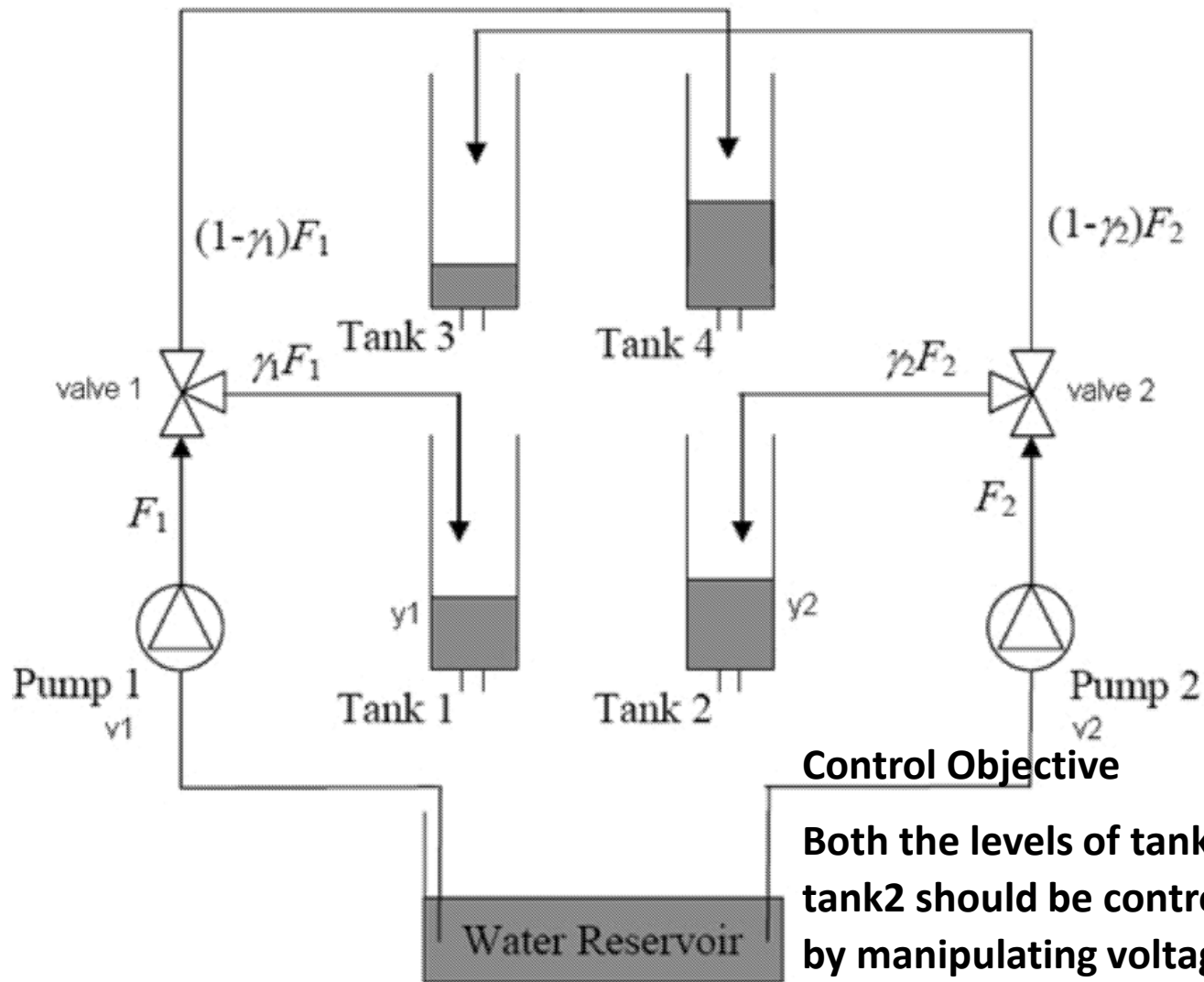# Process Dynamics & Control

Quadruple Tank problem

Control Objective

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

Quadruple Tank problem (Dynamic Model)

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

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

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

$$\frac{dh_4}{dt} = -\frac{a_4}{A_4}\sqrt{2gh_4} + \frac{(1-\gamma_1)k_1}{A_4}v_1$$

Data for simulation:

