Process Dynamics & Control

Development of Mathematical Model

Motivation:

- Develop understanding of process
- Build a mathematical hypothesis of process mechanisms
- Match observed process behavior
- useful in design, optimization and *control* of process

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Control:

- Interested in description of process dynamics

  - ➢ Dynamic model is used to predict how process responds to given input

  - ➢ Tells us how to react

Development of Mathematical Model

Mathematical Modeling of a process require

- Understanding of the process
- Writing conservation balance for Mass, Momentum and Energy
- Writing closure equations, i.e, constitutive relationships defining equilibrium and rate parameters
- Devising solution technique

What kind of model do we need?

Dynamic vs. Steady-state

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  - ➢Variables not a function of time
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- *Dynamic*
  - Variables are a function of time
  - Control requires dynamic model

What kind of model do we need?

Experimental vs Theoretical

- Experimental
  - ➢ Derived from tests performed on actual process
  - ➢ Simpler model forms
  - ➢ Easier to manipulate

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Experimental vs Theoretical

- Experimental
  - ➢ Derived from tests performed on actual process
  - ➢ Simpler model forms
  - ➢ Easier to manipulate
- Theoretical
  - ➢ Application of fundamental laws of physics and chemistry
  - ➢ more complex but provides understanding
  - ➢ Required in design stages

What kind of model do we need?

Empirical vs. Mechanistic models

- Empirical Models
  - only local representation of the process (no extrapolation)
  - model only as good as the data
  - do not rely on underlying mechanisms
  - Fit specific function to match process

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  - do not rely on underlying mechanisms
  - Fit specific function to match process

- Mechanistic Models
  - Rely on our understanding of a process
  - Derived from first principles
  - Observing laws of conservation of
    - Mass
    - Energy
    - Momentum
  - Useful for simulation and exploration of new operating conditions
  - May contain unknown constants that must be estimated

What kind of model do we need?

Linear vs Nonlinear

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  - simpler model form, easy to identify
  - easy to design controller
  - poor prediction, adequate control

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Linear vs Nonlinear

- Linear
  - basis for most industrial control
  - simpler model form, easy to identify
  - easy to design controller
  - poor prediction, adequate control
- Nonlinear
  - Reality
  - more complex and difficult to identify
  - need state-of-the-art controller design techniques to do the job
  - better prediction and control

What kind of model do we need?

In existing processes, we rely on

- Dynamic models obtained from experiments
- Usually of an empirical nature
- Linear

In new applications (or difficult problems)

- Focus on mechanistic modeling
- Dynamic models derived from theory
- Nonlinear

General modeling procedure

1. Identify modeling objectives
   - end use of model (e.g. control)
2. Identify fundamental quantities of interest
   - Mass, Energy and/or Momentum
3. Identify boundaries
4. Apply fundamental physical and chemical laws
   - Mass, Energy and/or Momentum balances
5. Make appropriate assumptions (Simplify)
   - ideality (e.g. isothermal, adiabatic, ideal gas, no friction, incompressible flow, etc,…)
6. Write down energy, mass and momentum balances
   - develop the model equations

General modeling procedure

7. Check model consistency
   - do we have more unknowns than equations
8. Determine unknown constants
   - e.g. friction coefficients, fluid density and viscosity
9. Solve model equations
   - typically nonlinear ordinary (or partial) differential equations
   - initial value problems
10. Check the validity of the model
    - compare to process behavior

Benchmark Systems to be used for the course

- Tank Level System
  - 3 tank in series
  - Quadruple Tank
- Continuous Stirred Tank Heater
- Continuous Stirred Tank Reactor system
  - Isothermal Reactor (Van de Vusse reaction)
  - Non-isothermal Reactor
  - Polymerization Reactor
- Distillation Column

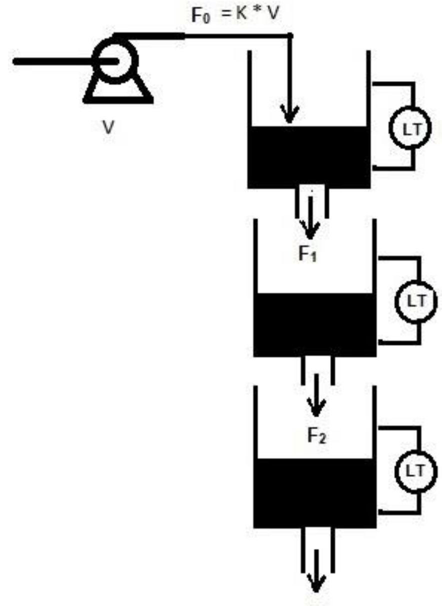
MATLAB / SIMULINK model will be developed based on nonlinear model

