Mathematical Modeling
CSTR Example

Develop a Dynamic Model

- Draw a schematic diagram, labeling process variables
- List all assumptions
- Classify Problem
  - Time Dependence Only
    - ODE: Ordinary differential equations
    - DAE: Differential algebraic equations
  - Time and Spatial Dependence
    - PDE: Partial differential equations
    - PDAE: Partial differential algebraic equations
- Write dynamic balances (mass, species, energy)
- Other relations (thermo, reactions, geometry, etc.)
- Degrees of freedom
  - Does # of eqns = # of unknowns?
- Simplify

Balances

- **Total Mass Balance:**

$$\frac{dm}{dt} = \frac{d(\rho V)}{dt} = \sum_{i=inlet} \dot{m}_i - \sum_{j=outlet} \dot{m}_j$$

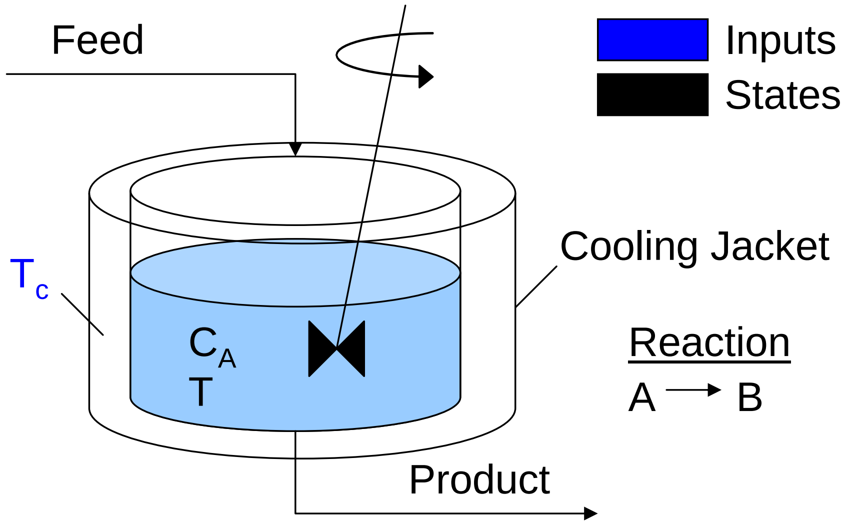
- **Species Mole Balance:**

$$\frac{dn_A}{dt} = \frac{d(c_A V)}{dt} = \sum_{i=inlet} c_{Ai} q_i - \sum_{j=outlet} c_{Aj} q_j + r_A V$$

- **Total Energy Balance:**

$$\frac{d[\rho C_p V(T - T_{ref})]}{dt} = \sum_{i:inlet} \dot{m}_i C_p (T_i - T_{ref}) - \sum_{j:outlet} \dot{m}_j C_p (T_j - T_{ref}) + Q + W_s$$

Process Diagram



Assumptions

1. Liquid-only system
2. Constant volume (tight level control)
3. First Order Reaction
4. No Jacket Temperature Dynamics
5. Negligible Heat Input from Stirring
6. Constant Density

Process Information

Manipulated Variables	
Tc = 270	Temperature of cooling jacket (K)
Disturbances	
q = 100	Volumetric Flowrate (m^3/sec)
V = 100	Volume of CSTR (m^3)
rho = 1000	Density of A-B Mixture (kg/m^3)
Cp = .239	Heat capacity of A-B Mixture (J/kg-K)
mdelH = 5e4	Heat of reaction for A->B (J/mol)
EoverR = 8750	EoverR = E/R = Activation energy (J/mol) / Universal Gas Constant (8.31451 J/mol-K)
k0 = 7.2e10	Pre-exponential factor (1/min)
UA = 5e4	UA = U * A = Overall Heat Transfer (W/m^2-K) / Area (m^2)
Caf = 1	Feed Concentration (mol/m^3)
Tf = 350	Feed Temperature (K)
Differential States	
Ca = 0.9	Concentration of A in CSTR (mol/m^3)
T = 305	Temperature in CSTR (K)

Model Equations

Species Mole Balance for Component A

$$\frac{dn_A}{dt} = \frac{d\left(c_A V\right)}{dt} = \sum_{i=inlet} c_{Ai} q_i - \sum_{j=outlet} c_{Aj} q_j + r_A V$$

$$V\frac{dc_A}{dt} = c_{A.in} q - c_A q + r_A V$$

Energy Balance

$$\frac{d[\rho C_p V(T - T_{ref})]}{dt} = \sum_{i:inlet} \dot{m}_i C_p (T_i - T_{ref}) - \sum_{j:outlet} \dot{m}_j C_p (T_j - T_{ref}) + Q + W_s$$

$$\rho C_p V\frac{dT}{dt} = \rho C_p q(T_{in} - T) + r_A \Delta H_r - UA(T - T_C)$$

