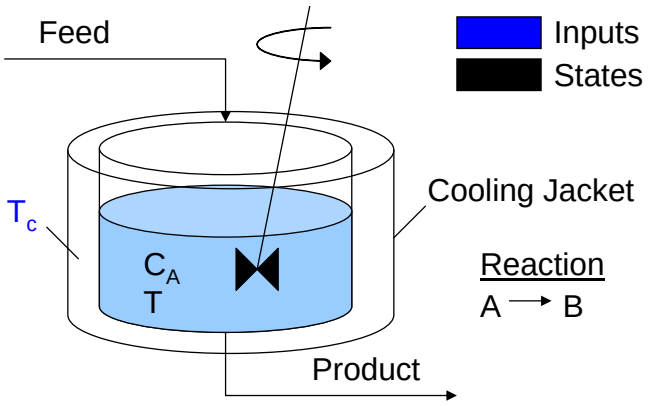
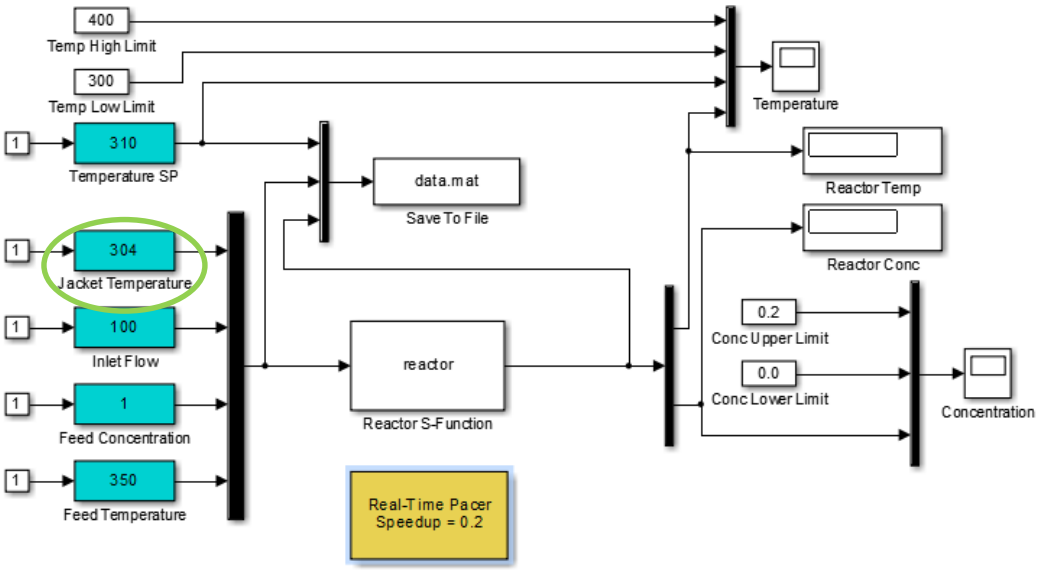
**Process Dynamics and Control: CSTR Case Study**




A reactor is used to convert a hazardous chemical "*A*" to an acceptable chemical "*B*" in waste stream before entering a nearby lake. This particular reactor is dynamically modeled as a Continuously Stirred Tank Reactor (CSTR) with a simplified kinetic mechanism that describes the conversion of reactant *A* to product *B* with an irreversible and exothermic reaction. It is desired to maintain the temperature at a constant setpoint that maximizes the destruction of *A* (highest possible temperature). You may use the MATLAB, Simulink, and Excel workbook resources to fit FOPDT models, simulate the system, and perform control studies for this project. Don't forget to open the plots by double-clicking the Temperature and Concentration plots. See Tutorial Video (first 1 min, 30 sec) for help. Download source files from http://apmonitor.com/che436/index.php/Main/CaseStudyCSTR

## Empirical Modeling Approach

a) Perform the necessary open loop dynamic modeling studies to determine a first order plus dead time (FOPDT) model which describes the relationship between cooling jacket temperature (MV=$T_c$) and reactor temperature (CV=$T$). Start at 280K for the cooling jacket temperature (green circled $T_c$) and step to 300K and down to 260K and back to 300K in a doublet test. Use the file *data.txt* to extract the information for the FOPDT model.