A_1, A_3 = 28 cm²

A_2, A_4 = 32 cm²

a_1, a_3 = 0.071 cm²
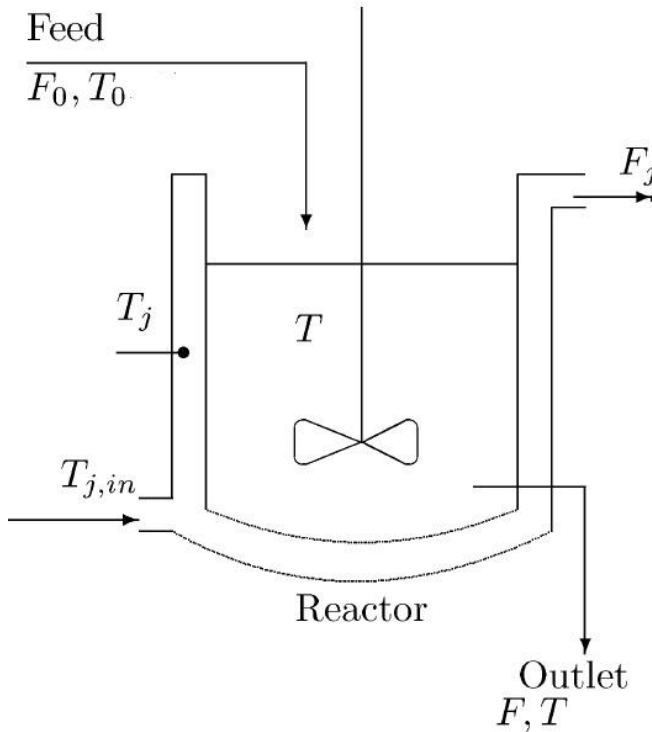
a_2, a_4 = 0.057 cm²

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

Feed
$\overline{F_0, T_0}$

T_j

T

F_j

$T_{j,in}$

Reactor

Outlet
F, T

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

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

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

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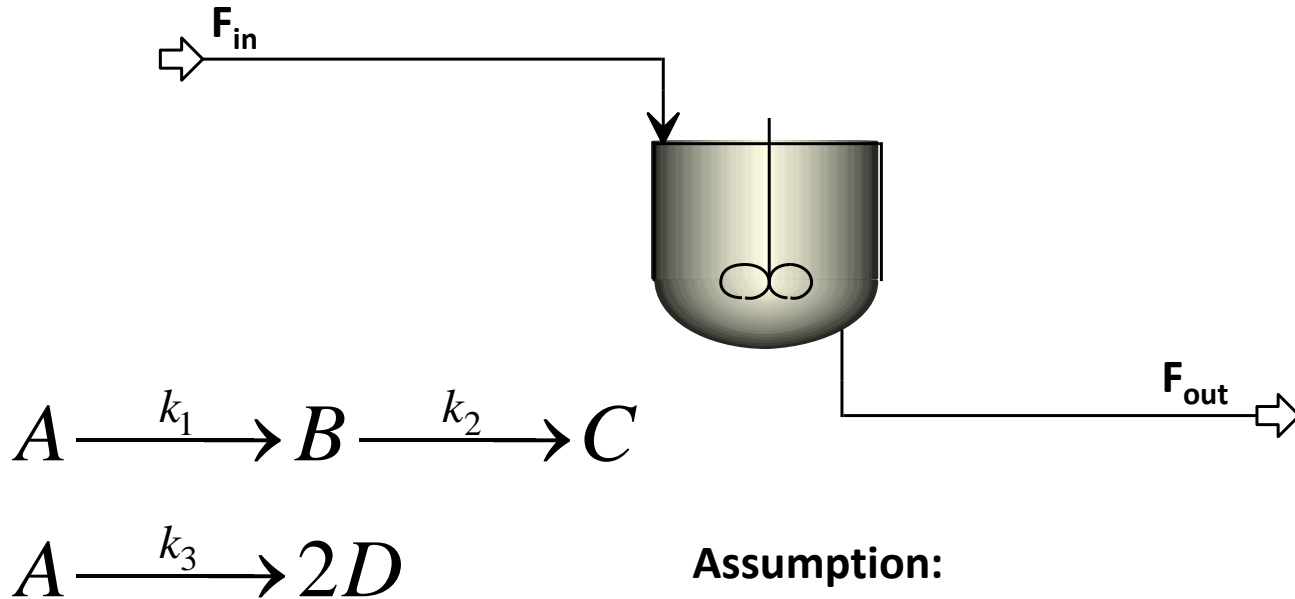
Control Objective
  Control T by manipulating F_j

