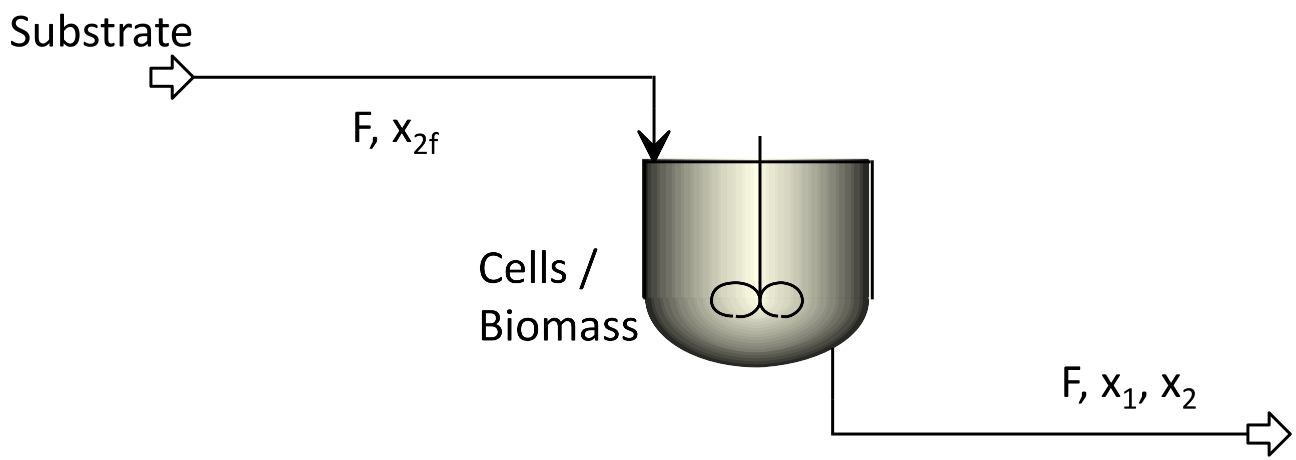
Process Dynamics & Control

Biochemical Reactor



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, $\mathrm{Y} = \frac{mass\ of\ cells\ produced}{mass\ of\ subsrtate\ consumed}$ 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: $\mu = \frac{\mu_{max}\, x_2}{k_m + x_2}$

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

Biochemical Reactor

Steady State equations:

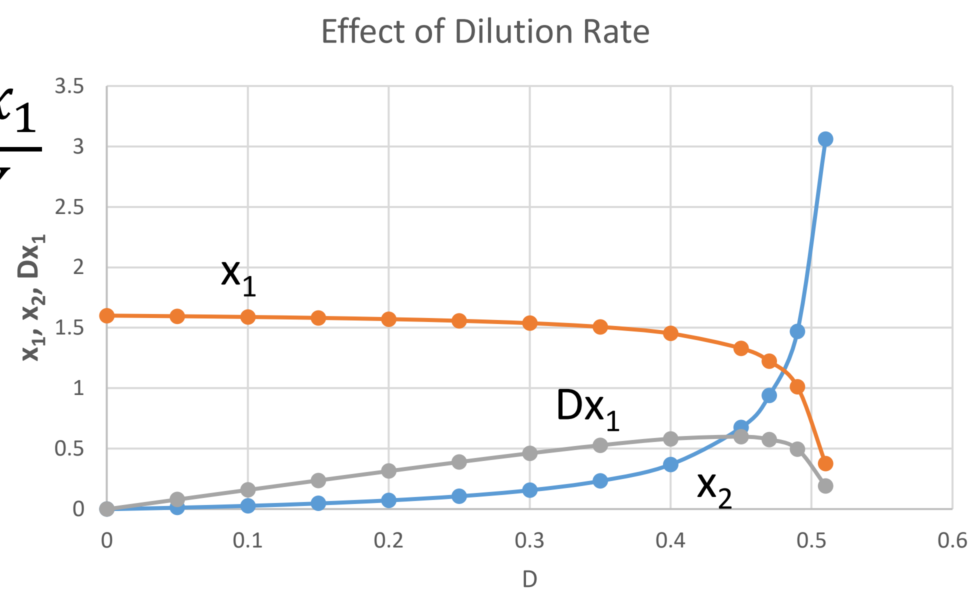
$$\frac{dx_1}{dt} = 0 = -\frac{F}{V}x_1 + \mu x_1 = (\mu - D)x_1 = (\frac{\mu_{max}\, x_2}{k_m + x_2} - D)x_1$$