Mathematical Model of tank level system

$$\frac{dh_1}{dt} = \frac{F_0}{A_1} - \frac{a_1}{A_1}\sqrt{2gh_1}$$

$$\frac{dh_2}{dt} = \frac{a_1}{A_2}\sqrt{2gh_1} - \frac{a_2}{A_2}\sqrt{2gh_2}$$

$$\frac{dh_3}{dt} = \frac{a_2}{A_3}\sqrt{2gh_2} - \frac{a_3}{A_3}\sqrt{2gh_3}$$



Control objective:

Control the 3rd tank level by manipulating pump voltage V, where $F_0 = K\,V$

Add q_2 input flow on the tanks 2 and set q_2 as manipulated variable.

Which one is difficult to control?

Data for Simulation in Matlab/Simulink

A_1, A_3 = 28 cm^2 A_2 = 32 cm^2 V^s = 3 V

a_1 = 0.06725 cm^2 a_2 = 0.05683 cm^2
a_3 = 0.07089 cm^2 K=3.14

- Transfer Function model

Define : $x_1 = h_1 - h_1^s$; $x_2 = h_2 - h_2^s$; $x_3 = h_3 - h_3^s$; $u = V - V^s$

Linearizing around steady state value h_1^s

$$\frac{dh_1}{dt} = \frac{K}{A_1}V - \frac{a_1}{A_1}\sqrt{2g}\left[\sqrt{h_1^s} + \frac{1}{2\sqrt{h_1^s}}(h_1 - h_1^s)\right]$$

Subtracting above from steady state equation,

$$\frac{dx_1}{dt} = \frac{K}{A_1}u - \frac{a_1\sqrt{g}}{A_1\sqrt{2h_1^s}}x_1 \quad \Rightarrow \text{Transfer function } \frac{x_1(s)}{u(s)} = \frac{K_{p_1}}{\tau_{p_1}s+1}$$

Where, $K_{p_1} = \frac{K}{a_1}\sqrt{\frac{2h_1^s}{g}}$ and $\tau_{p_1} = \frac{A_1}{a_1}\sqrt{\frac{2h_1^s}{g}}$

Similarly,

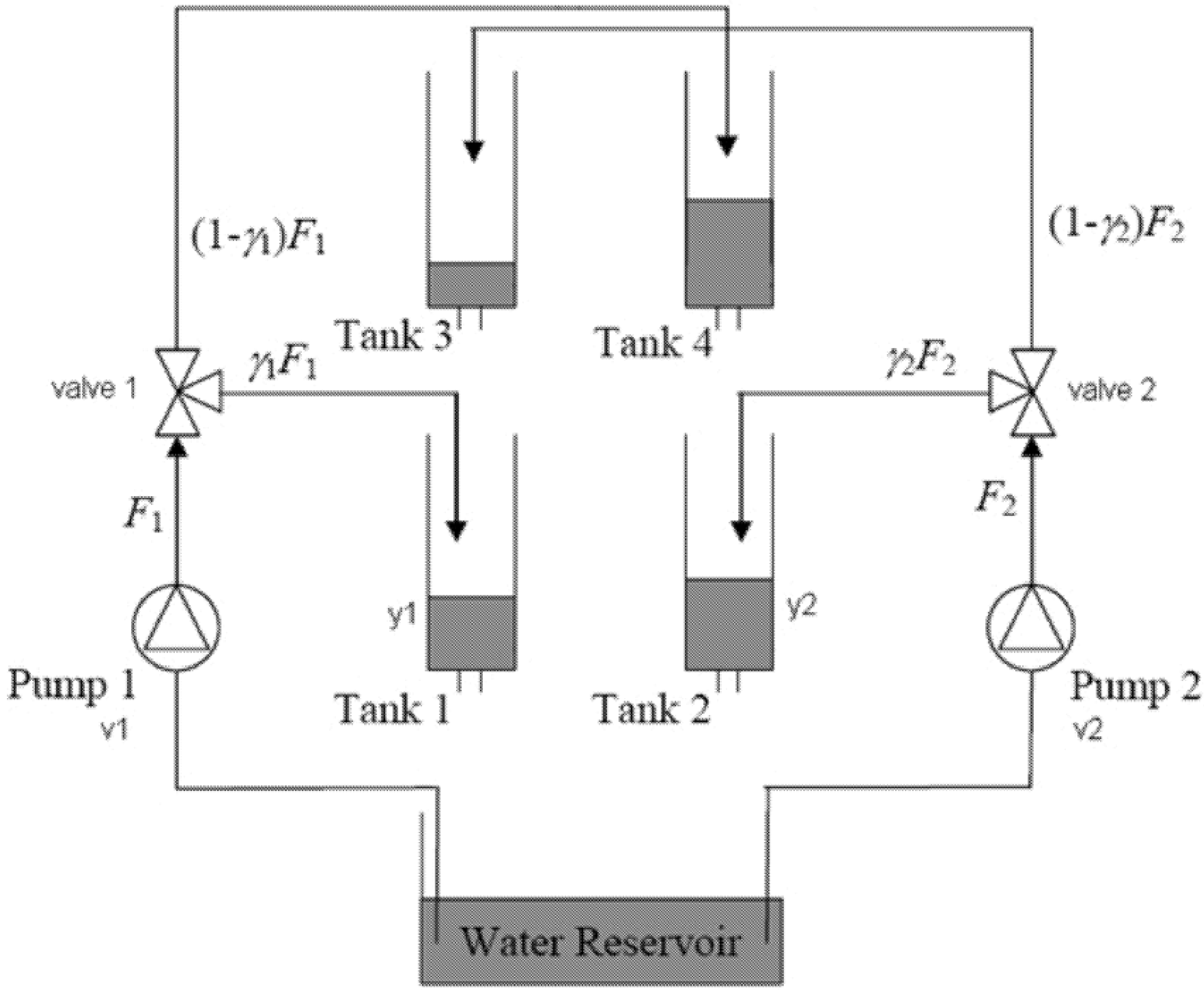
$$\frac{dx_2}{dt} = \frac{a_1}{A_2}\sqrt{\frac{g}{2h_1^s}}\,x_1 - \frac{a_2}{A_2}\sqrt{\frac{g}{2h_2^s}}\,x_2 \text{ and Transfer function } \frac{x_2(s)}{x_1(s)} = \frac{K_{p_2}}{\tau_{p_2}s+1}$$