Parameter and Steady State Values
F = 30 l/min; F_j^s = 50 l/min; T_0 = 15⁰C; T_{Jin} = 93⁰C; V = 300 l; V_j = 30 l;
ρC_p = 1 Kcal/K l; $\rho_j C_{pj}$ = 1.384 ; UA = 100 Kcal/min K; T^s = 60⁰C ; T_J = 73.5 ⁰C

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 (model)

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
$k_1 = 5/6$; $k_2 = 5/3$
$K_3 = 1/6$; $C_{af} = 10$

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

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

- $\frac{dC_B}{dt} = -\frac{F}{V} C_B + k_1 C_A - k_2 C_B = f_2(C_A, C_B, F/V)$

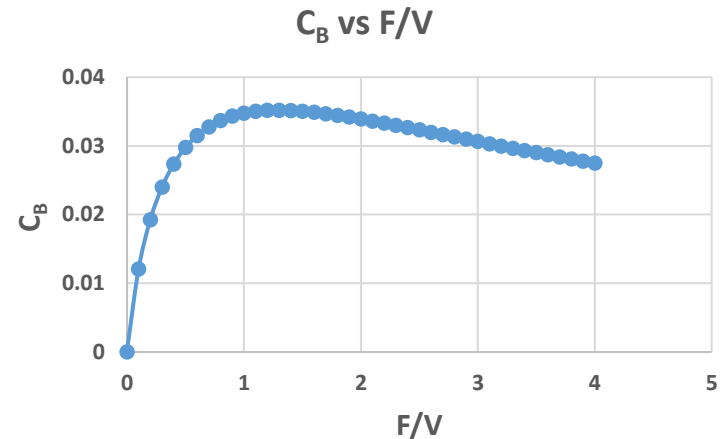# Continuous Stirred Tank Reactor

Find Maximum C_B with respect to F/V

- $\dfrac{dC_A}{dt} = \dfrac{F}{V}\left(C_{Af} - C_A\right) - k_1 C_A - k_3 C_A^2 = 0$