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.



Biochemical Reactor

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

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

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

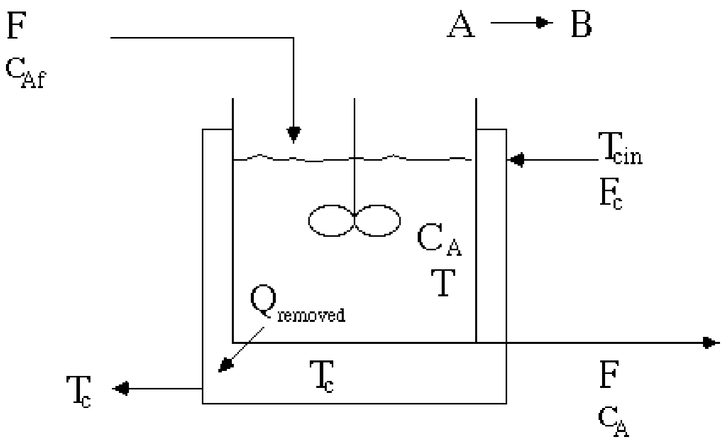
Or, $D^2\left(x_{2f} + k_m\right) - 2D\mu_{max}\left(x_{2f} + k_m\right) + x_{2f}\mu_{max}^2 = 0$

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



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

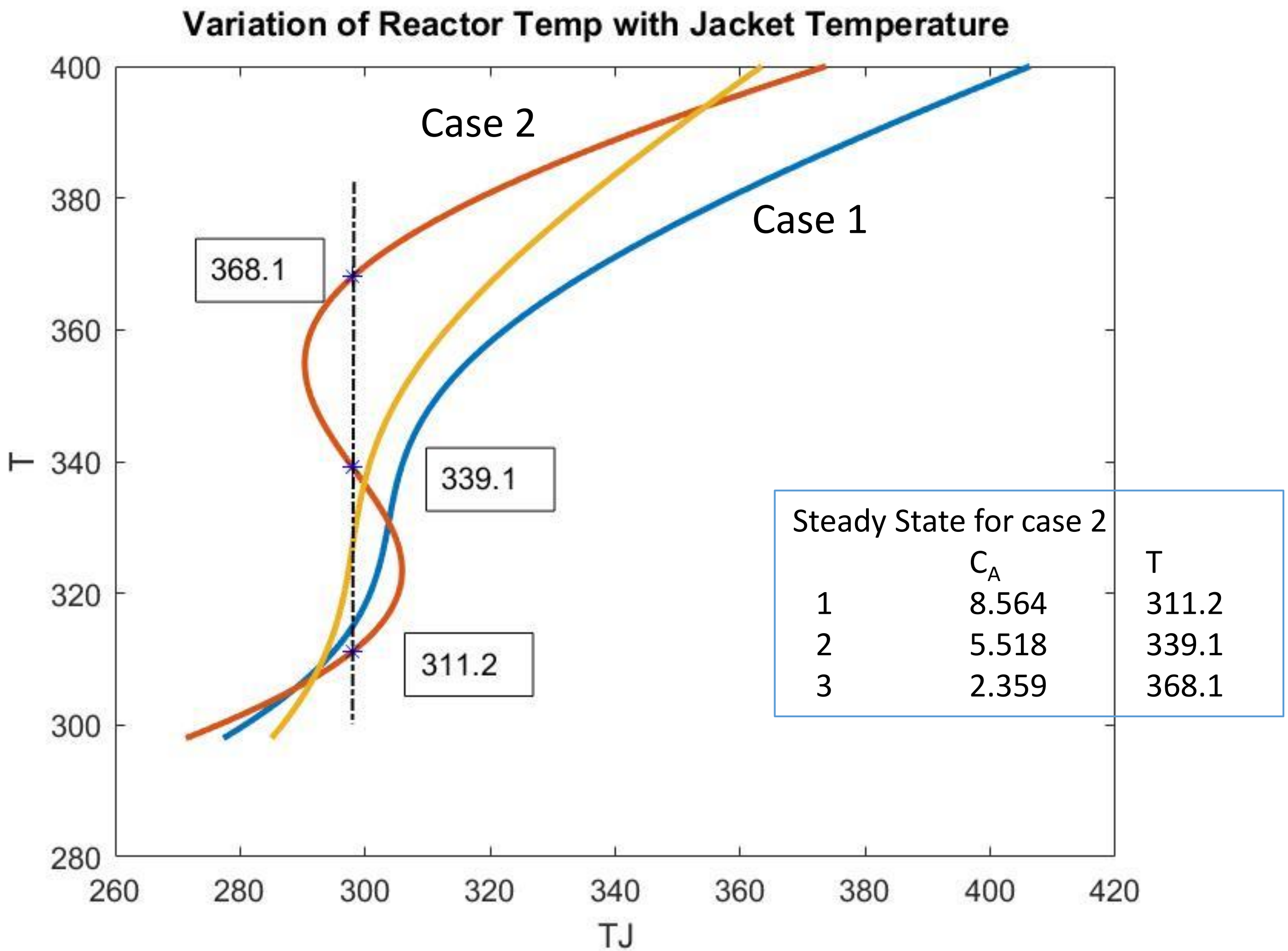
$$\frac{dT}{dt} = \frac{F}{V}\left(T_f - T\right) + \left(\frac{-\Delta H}{\rho C_p}\right)\mathrm{r} - \frac{\mathrm{UA}}{\mathrm{V}\rho C_p}(\mathrm{T} - \mathrm{T_C})$$

$$\frac{dT_c}{dt} = \frac{F_c}{V_c}(T_{ci} - T_c) + \frac{UA}{V_c \rho_c C_{pc}}(T - T_c)$$

Data:
F/V, hr^{-1} = 1;   E=11843 kcal/kgmol;
ρC_p=500; T_f = 25 ^{0}C ; C_{af} = 10,