$$\frac{dx_3}{dt} = \frac{a_2}{A_3}\sqrt{\frac{g}{2h_2^s}}\,x_2 - \frac{a_3}{A_3}\sqrt{\frac{g}{2h_3^s}}\,x_3 \text{ and Transfer function } \frac{x_3(s)}{x_2(s)} = \frac{K_{p_3}}{\tau_{p_3}s+1}$$

Where, $K_{p_j} = \frac{a_{j-1}}{a_j}\sqrt{\frac{h_j^s}{h_{j-1}^s}}$ and $\tau_{p_j} = \frac{A_j}{a_j}\sqrt{\frac{2h_j^s}{g}}$ for j = 2,3

So, Process Transfer function $G(s) = \frac{x_3(s)}{u(s)} = \frac{K_{p_1}K_{p_2}K_{p_3}}{(\tau_{p_1}s+1)(\tau_{p_2}s+1)(\tau_{p_3}s+1)}$

Quadruple Tank problem



Quadruple Tank problem

$$\frac{dh_1}{dt} = -\frac{a_1}{A_1}\sqrt{2gh_1} + \frac{a_3}{A_1}\sqrt{2gh_3} + \frac{\gamma_1 k_1}{A_1} v_1$$

$$\frac{dh_2}{dt} = -\frac{a_2}{A_2}\sqrt{2gh_2} + \frac{a_4}{A_2}\sqrt{2gh_4} + \frac{\gamma_2 k_2}{A_2} v_2$$

$$\frac{dh_3}{dt} = -\frac{a_3}{A_3}\sqrt{2gh_3} + \frac{(1-\gamma_2)k_2}{A_3} v_2$$

$$\frac{dh_2}{dt} = -\frac{a_4}{A_4}\sqrt{2gh_4} + \frac{(1-\gamma_1)k_1}{A_4} v_1$$

Control Objective

Both the levels of tank1 and tank2 should be controlled by manipulating voltages to the pumps.