- $\dfrac{dC_B}{dt} = -\dfrac{F}{V} C_B + k_1 C_A - k_2 C_B = 0$

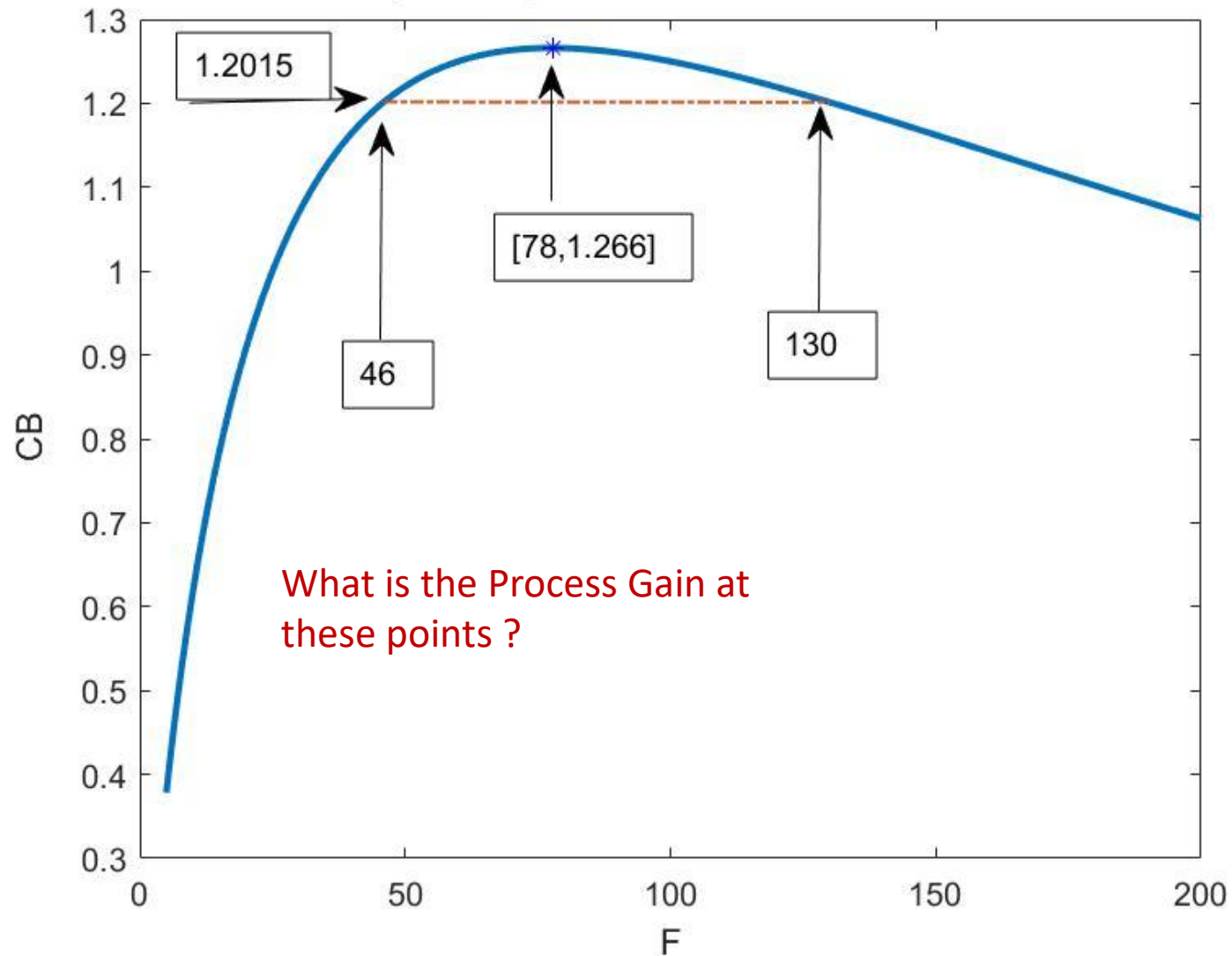- $C_A = \dfrac{-\left(k_1 + \frac{F}{V}\right) + \sqrt{\left(k_1 + \frac{F}{V}\right)^2 + 4 k_3 \frac{F}{V} C_{Af}}}{2 k_3}$ since, C_A can not be negative.

- $C_B = \dfrac{k_1 C_A}{\frac{F}{V} + k_2} = \dfrac{-k_1\left(k_1 + \frac{F}{V}\right) + k_1\sqrt{\left(k_1 + \frac{F}{V}\right)^2 + 4 k_3 \frac{F}{V} C_{Af}}}{2 k_3\left(\frac{F}{V} + k_2\right)}$
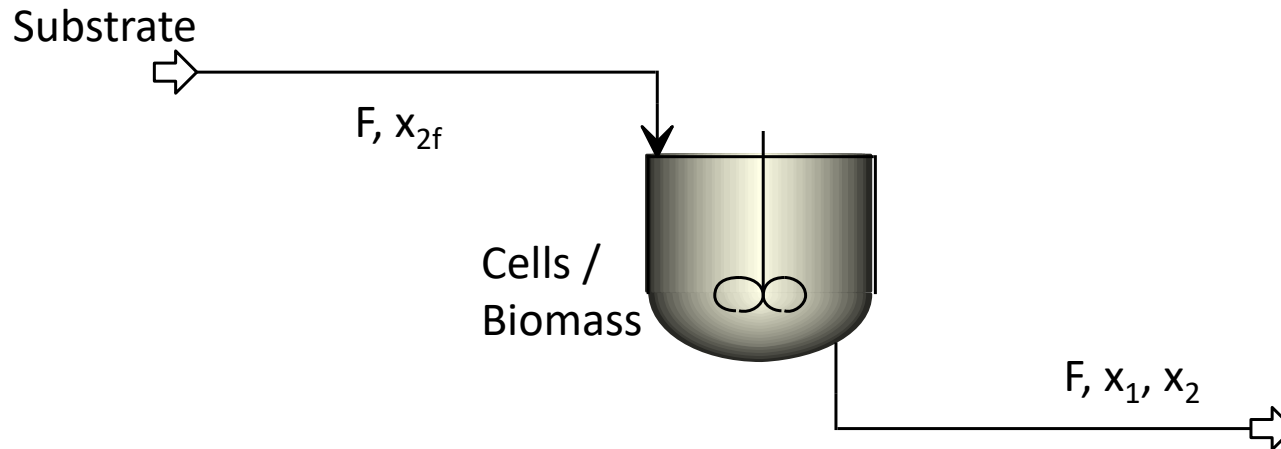
- $\dfrac{dC_B}{d\frac{F}{V}} = 0$ will give $\dfrac{F}{V_{opt}}$

C_B vs F/V

Steady State plot of Van-De-Vusse Reactor

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130

What is the Process Gain at these points ?