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

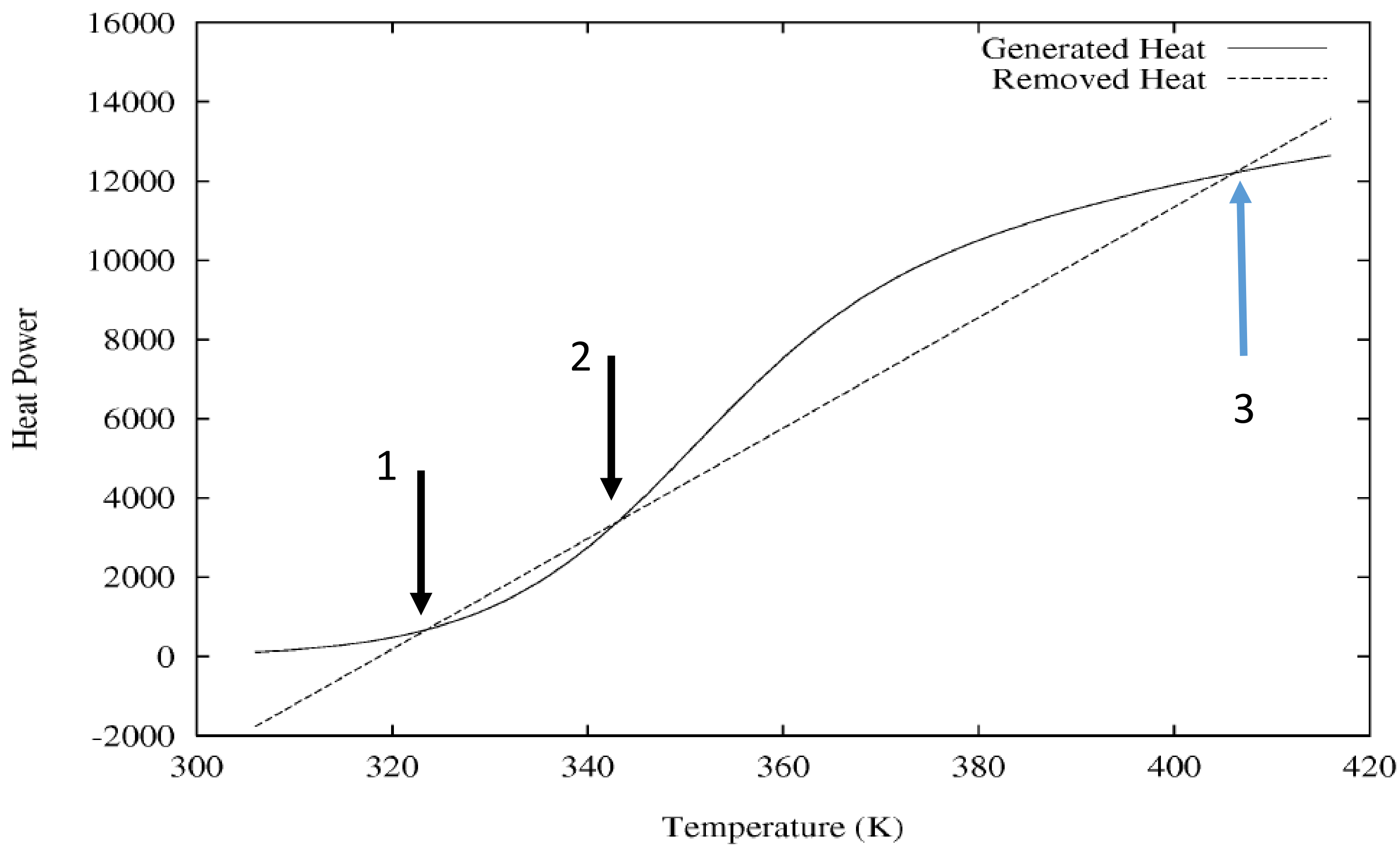
Case	k_0, 1/h	$(-\Delta H)$, kcal/kmol	UA/V
1	14825*3600	5215	250
2	9703*3600	5960	150
3	18194*3600	8195	750

