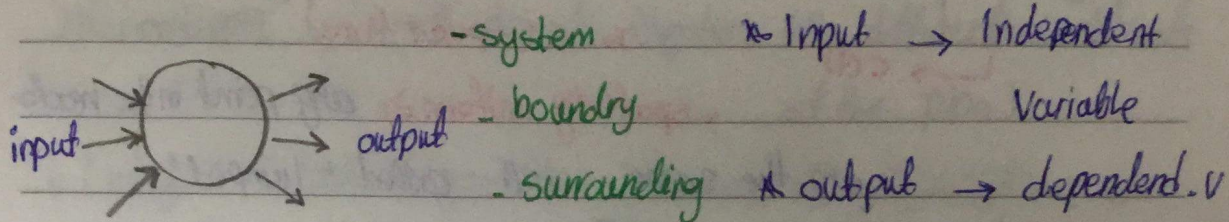


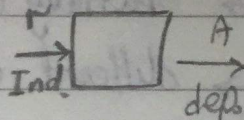
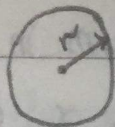
* Simulation.

1/2/2018

* Model (system):



* Circle:



* state of the goal $\Rightarrow$ Analytical OR technical goal

* boundary $\Rightarrow$ - Imaginary - Real.

* Modeling:

- Discription

- formulation $\Rightarrow$ (we need to write equation (mathematical))

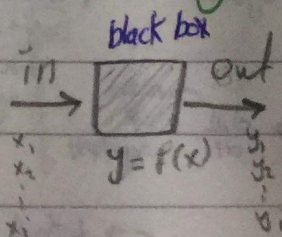
- DOF $\Rightarrow$ Degree of freedom Analogs

- Solution $\Rightarrow$ Optimization (Mathematical model + other)

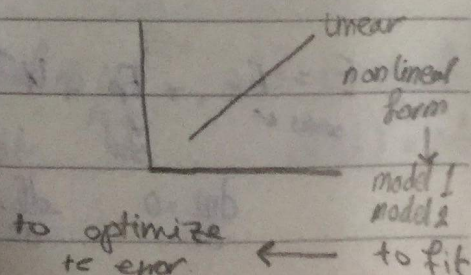
Relationships

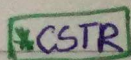
* Empirical modeling:

process modeling $\left\{ \begin{array}{l} \text{Fundamental} \rightarrow (\text{rigorous, theoretical}) \\ \text{Empirical} \rightarrow (\text{depends on experimental data}) \end{array} \right.$



Box possible data
out given in
 n data point

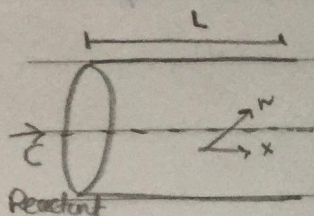




Not Steady state

* C (space time) position

* spatially uniform $\Rightarrow$ any point in the reactor same, will called "lumped"



* PFR

$c \rightarrow$ spatially uniform in r

$c \rightarrow$ different with x (distribution)

c (space time)

- * Empirical

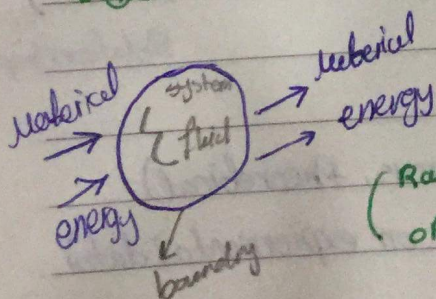
* Fundamental modeling

lumped
distributed

distribution $\Rightarrow$ under unsteady
state (Accumulated rate $\neq 0$)