Biochemical Reactor

Substrate

F, x_{2f}

Cells /
Biomass

F, x_1, x_2

x_1 is mass of cells per unit volume in the reactor
x_2 is mass of substrate per unit volume in the reactor
x_{2f} is mass of substrate per unit volume in the feed stream

Assumption:

1. **Exit Condition = Reactor Condition**
2. **Isothermal Reaction**
3. **Constant volume, i.e, $F_{in} = F_{out}=F$**
4. **No cell/biomass is present in the feed stream.**

Biochemical Reactor (Dynamic Model)

Dynamic Model

$$\frac{dx_1}{dt} = -\frac{F}{V}x_1 + \mu x_1 = (\mu - D)x_1$$

$$\frac{dx_2}{dt} = D\left(x_{2f} - x_2\right) - \frac{\mu x_1}{Y}$$

Where yield, $Y = \frac{mass\ of\ cells\ produced}{mass\ of\ subsrtate\ consumed}$ and μ is specific growth

rate coefficient for cell mass which is not constant but function of

substrate concentration. The most common functions are:

Monod model: $\qquad\qquad\qquad\mu = \frac{\mu_{max}\ x_2}{k_m + x_2}$

Substrate inhibition model: $\qquad\mu = \frac{\mu_{max}\ x_2}{k_m + x_2 + k_1 x_2^2}$

Biochemical Reactor

Steady State equations:

$$\frac{dx_1}{dt} = 0 = -\frac{F}{V}x_1 + \mu x_1 = (\mu - D)x_1 = (\frac{\mu_{max}\, x_2}{k_m + x_2} - D)x_1$$

if, $x_1 \neq 0$, then $x_2 = \frac{DK_m}{\mu_{max} - D}$

$$\frac{dx_2}{dt} = 0 = D\left(x_{2f} - x_2\right) - \frac{\mu x_1}{Y}$$
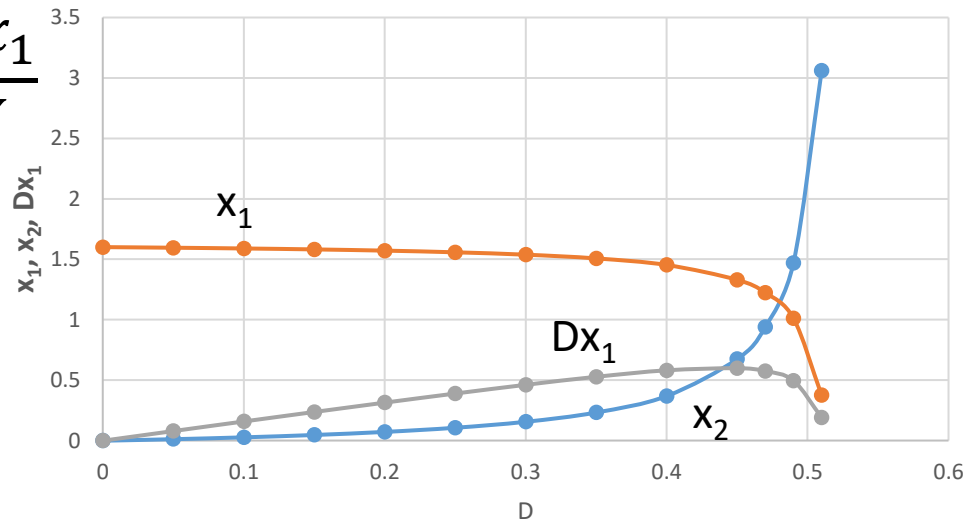
So, $x_1 = Y(x_{2f} - \frac{DK_m}{\mu_{max} - D})$

Dx_1 is the rate of cell Production per unit reactor Volume.