Other Equation(s): Reaction Rate

$$r_A = k_0 c_A \exp(-\frac{E}{RT})$$

Degrees of Freedom

Number of Variables

c_A T r_A

Number of Equations

$$V\frac{dc_A}{dt} = c_{A.in}q - c_A q + r_A V$$

$$\rho C_p V\frac{dT}{dt} = \rho C_p q(T_{in} - T) + r_A \Delta H_r - UA(T - T_C)$$

$$r_A = k_0 c_A \exp(-\frac{E}{RT})$$

$$N_{DOF} = N_{Variables} - N_{Equations}$$

Simplify

Variables

c_A T ~~r_A~~

Equations

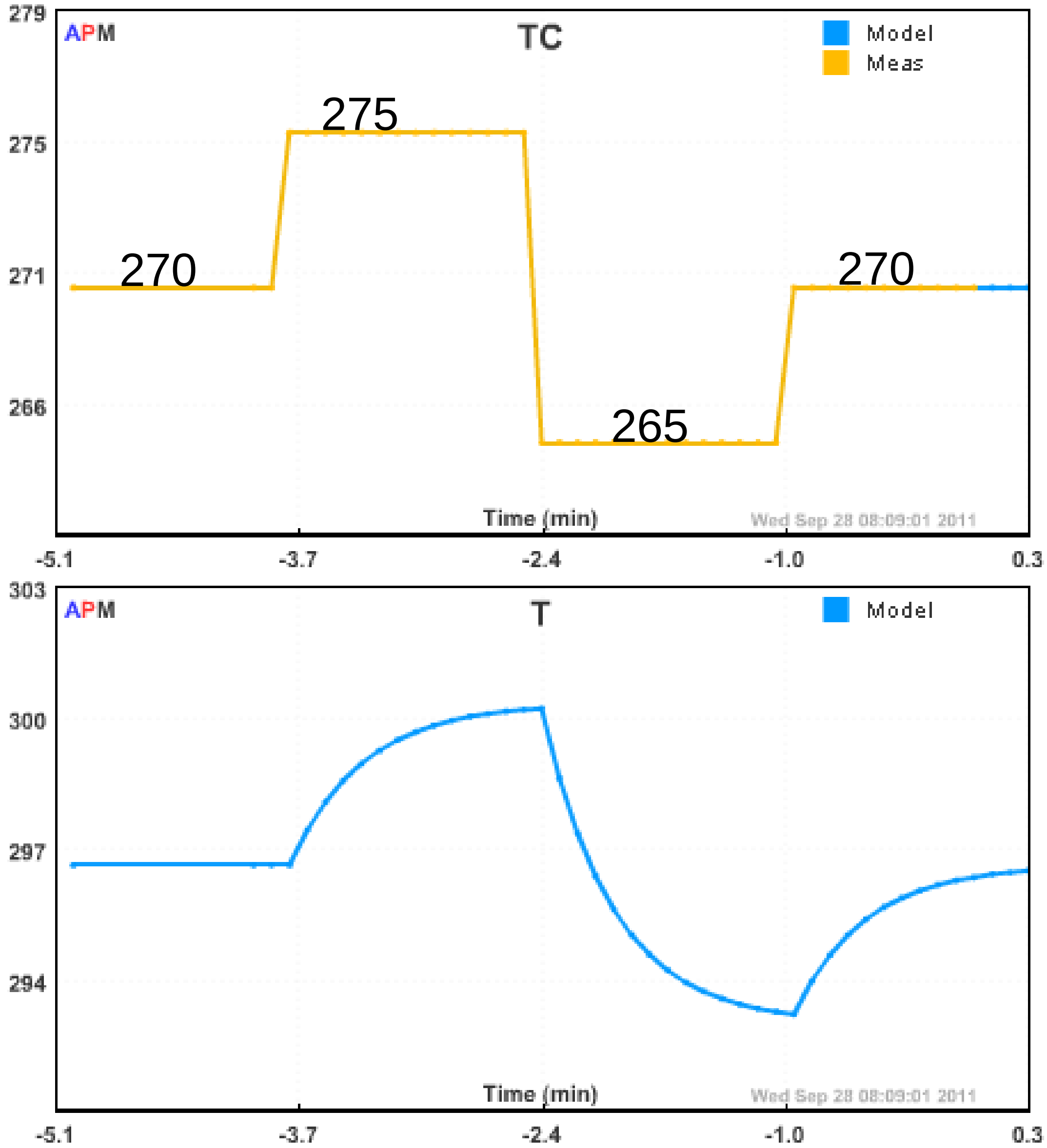
$$V\frac{dc_A}{dt} = c_{A.in}q - c_A q + r_A V$$

$$\rho C_p V\frac{dT}{dt} = \rho C_p q(T_{in} - T) + r_A \Delta H_r - UA(T - T_C)$$