* **lumped** : Algebraic equation

* distribution = Dof (unstable in $\frac{C}{D}$ order) $\rightarrow$ under 6.5



* Balance equation (Instantaneous modeling)

$$\left(\begin{array}{c} \text{Rate of mass} \\ \text{OR energy IN} \\ \text{To system} \end{array} \right) - \left(\begin{array}{c} \text{Rate of mass} \\ \text{or energy out} \\ \text{of system} \end{array} \right) = \left(\begin{array}{c} \text{Rate of mass} \\ \text{or energy} \\ \text{accumulation} \\ \text{with in} \end{array} \right)$$

$$E = E_K + E_p + U \rightarrow \text{instantaneous}$$

mass $\rightarrow \frac{dm}{dt}$ $\rightarrow$ mass of system

$$\frac{dm}{dt} = 0 \quad \frac{dE}{dt} = 0$$

energy $\rightarrow \frac{dE}{dt}$ $\rightarrow$ total energy of system

Simulation.

Macroscopic $\rightarrow$ tank full with water.

Microscopic $\rightarrow$ small elements (system like differential elements of the pipe)

* Integral balance approach:

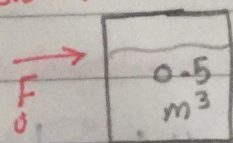
* Instantaneous balance approach

* Integral Approach:-

$$\left[\begin{array}{l} \text{mass or energy INTO} \\ \text{system from } t \text{ to } t+\Delta t \end{array} \right] - \left[\begin{array}{l} \text{mass or energy out} \\ \text{of system from } t \text{ to } t+\Delta t \end{array} \right] =$$

$$\left[\begin{array}{l} M \text{ or } E \text{ within} \\ \text{the system at } t+\Delta t \end{array} \right] - \left[\begin{array}{l} M \text{ or } E \text{ within} \\ \text{the system at } t \end{array} \right]$$

0.5 m³/hr



after 2 hr

$$2 \times 0.5 = 1 \text{ m}^3$$

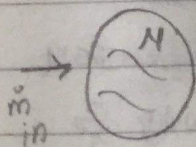
0.1 m³/hr

$$0.1 \times 2 = 0.2 \text{ m}^3$$

$$\Rightarrow 1 \text{ m}^3 - 0.2 = 0.8 \text{ m}^3$$

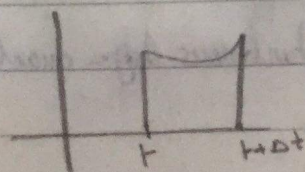
$$0.5 + 0.8 = 1.3 \text{ m}^3$$

Accumulation of mass.



$$\int_t^{t+\Delta t} \dot{m}_{in}(t) dt - \int_t^{t+\Delta t} \dot{m}_{out}(t) dt = M \Big|_{t+\Delta t} - M \Big|_t$$

$$\int_t^{t+\Delta t} (\dot{m}_{in} - \dot{m}_{out}) dt = M \Big|_{t+\Delta t} - M \Big|_t$$



$\Rightarrow$ if not constant $\dot{m}(t)$
 $\int_t^{t+\Delta t} \dot{m}(t) dt$

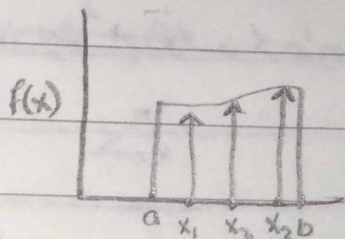
$\Rightarrow$ if constant $\dot{m}(t) \cdot \Delta t$

$t + \Delta t$

$$\int_t^{t+\Delta t} (\dot{m}_{in} - \dot{m}_{out}) dt = ??$$

* Remark 1:-

- Mean Value Theorem of Integral $f(t)$



$$\text{Area} = \int_a^b f(x) dx$$

Mean $f(b-a) = \text{Area}$.

$$\int_a^b f(x) dx = f(b-a) \cdot (b-a), \quad \bar{f} = \frac{1}{b-a} \int_a^b f(x) dx$$