Effect of Dilution Rate

Biochemical Reactor

We need to find optimum dilution rate to maximize Dx_1. so,

$$Dx_1 = Y(Dx_{2f} - \frac{D^2 K_m}{\mu_{max} - D})$$

$$\frac{d(\frac{Dx_1}{Y})}{dD} = x_{2f} - \frac{(\mu_{max} - D)2Dk_m - D^2 K_m(-1)}{(\mu_{max} - D)^2} = 0$$
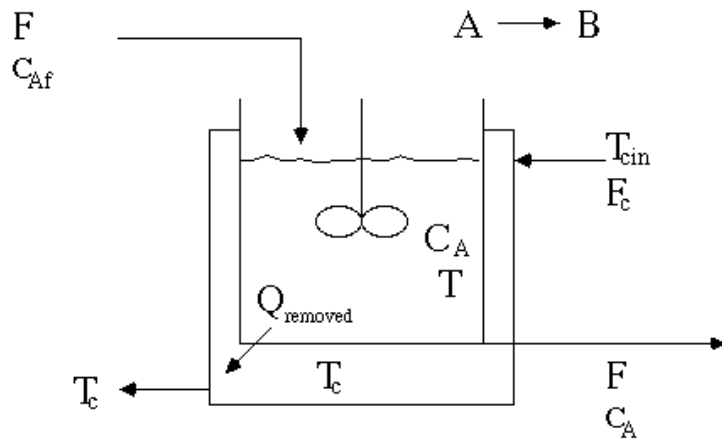
Or, $\quad D^2(x_{2f} + k_m) - 2D\mu_{max}(x_{2f} + k_m) + x_{2f}\mu_{max}^2 = 0$

Adding $K_m\mu_{max}^2$ both sides, we get

$$(D - \mu_{max})^2 = \frac{K_m\mu_{max}^2}{x_{2f} + K_m}$$

Or $D_{opt} = \mu_{max}\left(1 - \sqrt{\frac{K_m}{x_{2f} + K_m}}\right)$ since D can not be greater than μ_{max}

Non-Isothermal Jacketed CSTR

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

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

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

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
ρc_p, kcal/(m³ °C)	500	500	500
T_f, °C	25	25	25
C_{Af}, kgmol/m3	10	10	10
UA/V, kcal/(m³ °C hr)	250	150	750
T_C, °C	25	25	25