Data for simulation:

A_1, A_3 = 28 cm^2

A_2, A_4 = 32 cm^2

a_1, a_3 = 0.071 cm^2

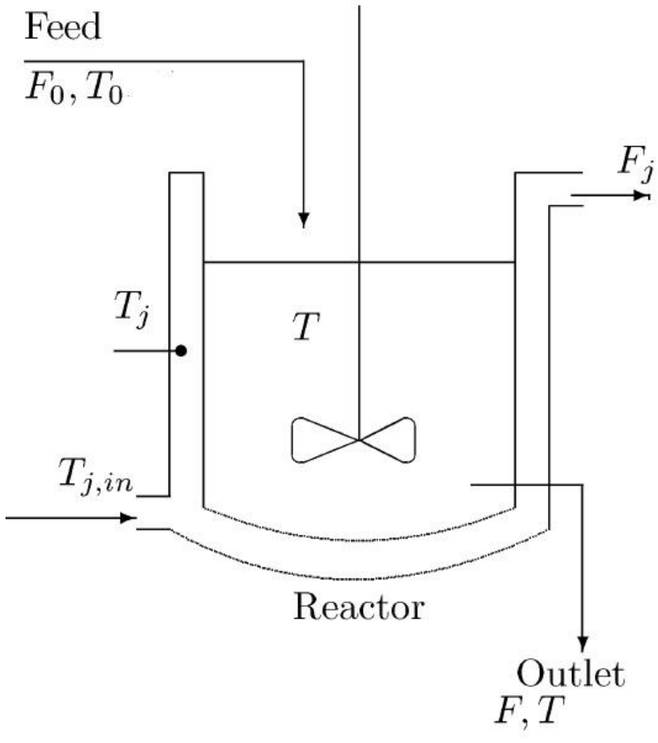
a_2, a_4 = 0.057 cm^2

k_1, k_2 = 3.33, 3.35

v_1, v_2 = 3.0, 3.0

γ_1, γ_2 = 0.7, 0.6

Jacketed heated stirred tank



Assumptions:

Constant hold-up in tank and jacket
Constant heat capacities and densities
Incompressible flow

$$\frac{dV}{dt} = F_0 - F = 0$$

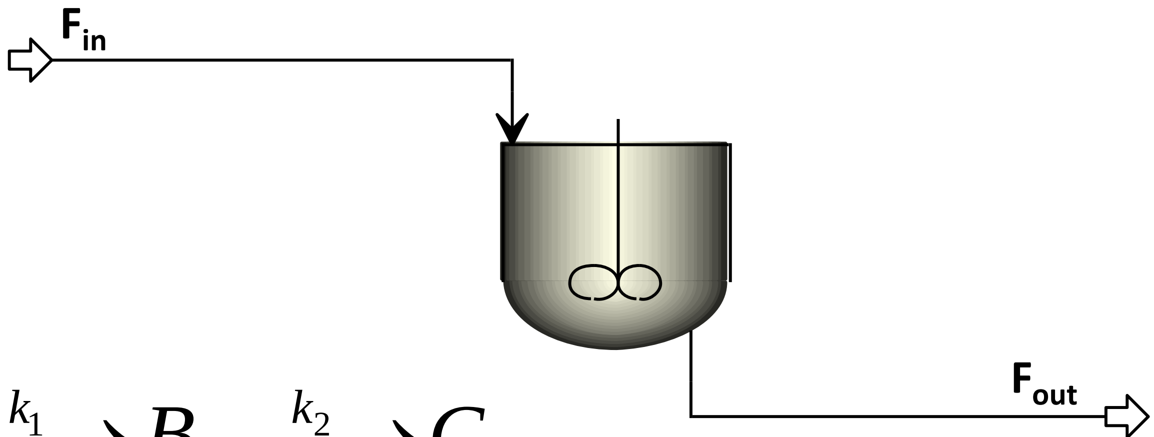
$$\frac{dT}{dt} = \frac{F}{V}(T_0 - T) + \frac{UA}{\rho C_P V}(T_j - T)$$

$$\frac{dT_j}{dt} = \frac{F_j}{V_j}(T_{ji} - T_j) - \frac{UA}{\rho_j C_{Pj} V_j}(T_j - T)$$

Parameter and Steady State Values

F = 30 l/min; F_j^s = 50 l/min; T_0 = 15^{0}C; T_{Jin} = 93^{0}C; V = 300 l; V_j = 30 l;
ρC_p = 1 Kcal/K l; ρC_{pj} = 1.384 ; UA = 100 Kcal/min K; T^s = 60^{0}C ; T_J = 73.5 ^{0}C

Continuous Stirred Tank Reactor



$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

$$A \xrightarrow{k_3} 2D$$

Assumption:

1. **Exit Condition = Reactor Condition**
2. **Isothermal Reaction**
3. **Constant volume, i.e, F_{in} = F_{out}=F**
4. **Only reactant A in feed is consumed, i.e, other reactant is in large excess. No product in the feed**