* $c_p \rightarrow T \in [a, b]$

$$\bar{c}_p = \frac{1}{b-a} \int_a^b c_p(T) dT$$

So, $\int_t^{t+\Delta t} (\dot{m}_{in} - \dot{m}_{out}) dt = (\dot{m}_{in} - \dot{m}_{out}) \cdot \Delta t = M \Big|_t^{t+\Delta t}$

$$(\dot{m}_{in} - \dot{m}_{out}) = \frac{M \Big|_t^{t+\Delta t}}{\Delta t} = \frac{\Delta M}{\Delta t}$$

$\Delta t \rightarrow 0$ quantity given Avg

if $\Delta t \rightarrow 0 \Rightarrow \frac{\Delta M}{\Delta t} = \frac{dM}{dt}$

$\frac{dM}{dt} = \dot{m}_{in} - \dot{m}_{out} \rightarrow$ In Instantaneous Avg = quantity

in out $\rightarrow \dot{V} \rightarrow \dot{m}$
system $\rightarrow M \rightarrow V$

$p_{in} p_{out} \rightarrow$ Isothermal.

$$\dot{m} = \rho \dot{V}$$

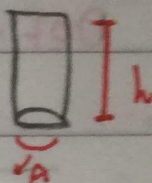
$$M = \rho V$$

$$\rho \dot{V}_{in} - \rho \dot{V}_{out} = \frac{d(\rho V)}{dt}$$

$$\dot{V}_{in} - \dot{V}_{out} = \frac{dV}{dt} \rightarrow \text{geometry}$$

$$V = A h(t)$$

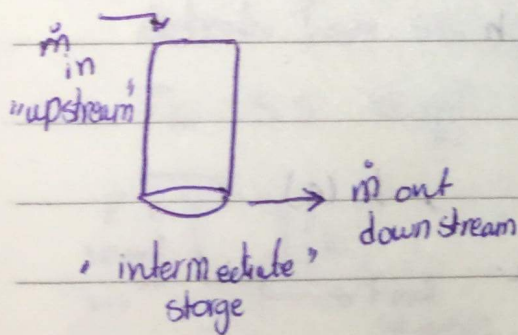
$\downarrow$ constant $\downarrow$ variable
 $\downarrow$
 $A \frac{dh}{dt}$



* Variable 8

- state variable $\rightarrow h = f(V_{in}, V_{out})$
input output
- Input - Output.

* Instantaneous (differential) modeling:



$$\rho \frac{dV}{dt} = m_{in} - m_{out}$$

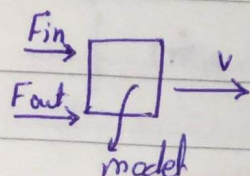
$\rightarrow$ Accumulate in up stream
 down

eq. (1) $\Rightarrow \rho \frac{dV}{dt} = \rho F_{in} - \rho F_{out}$

$$\frac{dV}{dt} = F_{in} - F_{out}$$

$V \rightarrow$ state variable

$F_{in}, F_{out} \rightarrow$ Input variable



$$\frac{dv}{dt} = F_{in} - F_{out} \Rightarrow \text{ODE}$$

So, I need Initial $\&$ condition
 "select input variable"

$$\text{DoF} = \# \text{ of eq. (1)}$$

$$\# \text{ of variable } [v / F_{in} / F_{out}] = 3$$

$$\text{DoF} = 2$$

$\xrightarrow{F_{in}, F_{out}}$
~~depend~~ variable v
 state variable

$$F_{in}(t), F_{out}(t), v(t)$$

$$F_{in} = f(t), \quad F_{out} = f(t)$$

* specific geometry of tank:

spherical

cylindrical

$$V = Ah$$

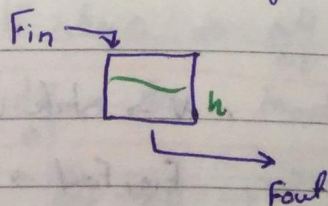
$$\frac{Ad}{h(t)}$$



$$A \frac{dh}{dt} = F_{in} - F_{out}, \quad h(t)$$

$A \rightarrow$ cross sectional Area

$\rho \rightarrow$ density



$$F_{out} \propto h \quad (\text{level of tank})$$

$$x, y, y = f(x)$$

$$y = ax + b$$

$$F_{out} = Bh(t) \rightarrow \text{linear, in reality} \quad F_{out} = B\sqrt{h(t)}$$