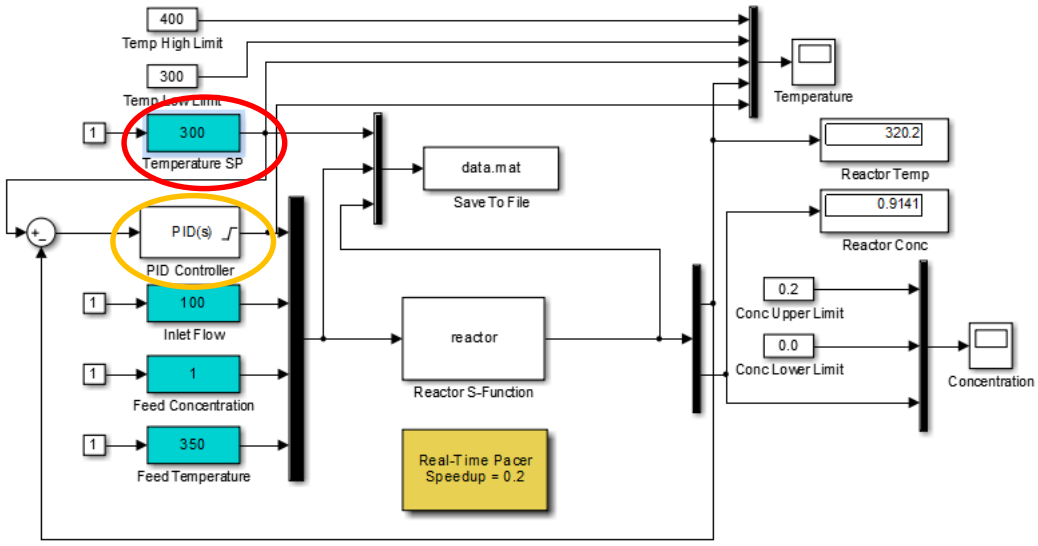
b) Use the $K_p$, $\tau_p$, and $\theta_p$ from part *a* in the Internal Model Control (IMC) tuning correlation and compute the tuning parameters for a PI controller. Assume that the closed loop time constant, $\tau_c$, equals 0.1 $\tau_p$ for aggressive tuning.

**IMC (lambda) Tuning**

Aggressive Tuning: $\tau_C$ is the larger of $0.1\,\tau_P$ or $0.8\,\theta_P$
Moderate Tuning: $\tau_C$ is the larger of $1.0\,\tau_P$ or $8.0\,\theta_P$
Conservative Tuning: $\tau_C$ is the larger of $10\,\tau_P$ or $80\,\theta_P$

| | $K_C$ | $\tau_I$ | $\tau_D$ |
|---|---|---|---|
| P-Only* | $K_C = \frac{0.2}{K_p}(\tau_p/\theta_p)^{1.22}$ | | |
| PI | $\frac{1}{K_P}\frac{\tau_P}{(\theta_P+\tau_C)}$ | $\tau_P$ | |
| PID Ideal | $\frac{1}{K_P}\left(\frac{\tau_P+0.5\theta_P}{\tau_C+0.5\theta_P}\right)$ | $\tau_P+0.5\theta_P$ | $\frac{\tau_P\theta_P}{2\tau_P+\theta_P}$ |
| PID Interacting | $\frac{1}{K_P}\left(\frac{\tau_P}{\tau_C+0.5\theta_P}\right)$ | $\tau_P$ | $0.5\theta_P$ |

c) Using your $K_C$ and $\tau_I$ from part *b*, implement a PI controller (orange circled PID controller) with anti-reset windup (be sure to turn off the derivative action). Test the set point tracking capability (red circled reactor SP) of this controller by plotting the response of the process to steps in setpoint of the reactor temperature (not cooling jacket temperature) from 300K up to 320K and then down to 280K. Comment on how the nonlinear behavior of this process impacts your observed set point response performance.




d) Determine a "best" tuning by adjusting $K_c$ and $\tau_I$ by trial and error until the controller displays a 10% to 15 % overshoot in response to set point steps from 300K up to 320K and plot this set point step response.

e) Step up the setpoint to achieve a maximum temperature in the reactor without exceeding the maximum allowable temperature of 400K (don't cause a reactor run-away). What is the lowest concentration that can be achieved without exceeding the maximum allowable temperature?