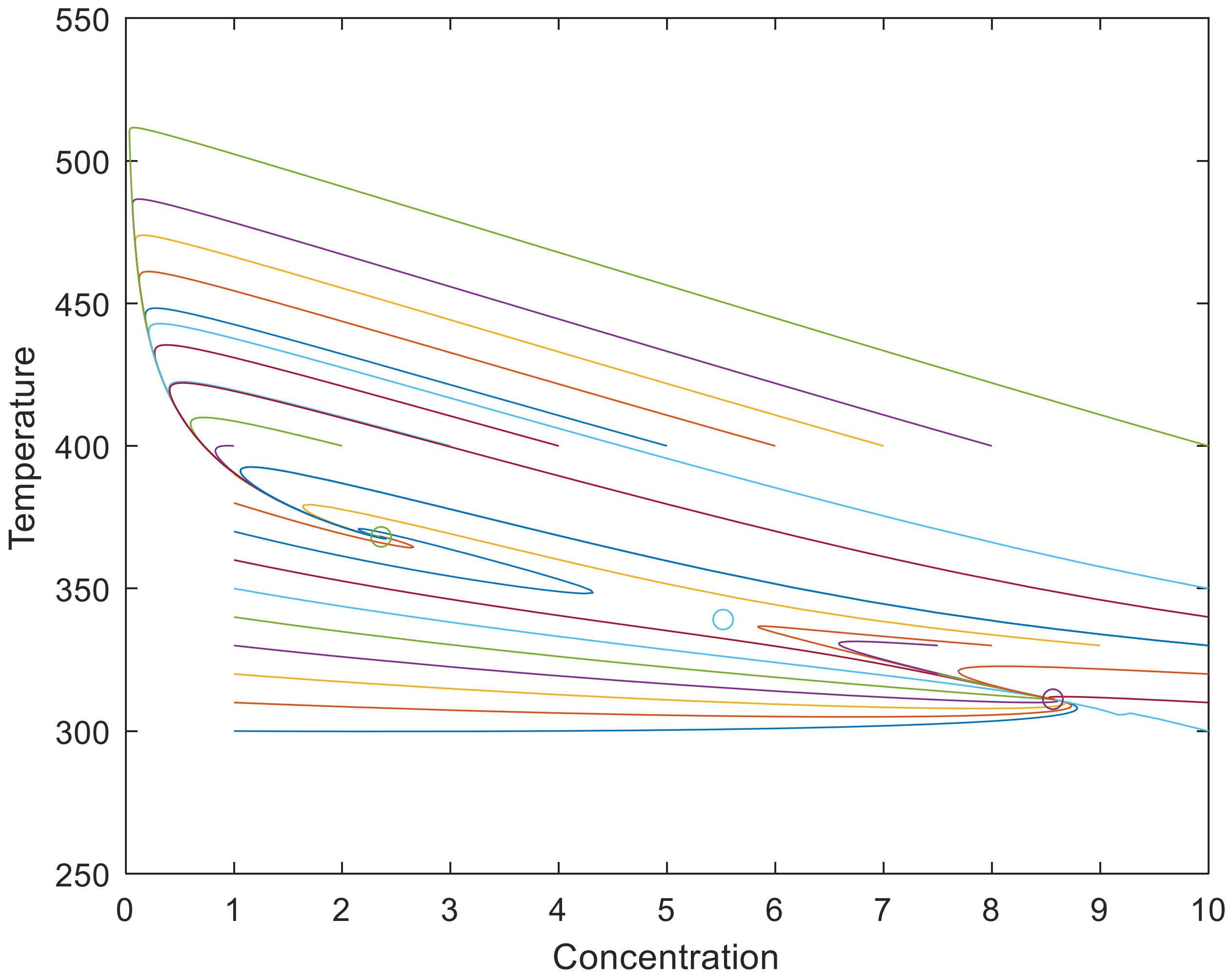


Steady State for case 2

	C_A	T
1	8.564	311.2
2	5.518	339.1
3	2.359	368.1

Steady State Heat Power vs Reactor Temperature





550
500
450
400
350
300
250
Temperature
0
1
2
3
4
5
6
7
8
9
10
Concentration

Developing Control Relevant Models

1. Develop dynamic model from 1st principles i.e,

$$\dot{x} = f(x,u) \quad \ldots(1)$$

2. Define control objective $y = h(x,u) \ldots\ldots(2)$

3. Rearrange equation (1) and (2) to get control-affine nonlinear state space form

$$\dot{x} = f(x) + g(x)u$$
$$y = h(x,u)$$

4. Linearize equation (1) and (2) around nominal values of x_s and u_s and form linear state space equation after subtracting steady state equation $f(x_{s,}\ u_s) = 0$; $h(x_{s,}\ u_s) = 0$