$$F_{out} \propto \sqrt{h(t)}$$

$$A \frac{dh(t)}{dt} = F_{in}(t) - Bh(t)$$

$$A \frac{dh(t)}{dt} + Bh(t) = F_{in}(t)$$

→ linear ODE. i.e. $h(0)$

* non linear → $F_{out} \propto \sqrt{h}$

$$A \frac{dh(t)}{dt} + B\sqrt{h(t)} = F_{in}(t)$$

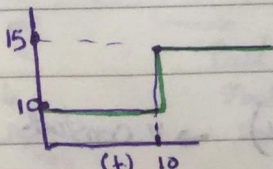
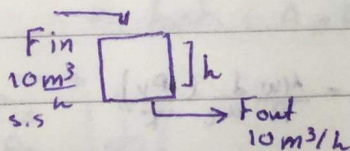
* need to specify $F_{in}(t)$ at S.S level (h) constant

$$F_{in} = F_{out}$$

* time of change:

distrib. from S.S

$$F_{in} \text{ S.S } 10 \frac{m^3}{h} \rightarrow 15 \frac{m^3}{h}$$

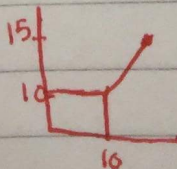


time of change when change system

$$(\text{step change}) \rightarrow F_{in}(t) = \begin{cases} 10 \frac{m^3}{h} & t \leq 0 \\ 15 \frac{m^3}{h} & t \geq 0 \end{cases}$$

$$A \frac{dh}{dt} + B\sqrt{h(t)} = F_{in}(t)$$

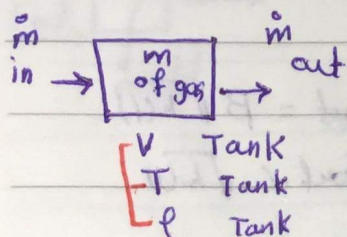
$$A \frac{dh}{dt} + B\sqrt{h(t)} = 15$$



$$F_{in} = \alpha t + \gamma$$

$$F_{in} = \gamma = F_{in} \text{ at S.S} = 10$$

*
gas intermediate storage tank:



⇒ overall material balance:-

$$\dot{m}_{in} - \dot{m}_{out} = \frac{d}{dt} (mg)$$

n moles,

$$m = n \frac{M_w}{\text{mol} \cdot \text{kg/mol}}$$

$$M_w n_{in} - M_w n_{out} = \frac{d}{dt} (mg)$$

gas behavior $\rightarrow$ ideal
 $\rightarrow$ non ideal.

→ Assume ideal behavior:

$$PV = nRT$$

$$PV = \frac{mg}{M_w} RT$$

$$mg = \frac{M_w PV}{RT} \quad \dots **$$

$$M_w n_{in} - M_w n_{out} = \frac{d}{dt} \left(\frac{M_w PV}{RT} \right) = \frac{M_w}{R} \frac{d}{dt} \left(\frac{PV}{T} \right)$$

→ assumptions:-

① $V \rightarrow$ constant

$$M_w n_{in} - M_w n_{out} = \frac{d}{dt} \left(\frac{M_w PV}{RT} \right) \rightarrow V \text{ constant}$$

$$\Rightarrow \frac{VM_w}{R} \frac{d}{dt} \left(\frac{P}{T} \right)$$

② isothermal (T constant)

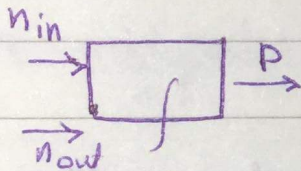
$$\frac{M_w V}{R T} \frac{dp}{dt} = M_w n_{in} - m_w n_{out}$$

$$\left[\frac{dp}{dt} = \frac{R T}{V} (n_{in} - n_{out}) \right]$$

→ P state variable p(t)

n_{in} , n_{out} , input variable.