Variation of Reactor Temp with Jacket Temperature

Steady State for case 2		
	C_A	T
1	8.564	311.2
2	5.518	339.1
3	2.359	368.1
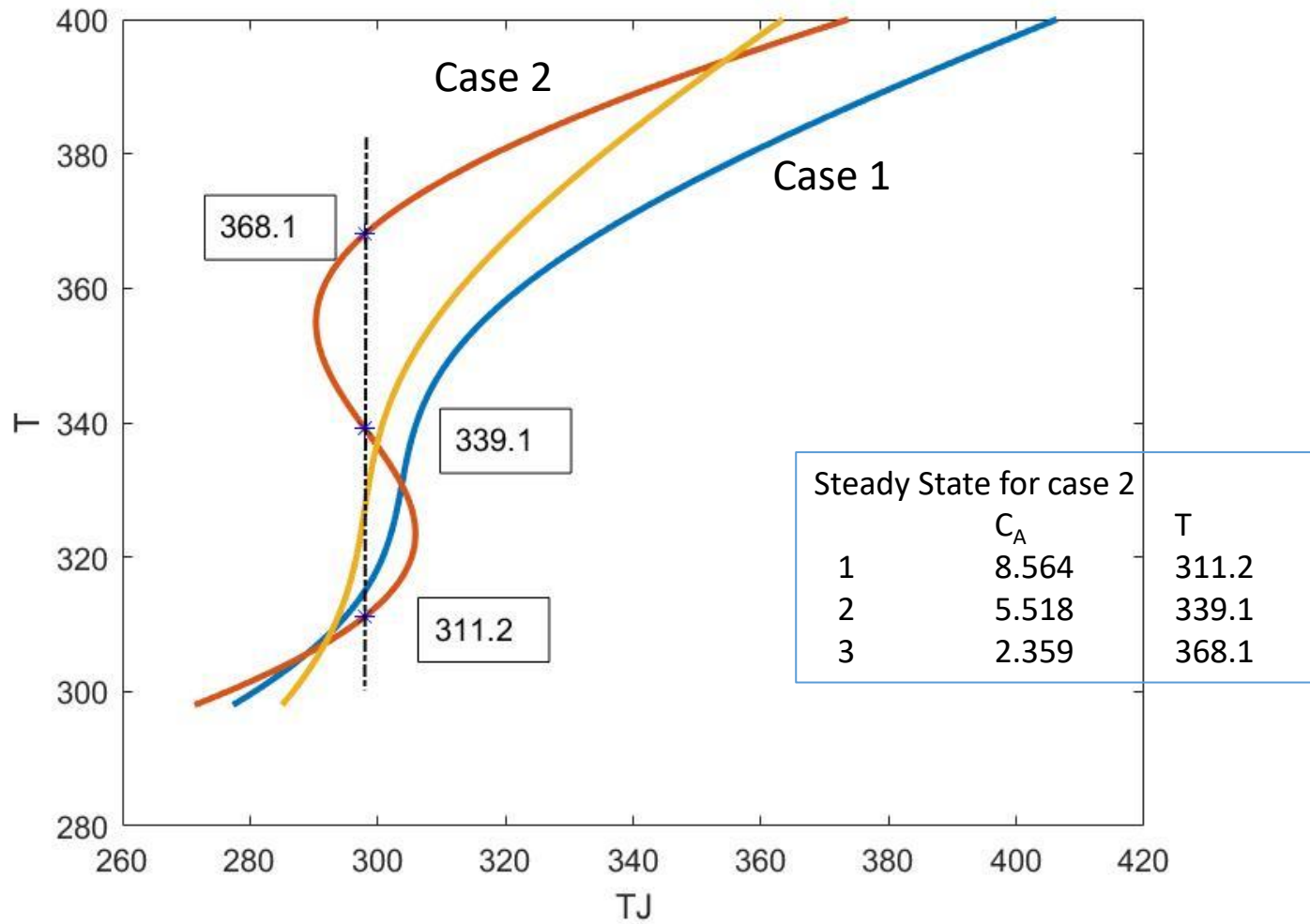
Styrene Polymerization Reactor

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

$$\dot{x}_1 = \frac{(F_i\,C_{ia} - F_o\,x_1)}{V} - k_d\,x_1$$

$$\dot{x}_2 = \frac{(F_m\,C_{ma} - F_o\,x_2)}{V} - k_p\,x_2\,\mathcal{R}$$

$$\dot{x}_3 = \frac{F_o\,(T_a - x_3)}{V} - \frac{\Delta H}{\rho\,C_p}\,k_p\,x_2\,\mathcal{R} - \frac{U A}{\rho\,C_p\,V}\,(x_3 - x_4)$$

$$\dot{x}_4 = \frac{F_j(T_{j,in} - x_4)}{V_j} + \frac{U A}{\rho_j\,C_{pj}\,V_j}\,(x_3 - x_4)$$