Continuous Stirred Tank Reactor

Constant volume : dV/dt = 0

Dynamic model

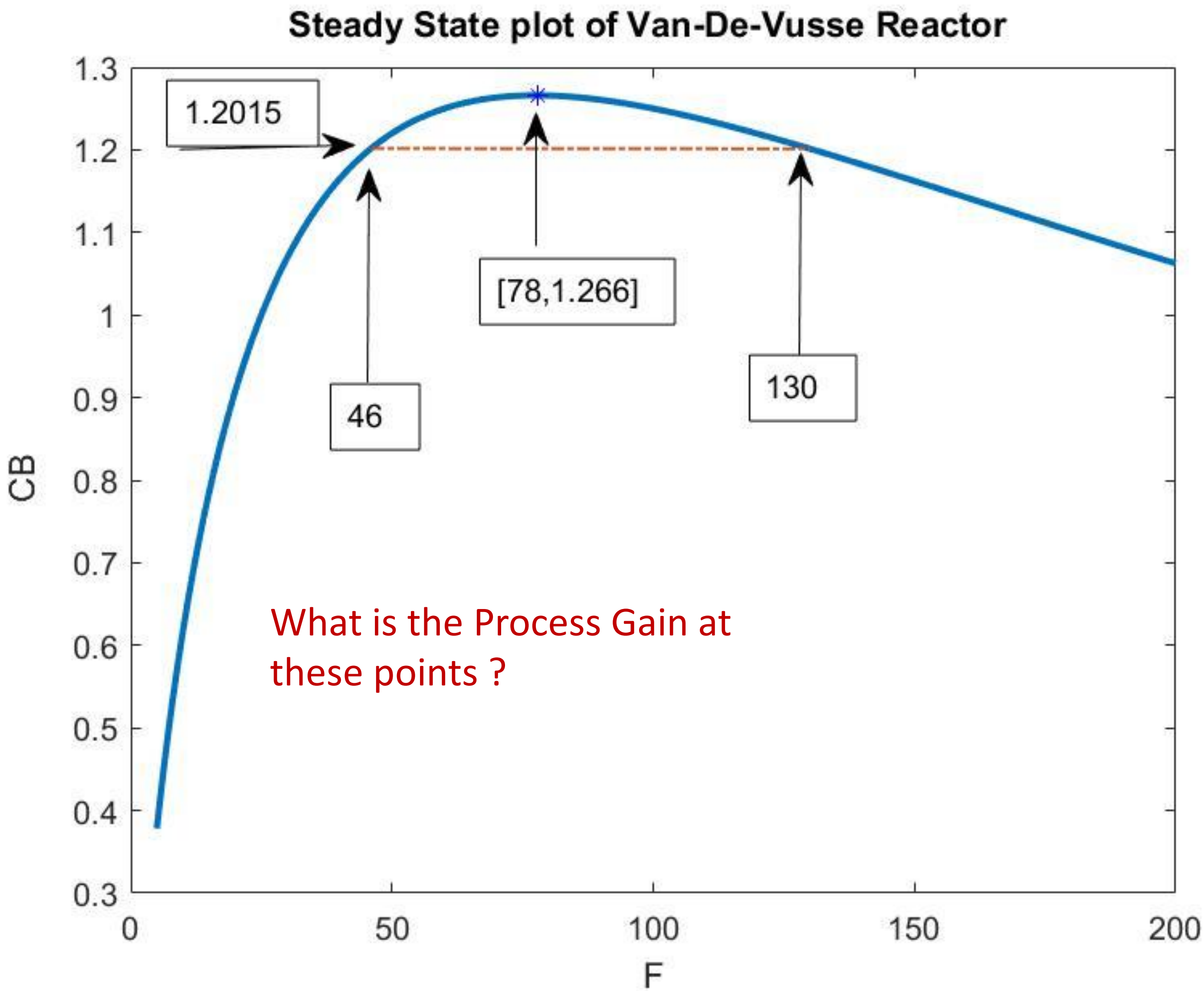
- $\frac{dC_A}{dt} = \frac{F}{V}\left(C_{Af} - C_A\right) - k_1 C_A - k_3 C_A^2$
- $\frac{dC_B}{dt} = -\frac{F}{V} C_B + k_1 C_A - k_2 C_B$
- $\frac{dC_C}{dt} = -\frac{F}{V} C_C + k_2 C_B$
- $\frac{dC_D}{dt} = -\frac{F}{V} C_D + \frac{1}{2} k_3 C_A^2$

Data for the CSTR

V = 1 l
F = 78 l/h
C_{Af} = 10 mol/l
kl = 50 h-1
k2 = 100 h-1
k3 = 10 l.mol-1.h-1