T, V, R, Parameters.



$$\frac{dp}{dt} = \frac{R T}{V} (n_{in} - n_{out})$$

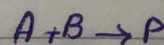
$$\underline{i.c} = \frac{R T}{V} (n_{in} - n_{out}), \underline{i.c} p(0)$$

Dof $\Rightarrow P, n_{in}, n_{out} \rightarrow 3 - 1 \text{ (eq)} = 2$ ① n_{in}, n_{out}
② Initial condition

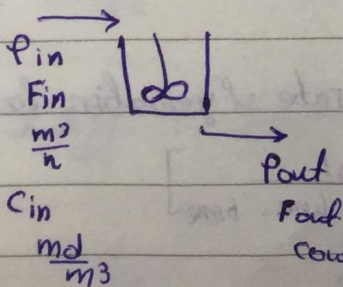
material + energy
balance not enough.

③

ex isothermal chemical Reaction.



Reactants: A + B, Product: P



$$F_c = \left[\frac{m^3}{n} \cdot \frac{mol}{m^3} \right] = \frac{mol}{hr}$$

* Rxn irreversible

* T is constant 'not need energy balance'

* perfectly mixing

C (space, time) ← in general

C (time) depend only time
"perfect mix."

① overall MB:

$$\frac{dM}{dt} = \dot{m}_{in} - \dot{m}_{out}$$

$\rho \rightarrow$ "density" function of concentration.

Assume ρ is not function of concentration

$$\rho = aC + b$$

$$M = \rho V$$

$$\left[\frac{dV}{dt} \rho = \dot{F}_{in} - \dot{F}_{out} \right] \dots \textcircled{1}$$

$$\frac{dM}{dt} = \dot{m}_{in} + \text{rate of generation} - \dot{m}_{out} - \text{rate of consumption}$$

$$\frac{dM}{dt} = \dot{m}_{in} - \dot{m}_{out} \quad * \text{Total mass in-out}$$

$$* C_0 V = \text{mol}$$

$\frac{\text{mol}}{\text{m}^3} \cdot \text{m}^3$

consump. or generation

For (A)

$$\left[\frac{d(VCA)}{dt} = \dot{F}_{in} C_{A0} - \dot{F}_{out} C_A - \dot{r}_A \right] \dots \textcircled{2}$$

$$\left[\frac{d(VCB)}{dt} = \dot{F}_{in} C_{B0} - \dot{F}_{out} C_B - \dot{r}_B \right] \dots \textcircled{3} \quad \text{rate of consumption for B mol/time}$$

$$\left[\frac{d(VCA)}{dt} = \dot{F}_{in} C_{P0} - \dot{F}_{out} C_P + \dot{r}_P \right] \dots \textcircled{4} \quad \text{rate of generation for P}$$

$\dot{r}$ rate of reaction $\left[\frac{\text{mol}}{\text{volume} \cdot \text{time}} \right]$

$$r_V = \left[\frac{\text{mol}}{\text{V} \cdot \text{time}} \right] \cdot V = \frac{\text{mol}}{\text{time}}$$

$$\dot{r}_A = r_A V$$

$$\dot{r}_B = r_B V$$

$$\dot{r}_P = r_P V$$

11/2/2018

simulation.

$$\frac{dv}{dt} = F_{in} - F \quad \text{--- (1)} \quad [\text{assume } C_{p0} = 0]$$

$$A: \frac{d(VCA)}{dt} = F_{in} C_{A0} - F C_A - V r_A \quad \text{--- (2)}$$

$$B: \frac{d(VCB)}{dt} = F_{in} C_{B0} - F C_B - V r_B \quad \text{--- (3)}$$

$$P: \frac{d(VCP)}{dt} = F_{in} C_{p0} - F C_p - V r_p \quad \text{--- (4)}$$

$$\begin{aligned} \frac{d(VCA)}{dt} &= V \frac{dC_A}{dt} + C_A \frac{dV}{dt} \quad \text{From eq. (1)} \\ &= V \frac{dC_A}{dt} + C_A (F_{in} - F) \quad \text{--- (5)} \end{aligned}$$