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

Initiator F_i

Monomer F_m

Solvent F_s

T_j

T

$T_{j,in}$

Reactor
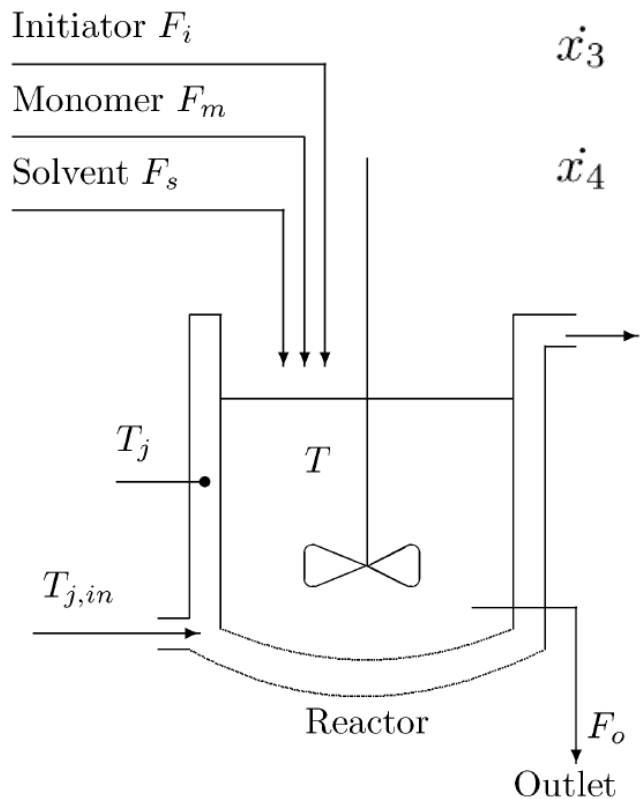
F_o

Outlet

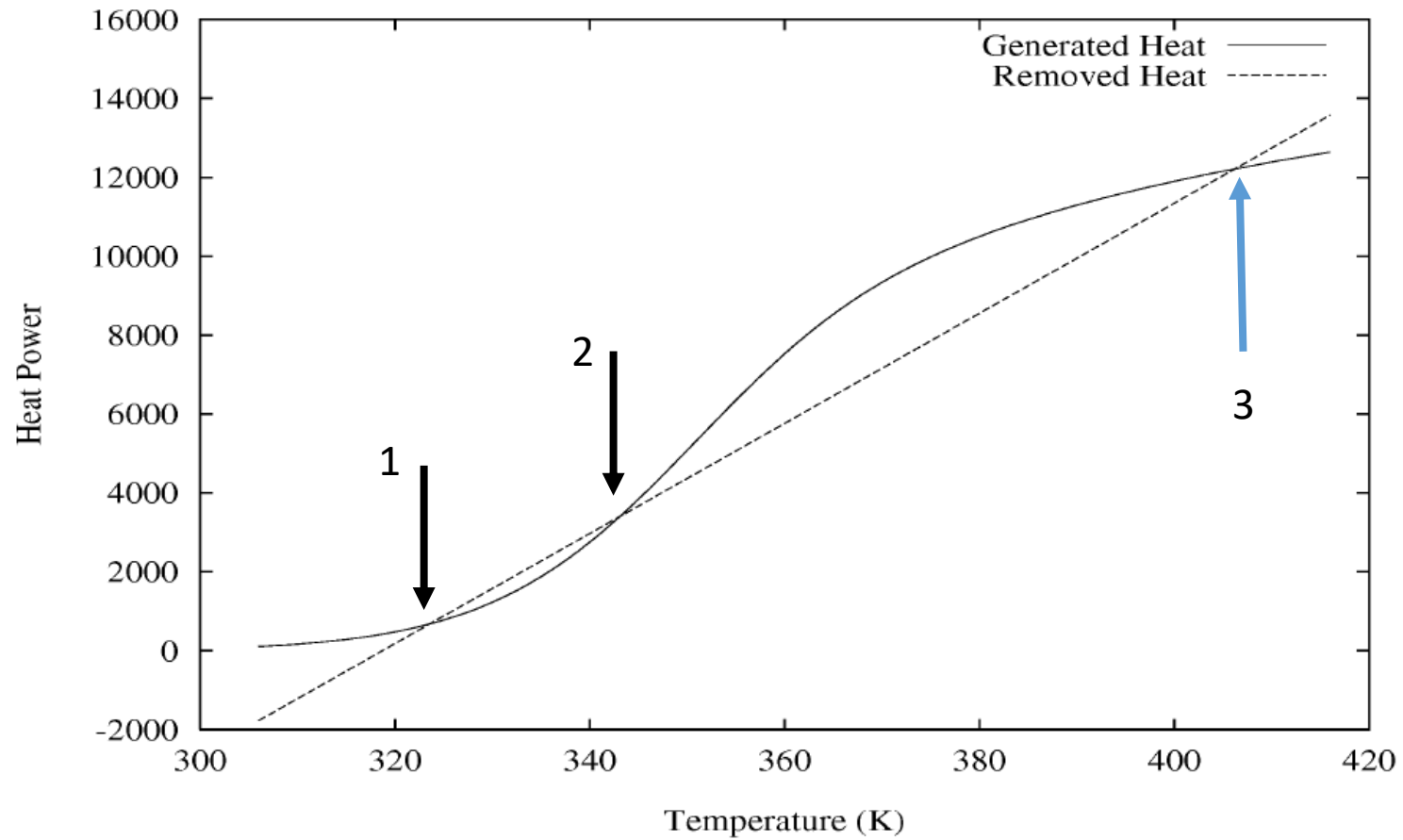The chain concentration of growing polymer is equal to

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

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