

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

$$\frac{dC_a}{dt} = q(C_{ai} - C_a) - V k C_a$$
$$\frac{dT}{dt} = (w C_p (T_{in} - T) + U A (T_c - T) + (-\Delta H) V k C_a) / (V \rho C_p)$$

Arrhenius law:

$$k = k_0 \cdot \exp(-E/(R \cdot T))$$

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');
```