$$V \frac{dC_A}{dt} + \cancel{C_A (F_{in} - F)} = F_{in} C_{A0} - \cancel{F C_A} - V r_A$$

$$V \frac{dC_A}{dt} = F_{in} (C_{A0} - C_A) - V r_A$$

$$V \frac{dC_B}{dt} = F_{in} (C_{B0} - C_B) - V r_B$$

$$V \frac{dC_p}{dt} = -F_{in} C_p + V r_p$$

$$\frac{dv}{dt} = F_{in} - F$$

→ 4 state variables

 V, C_A, C_B, C_p

→ initial condition

$$\begin{aligned} V(0) &= V(t=0) & C_A(0) &= C_{A0} \\ C_B(0) &= C_B(t=0) & C_p(0) &= 0 \end{aligned}$$

→ input variables

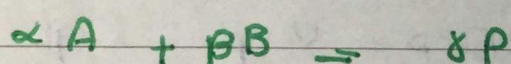
 C_{A0}, C_{B0}, F_{in}

variables $\Rightarrow F, F_{in}, V, C_A, C_B, C_P, C_{A_0}, C_{B_0}$
 r_A, r_B, r_P

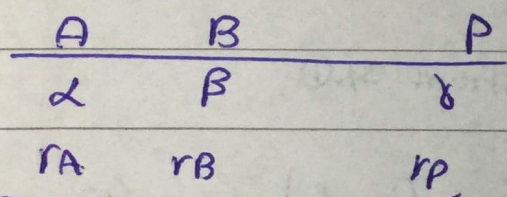
need to know $\rightarrow r_B, r_A, r_P$ kinetics.

Reaction $\rightarrow$ irreversible

Stoich. Eqn



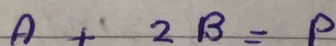
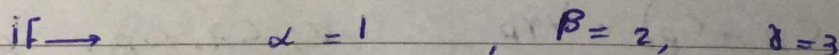
$[\alpha, \beta, \gamma]$ stoichiometry



$$r_B = \left(\frac{\beta}{\alpha}\right) r_A \quad r_P = \left(\frac{\gamma}{\alpha}\right) r_A$$

* need expression of r_A

$$r_A = f(C_A, C_B) \text{ of reactants} \quad - \quad r_A = \frac{\text{mol of A}}{V-t}$$