$$\dot{X} = AX + BU$$
$$Y = CX + DU$$

Developing Control Relevant Models

5. Derive transfer function model by taking Laplace transform of linear state space model:

$$Y(s) = G_P(s)M(s) + G_L(s)L(s)$$

6. Put s=jω and convert Laplace domain model to Frequency Domain transfer function model

$$Y(\omega) = G_P(\omega)M(\omega) + G_L(\omega)L(\omega)$$

7. Take inversion of Laplace domain transfer function model and get Convolution model

$$Y(t) = \int_0^t G_p(t-\tau)\,\mathrm{M}(\tau)d\tau + \int_0^t G_L(t-\tau)\,L\,(\tau)\mathrm{d\tau}$$

$$\dot{X} = AX + BU$$
$$Y = CX + DU$$

Taking Laplace Transform,

$$sX(s) = AX(s) + BU(s)$$
$$Y(s) = CX(s) + DU(s)$$

Or,

$$(sI - A)X(s) = BU(s); i.e, X(s) = (sI - A)^{-1}BU(s)$$

So,

$$Y(s) = [C(sI - A)^{-1}B + D]U(s)$$

Normally transfer function model is expressed in terms of process and disturbance transfer function. So, input variables U are partitioned to manipulated M and load/disturbance variable L i.e, U = [M L]

$$Y(s) = [C(sI - A)^{-1}B_M + D_M]M(s) + [C(sI - A)^{-1}B_L + D_L]L(s)$$

$$Y(s) = G_P(s)M(s) + G_L(s)L(s)$$

Dynamic model:

$$\dot{x} = f(x,u) \quad \ldots(1)$$
$$y = h(x,u) \ldots\ldots(2)$$

Using Taylor series approximation around (x^s , u^s) and neglecting HOT

$$\dot{x}_1 = f_1(x_1^s, x_2^s, \ldots\ldots. x_n^s, u_1^s, u_2^s, \ldots\ldots u_m^s) +$$

$$\frac{\partial f_1}{\partial x_1}(x_1 - x_1^s) + \frac{\partial f_1}{\partial x_2}(x_2 - x_2^s) + \ldots\ldots + \frac{\partial f_1}{\partial x_n}(x_n - x_n^s)$$

$$+ \frac{\partial f_1}{\partial u_1}(u_1 - u_1^s) + \frac{\partial f_1}{\partial u_2}(u - u_2^s) + \ldots\ldots + \frac{\partial f_1}{\partial u_m}(u_m - u_m^s)$$

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$$\dot{x}_n = f_n(x_1^s, x_2^s, \ldots\ldots. x_n^s, u_1^s, u_2^s, \ldots\ldots u_m^s) +$$

$$\frac{\partial f_n}{\partial x_1}(x_1 - x_1^s) + \frac{\partial f_n}{\partial x_2}(x_2 - x_2^s) + \ldots\ldots + \frac{\partial f_n}{\partial x_n}(x_n - x_n^s)$$

$$+ \frac{\partial f_n}{\partial u_1}(u_1 - u_1^s) + \frac{\partial f_n}{\partial u_2}(u - u_2^s) + \ldots\ldots + \frac{\partial f_n}{\partial u_m}(u_m - u_m^s)$$

Subtracting the steady state equations, we can write:

$$\begin{bmatrix} \dot{X}_1 \\ \dot{X}_2 \\ . \\ . \\ \dot{X}_n \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \cdots & \frac{\partial f_n}{\partial x_n} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ . \\ . \\ X_n \end{bmatrix} + \begin{bmatrix} \frac{\partial f_1}{\partial u_1} & \cdots & \frac{\partial f_1}{\partial u_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial u_1} & \cdots & \frac{\partial f_n}{\partial u_m} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ . \\ . \\ U_m \end{bmatrix}$$

i.e,

$$\dot{X} = AX + BU$$

Where,

A= $\begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \cdots & \frac{\partial f_n}{\partial x_n} \end{bmatrix}$ $a_{ij} = \frac{\partial f_i}{\partial x_j}$ *and B =* $\begin{bmatrix} \frac{\partial f_1}{\partial u_1} & \cdots & \frac{\partial f_1}{\partial u_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial u_1} & \cdots & \frac{\partial f_n}{\partial u_m} \end{bmatrix}$ $b_{ij} = \frac{\partial f_i}{\partial u_j}$

