T,Tc) [ ...
  (q/V)*(cAi - cA) - k(T)*cA;
  (q/V)*(Ti - T) + (-dHr/rho/C)*k(T)*cA + (UA/V/rho/C)*(Tc-T)];
```

Solution of the Differential Equations

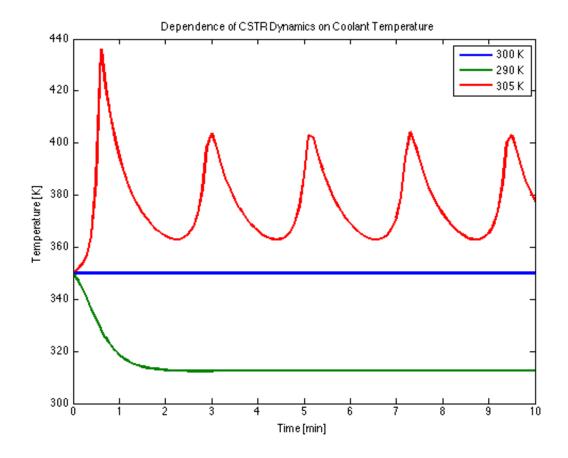
```
% Time grid
t = 0:0.1:10;
% Solutions for three values of Tc

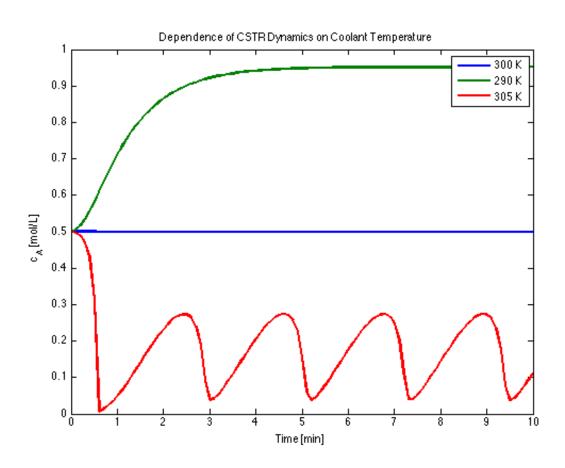
s300 = ode15s(@(t,x) deriv(x(1),x(2),300),t,[cA0,T0]);
s290 = ode15s(@(t,x) deriv(x(1),x(2),290),t,[cA0,T0]);
s305 = ode15s(@(t,x) deriv(x(1),x(2),305),t,[cA0,T0]);
```

Display Solutions

```
figure(1);clf
plot(t,deval(s300,t,2),t,deval(s290,t,2),t,deval(s305,t,2),'Linewidth',2);
xlabel('Time [min]');
ylabel('Temperature [K]');
title('Dependence of CSTR Dynamics on Coolant Temperature');
legend('300 K','290 K','305 K');

figure(2);clf
plot(t,deval(s300,t,1),t,deval(s290,t,1),t,deval(s305,t,1),'Linewidth',2);
xlabel('Time [min]');
ylabel('c_A [mol/L]');
title('Dependence of CSTR Dynamics on Coolant Temperature');
legend('300 K','290 K','305 K');
```





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