Substitute

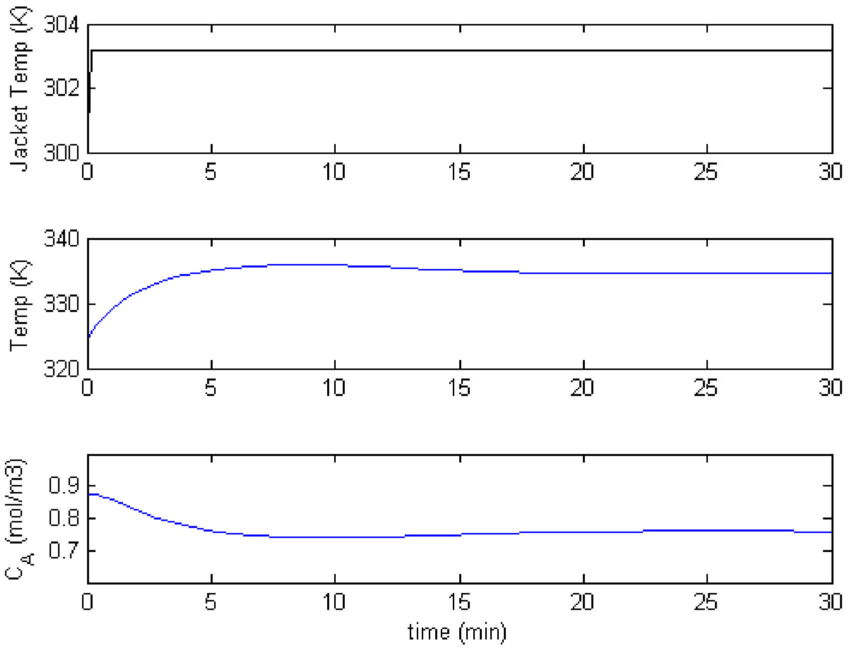
$$r_A = k_0 c_A \exp(-\frac{E}{RT})$$

Simulate: Doublet Test

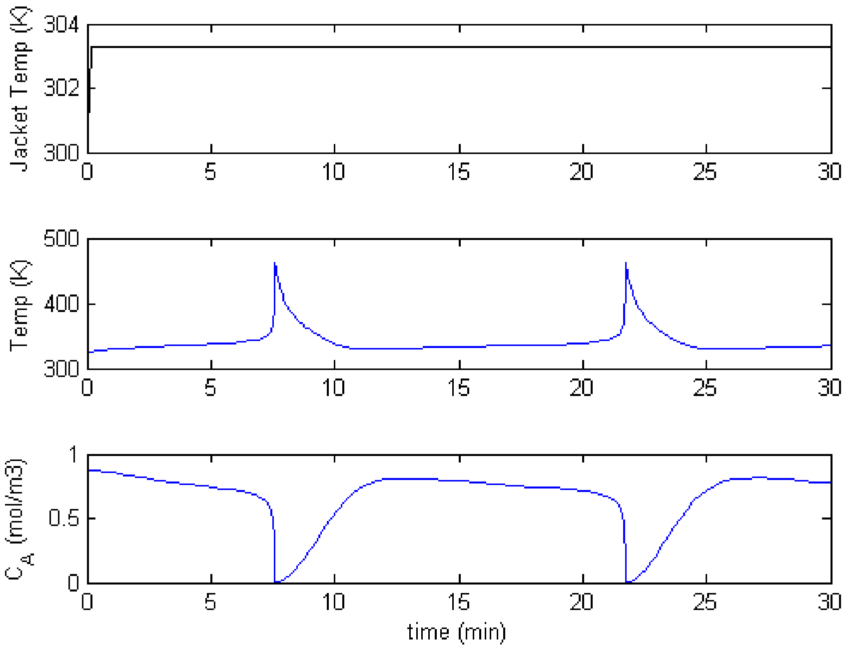


Stability Analysis

Tc = 303.2 K



Tc = 303.3 K



Model-Based Control

How does the controller achieve 380 K when manual control to 335 K appeared to cause run-away reaction?