Similarly for equation (2),

$$y_1 = h_1(x_1^s, x_2^s, \dots \dots . x_n^s, u_1^s, u_2^s, \dots . . u_m^s) +$$

$$\frac{\partial h_1}{\partial x_1}(x_1 - x_1^s) + \frac{\partial h_1}{\partial x_2}(x_2 - x_2^s) + \dots \dots + \frac{\partial h_1}{\partial x_n}(x_n - x_n^s)$$

$$+ \frac{\partial h_1}{\partial u_1}(u_1 - u_1^s) + \frac{\partial h_1}{\partial u_2}(u - u_2^s) + \dots \dots + \frac{\partial h_1}{\partial u_m}(u_m - u_m^s)$$

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$$y_p = h_p(x_1^s, x_2^s, \dots \dots . x_n^s, u_1^s, u_2^s, \dots . . u_m^s) +$$

$$\frac{\partial h_p}{\partial x_1}(x_1 - x_1^s) + \frac{\partial h_p}{\partial x_2}(x_2 - x_2^s) + \dots \dots + \frac{\partial h_p}{\partial x_n}(x_n - x_n^s)$$

$$+ \frac{\partial h_p}{\partial u_1}(u_1 - u_1^s) + \frac{\partial h_p}{\partial u_2}(u - u_2^s) + \dots \dots + \frac{\partial h_p}{\partial u_m}(u_m - u_m^s)$$

Subtracting the steady state equations, we can write:

$$\begin{bmatrix} Y_1 \\ Y_2 \\ . \\ . \\ Y_p \end{bmatrix} = \begin{bmatrix} \frac{\partial h_1}{\partial x_1} & \cdots & \frac{\partial h_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial h_p}{\partial x_1} & \cdots & \frac{\partial h_p}{\partial x_n} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ . \\ . \\ X_n \end{bmatrix} + \begin{bmatrix} \frac{\partial h_1}{\partial u_1} & \cdots & \frac{\partial h_1}{\partial u_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial h_p}{\partial u_1} & \cdots & \frac{\partial h_p}{\partial u_m} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ . \\ . \\ U_m \end{bmatrix}$$

i.e,

$$Y = CX + DU$$

Where,

C= $\begin{bmatrix} \frac{\partial h_1}{\partial x_1} & \cdots & \frac{\partial h_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial h_p}{\partial x_1} & \cdots & \frac{\partial h_p}{\partial x_n} \end{bmatrix}$ $c_{ij} = \frac{\partial h_i}{\partial x_j}$ *and D =* $\begin{bmatrix} \frac{\partial h_1}{\partial u_1} & \cdots & \frac{\partial h_1}{\partial u_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial h_p}{\partial u_1} & \cdots & \frac{\partial h_p}{\partial u_m} \end{bmatrix}$ $d_{ij} = \frac{\partial h_i}{\partial u_j}$

Example: Van De Vusse Reactor

Dynamic Model:

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

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

Non-linear state space model:

States are : $x_1 = C_A$, $x_2 = C_B$ input : u = F/V and output $y = C_B$

State equation:

$$\frac{dx_1}{dt} = (-k_1 x_1 - k_3 x_1^2) + \left(x_{1f} - x_1\right) u$$

$$\frac{dx_2}{dt} = k_1 x_1 - k_2 x_2 + (-x_2) u$$

i.e, $\dot{x} = \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{Bmatrix} (-k_1 x_1 - k_3 x_1^2) \\ k_1 x_1 - k_2 x_2 \end{Bmatrix} + \begin{Bmatrix} \left(x_{1f} - x_1\right) \\ (-x_2) \end{Bmatrix} \mathrm{u} = \mathrm{f(x) + g(x)u}$