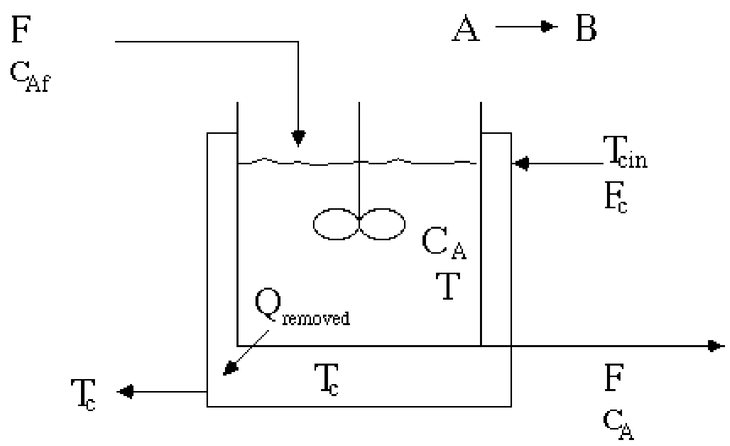
Since our objective is to control C_B, the reduced order model should be

- $\frac{dC_A}{dt} = \frac{F}{V}\left(C_{Af} - C_A\right) - k_1 C_A - k_3 C_A^2 = f_1(C_A, C_B, F)$
- $\frac{dC_B}{dt} = -\frac{F}{V} C_B + k_1 C_A - k_2 C_B = f_2(C_A, C_B, F)$



What is the Process Gain at these points ?