## First Principles Modeling Approach

f) Using the Species for *A* and Energy Balance, derive a model of the CSTR response of $C_a$ and $T$ to changes in the inputs $C_{a,i}$, $T_i$, and $T_c$. See Solution Video starting at 1 min 33 sec for help.

```
Tc = 270                % Temperature of cooling jacket (K)
q = 100                 % Volumetric Flowrate (m^3/sec)
V = 100                 % Volume of CSTR (m^3)
ρ = 1000                % Density of A-B Mixture (kg/m^3)
Cp = .239               % Heat capacity of A-B Mixture (J/kg-K)
ΔHr = 5e4               % Heat of reaction for A->B (J/mol)
E/R = 8750              % EoverR = E/R
k0 = 7.2e10             % Pre-exponential factor (1/sec)
UA = 5e4                % Overall heat transfer coefficient (U=W/m^2-K)
Ca,i = 1                % Feed Concentration (mol/m^3)
Ti = 350                % Feed Temperature (K)
Ca = 0.989              % Concentration of A in CSTR (mol/m^3)
T = 296.6               % Temperature in CSTR (K)

k = k0*exp(-EoverR/T)
rate = k * Ca
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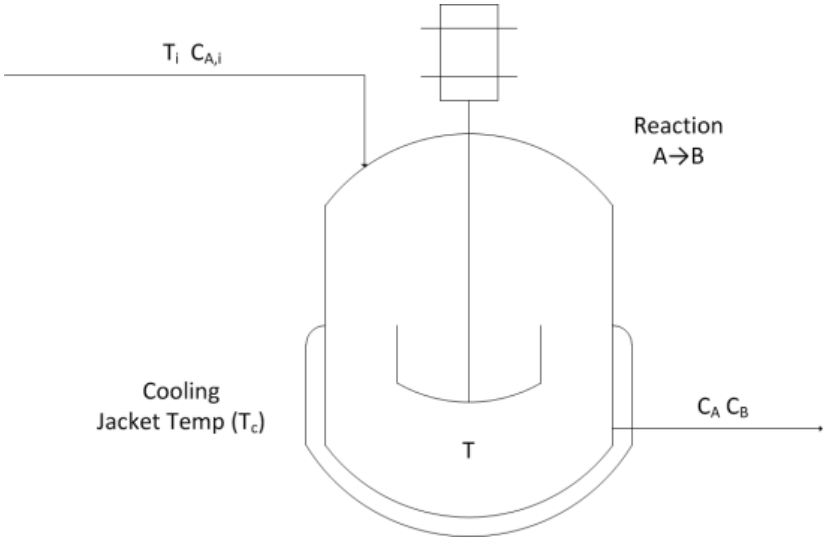


g) Linearize the first principles model from part *f* and obtain values of the constants $\alpha_1 - \alpha_4$ and $\beta_1 - \beta_3$. The prime indicates deviation variable form (e.g. $T' = T - \bar{T}$).

$$\frac{dC'_a}{dt} = \alpha_1 C'_a + \alpha_2 T' + \beta_1 C'_{a,i}$$

$$\frac{dT'}{dt} = \alpha_3 C'_a + \alpha_4 T' + \beta_2 T'_i + \beta_3 T'_c$$

h) Put the model into State Space form:

$$\frac{dx}{dt} = Ax + Bu$$

$$y = Cx + Du$$

where

$$\frac{dx}{dt} = \begin{bmatrix} \frac{dC'_a}{dt} \\ \frac{dT'}{dt} \end{bmatrix},\ x = \begin{bmatrix} C'_a \\ T' \end{bmatrix},\ u = \begin{bmatrix} C'_{a,i} \\ T'_i \\ T'_c \end{bmatrix},\ y = [T']$$

$$A = \begin{bmatrix} \alpha_1 & \alpha_2 \\ \alpha_4 & \alpha_5 \end{bmatrix},\ B = \begin{bmatrix} \beta_1 & 0 & 0 \\ 0 & \beta_2 & \beta_3 \end{bmatrix},\ C = [0 \quad 1],\ D = [0 \quad 0 \quad 0]$$

i) Simulate the linear (State Space) and nonlinear models in MATLAB / Simulink. How well does the linear model approximate the nonlinear behavior?

j) Implement a Model Predictive Controller to regulate temperature within safety limits (<400 K) and minimize $C_a$ output below a concentration of 0.2 mol/L. See Solution Video (last 30 seconds) for one possible implementation.