Output map: $y = h(x) = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$

Example: Van De Vusse Reactor

Linear State Space Model:

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

$$f_2(C_A, C_B, {}^F/_V) = -\frac{F}{V} C_B + k_1 C_A \; - k_2 C_B$$

Let, $\quad X_1 = C_A - C_A^s \; ; \;\; X_2 = C_B - C_B^s ; U = \frac{F}{V} - \frac{F^s}{V}$

$$A = \begin{bmatrix} \frac{\partial f_1}{\partial C_A} & \frac{\partial f_1}{\partial C_B} \\ \frac{\partial f_2}{\partial C_A} & \frac{\partial f_2}{\partial C_B} \end{bmatrix} = \begin{bmatrix} -{}^{F^s}/_V - k_1 - 2k_3 C_A^s & 0 \\ k_1 & -{}^{F^s}/_V - k_2 \end{bmatrix}$$

$$B = \begin{bmatrix} \frac{\partial f_1}{\partial (\frac{F}{V})} \\ \frac{\partial f_2}{\partial (\frac{F}{V})} \end{bmatrix} = \begin{bmatrix} C_{Af} - C_A^s \\ -C_B^s \end{bmatrix} \qquad C = [0 \quad 1] \quad D = 0$$

$$\dot{X} = AX + BU$$

$$Y = CX + DU$$

Example: Van De Vusse Reactor

Transfer Domain Model -- Laplace Domain:

$$Y(s) = [C(sI - A)^{-1}B + D]U(s) = [C(sI - A)^{-1}B]U(s)$$

$$sI - A = \begin{bmatrix} s + {F^s}/{V} + k_1 + 2k_3C_A^s & 0 \\ -k_1 & s + {F^s}/{V} + k_2 \end{bmatrix} = \begin{bmatrix} s - a_{11} & -a_{12} \\ -a_{21} & s - a_{22} \end{bmatrix}$$

$$(sI - A)^{-1} = \frac{1}{det}\begin{bmatrix} s - a_{22} & a_{12} \\ a_{21} & s - a_{11} \end{bmatrix}$$

where, $det = (s - a_{11})(s - a_{22}) - a_{12}a_{21}$

$$C(sI - A)^{-1} = [0 \quad 1]\frac{1}{det}\begin{bmatrix} s - a_{22} & a_{12} \\ a_{21} & s - a_{11} \end{bmatrix} = \frac{1}{det}[a_{21} \quad s - a_{11}]$$

$$C(sI - A)^{-1}\mathrm{B} = \frac{1}{det}[a_{21} \quad s - a_{11}]\begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \frac{a_{21}b_1 + (s - a_{11})b_2}{(s - a_{11})(s - a_{22}) - a_{12}a_{21}}$$

Example: Van De Vusse Reactor

Transfer Domain Model -- Laplace Domain:

$$C(sI - A)^{-1}\mathrm{B} = \frac{a_{21}b_1 + (s - a_{11})b_2}{(s - a_{11})(s - a_{22}) - a_{12}a_{21}}$$

$$= \frac{k_1\left(C_{Af} - C_A^s\right) - C_B^s s - C_B^s\left({F^s}/{V} + k_1 + 2k_3C_A^s\right)}{(s + {F^s}/{V} + k_1 + 2k_3C_A^s)(s + {F^s}/{V} + k_2)}$$

$$= \frac{-C_B^s s + [k_1\left(C_{Af} - C_A^s\right) - C_B^s\left({F^s}/{V} + k_1 + 2k_3C_A^s\right)]}{(s + {F^s}/{V} + k_1 + 2k_3C_A^s)(s + {F^s}/{V} + k_2)}$$