Non-Isothermal Jacketed CSTR

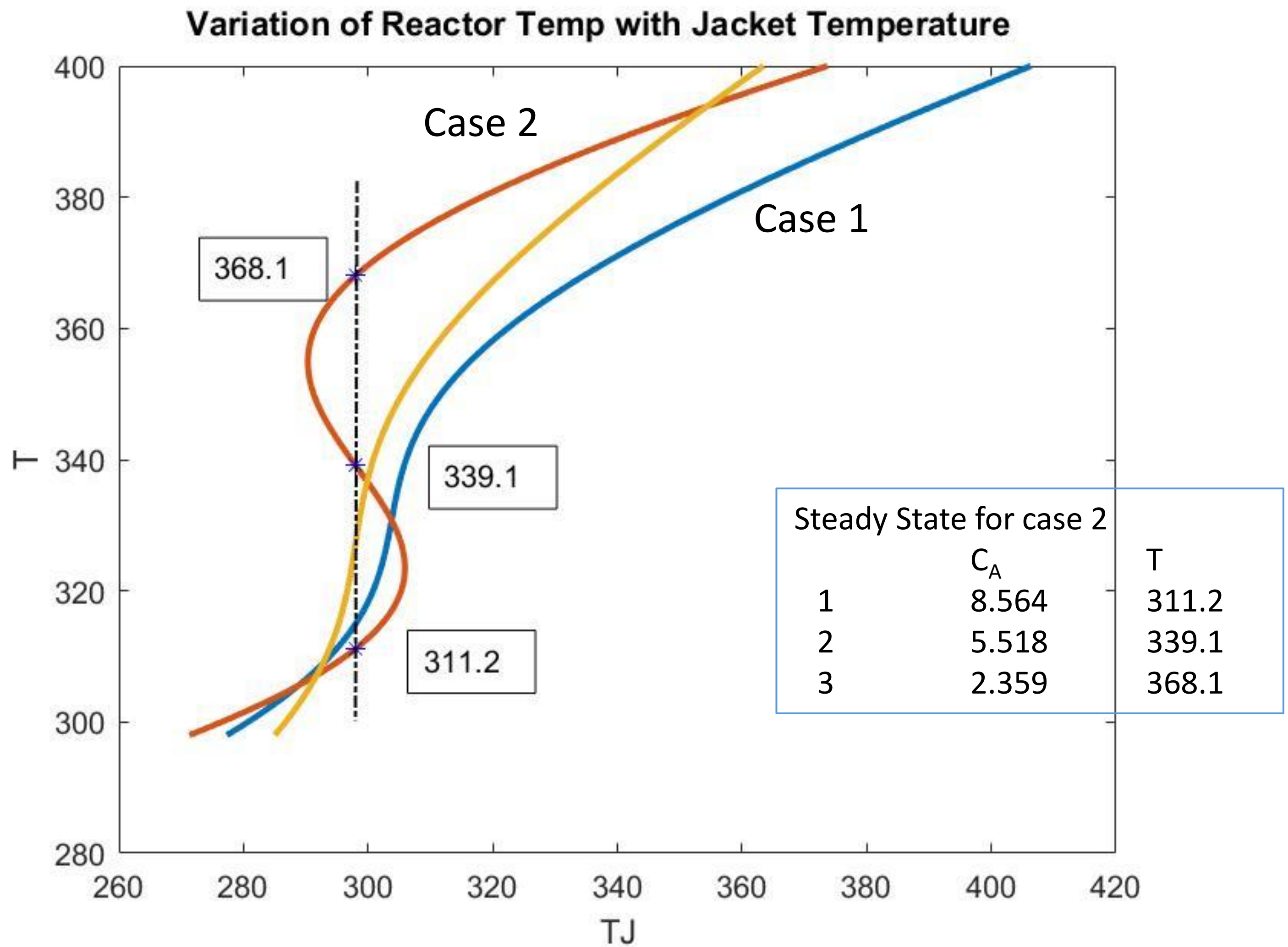


$$\frac{dC_A}{dt} = \frac{F}{V}\left(C_{A_f} - C_A\right) - r$$

$$\frac{dT}{dt} = \frac{F}{V}\left(T_f - T\right) + \left(\frac{-\Delta H}{\rho C_p}\right)\mathrm{r} - \frac{\mathrm{UA}}{\mathrm{V}\rho C_p}(\mathrm{T} - \mathrm{T_C})$$

$$r = k_0 e^{-\frac{E}{RT}} C_A$$

parameter	case 1	case 2	case 3
F/V, hr-1	1	1	1
k_0, hr-1	14,825*3600	9,703*3600	18,194*3600
$(-\Delta H)$, kcal/kgmol	5215	5960	8195
E, kcal/kgmol	11,843	11,843	11,843
ρcp, kcal/(m^3 °C)	500	500	500
T_f, °C	25	25	25
C_{Af}, kgmol/m3	10	10	10
UA/V, kcal/(m^3 °C hr)	250	150	750
T_C, °C	25	25	25

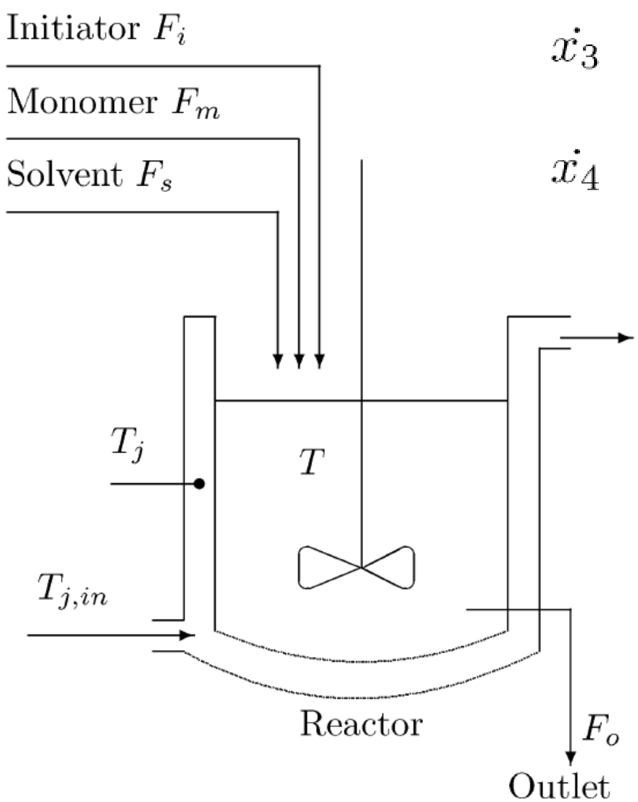


Variation of Reactor Temp with Jacket Temperature
Case 2
Case 1
368.1
339.1
311.2
Steady State for case 2
C_A
T
1 8.564 311.2
2 5.518 339.1
3 2.359 368.1
T
TJ
400
380
360
340
320
300
280
260
280
300
320
340
360
380
400
420

Styrene Polymerization Reactor

x_1 Initiator Conc
x_2 Monomer Conc
x_3 Reactor Temp
x_4 Jacket Temp.

$$
\begin{aligned}
\dot{x_1} &= \frac{(F_i\,C_{ia} - F_o\,x_1)}{V} - k_d\,x_1 \\
\dot{x_2} &= \frac{(F_m\,C_{ma} - F_o\,x_2)}{V} - k_p\,x_2\,\mathcal{R} \\
\dot{x_3} &= \frac{F_o\,(T_a - x_3)}{V} - \frac{\Delta H}{\rho\,C_p}\,k_p\,x_2\,\mathcal{R} - \frac{U\,A}{\rho\,C_p\,V}\,(x_3 - x_4) \\
\dot{x_4} &= \frac{F_j(T_{j,in} - x_4)}{V_j} + \frac{U\,A}{\rho_j\,C_{pj}\,V_j}\,(x_3 - x_4)
\end{aligned}
$$



$$F_o = F_i + F_m + F_s.$$

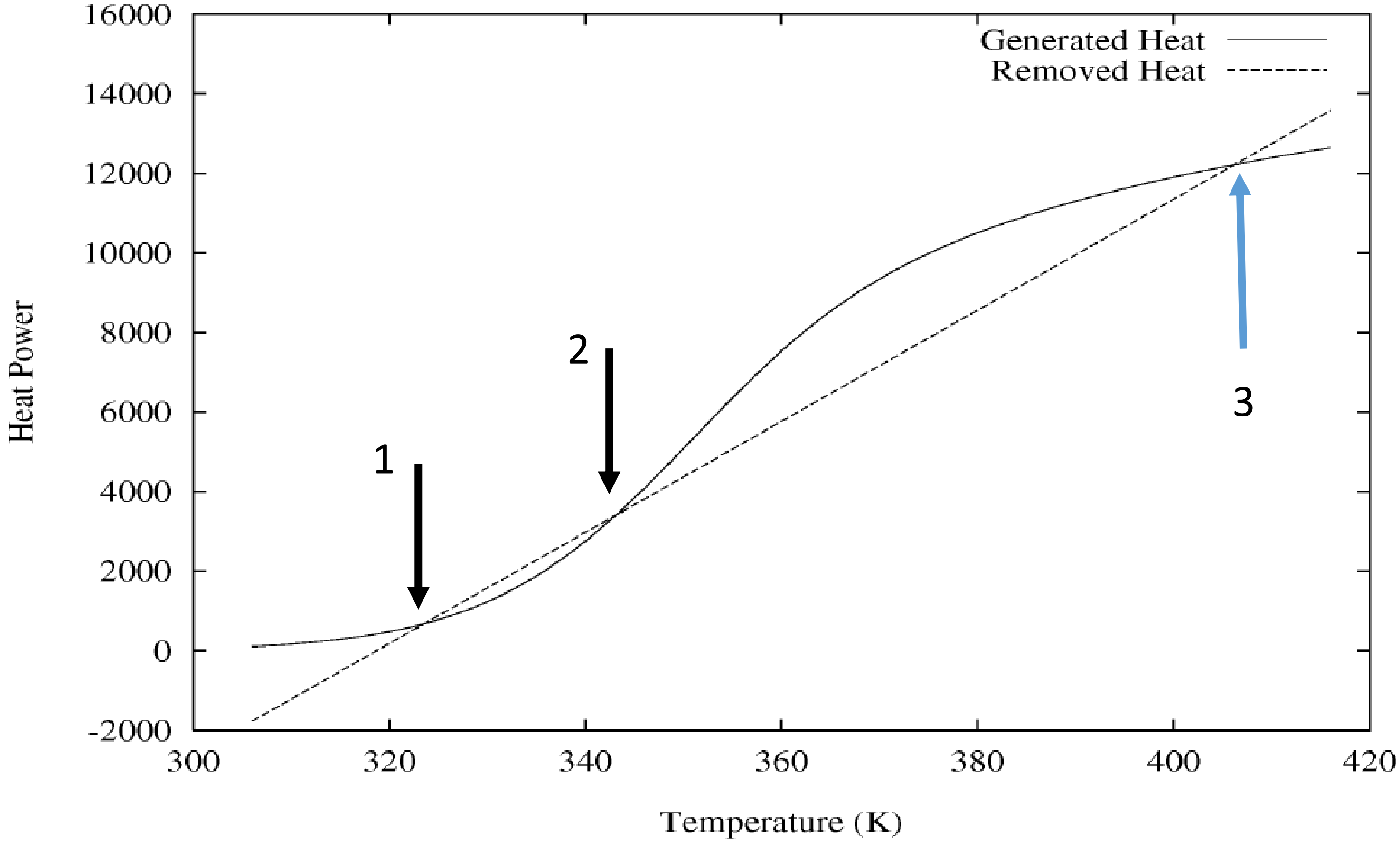
The chain concentration of growing polymer is equal to

$$\mathcal{R} = (2\,f\,k_d\,x_1/k_t)^{0.5}$$

The dissociation, propagation and termination Rate constants follow Arrhenius law :

$$k_i = k_{i0}\,e^{-\frac{E_i}{RT}} \quad \text{for I =d, p or t}$$

Steady State Heat Power vs Reactor Temperature



Phase Portrait