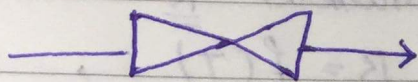
rate = 2nd order in $(C_A \times C_B)$

$$r_A = k C_A C_B$$

$$r_B = 2 k C_A C_B$$

$$r_P = k C_A C_B$$

flow through valves :-



$$F = C_v f(x) \sqrt{\frac{\Delta P}{S \cdot G}}$$

$F \Rightarrow$ Volumetric flow rate

$C_v \Rightarrow$ valve coefficient

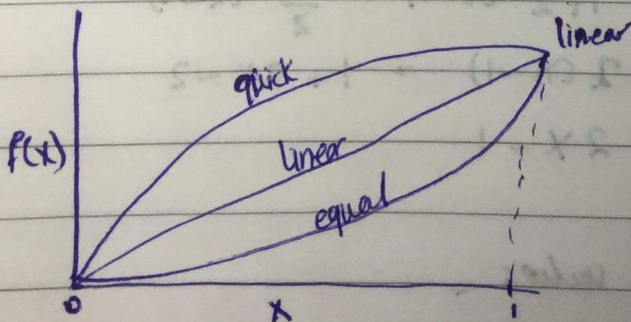
$f(x) \Rightarrow$ flow characteristic

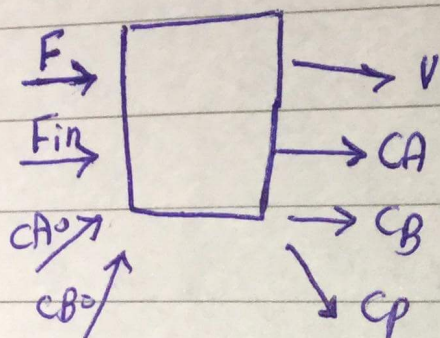
$x \Rightarrow$ valve opening

$\Delta P \Rightarrow$ pressure drop

$SG \Rightarrow$ specific gravity, $SG = \frac{\rho}{\rho_{ref}}$

$$f(x) = \begin{cases} x & \text{linear} \\ \sqrt{x} & \text{quick opening} \\ x-1 & \text{equal percentage valve} \end{cases}$$





parameter K

$$K = f(T)$$

Function of Temperature

$$K = K_0 e^{-E/RT}$$

not linear eq., on graph is linear. $\left[\ln K = \ln K - \frac{E}{R_T} \right]$

Draw $\ln K$ vs. $\frac{1}{T}$, slope = E/R .

* Linearization.

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2}(x - x_0)^2$$

$$f(x) = x^2 \quad , \quad x_0 = 1$$

$$f'(x) = 2x \quad , \quad f''(x) = 2$$

$$f' \Big|_{x_0} = 2 \quad , \quad f'' \Big|_{x_0} = 2 \quad f(x_0 = 1) = 1$$

$$f(x) = x^2 = 1 + 2(x - 1) + \frac{2}{2}(x - 1)^2$$

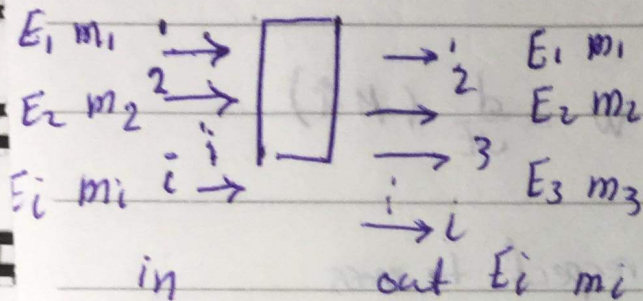
$$x^2 = 1 + 2(x - 1) = 1 + 2x - 2 = 2x - 1$$

* Flow through valves

13/2/2018

⇒ Simulation.

Energy balance :-



$\sum E_i$

$\sum E_i$

$$\text{Rate of energy accumulation} = \left[\begin{array}{c} \text{Rate of} \\ E \\ \text{by} \\ \text{convection} \end{array} \right] - \left[\begin{array}{c} \text{Rate of} \\ E \text{ out} \\ \text{by stream} \end{array} \right]$$

$$+ \left[\begin{array}{c} \text{Net rate of} \\ \text{Heat in sys} \\ \text{from surrounding} \end{array} \right] + \left[\begin{array}{c} \text{Net Rate of} \\ \text{work} \\ \text{performed by} \\ \text{surrounding in} \\ \text{system} \end{array} \right]$$

$$U = m \hat{U}$$

$$[J] = [kg] [\hat{U}/kg]$$

$$E = \dot{E}_K + \dot{E}_P + \dot{U}$$

$$= \frac{1}{2} \dot{m} v^2 + \dot{m} g z + \dot{U}$$

Go to eq. ① in principle ① CH-7

$$\Delta \dot{E} = \Delta \dot{H} + \Delta \dot{E}_K + \Delta \dot{E}_P = \frac{d}{dt} (\text{energy with system})$$

$$\Delta H = \sum m_j \hat{H}_j - \sum m_j \hat{H}_j^?$$

$$\sum m_i \hat{H}_i = \sum m_i H_i + Q + \dot{W} = \frac{d}{dt} (U)$$

$$\sum_i \dot{m}_i \hat{H}_i = \sum \dot{m}_i H_i + Q + W = \frac{d}{dt} (MA)$$

⇒ if system at steady state with respect to mass

$$\sum \dot{m}_e = \sum \dot{m}_i = \frac{d}{dt} (M_{\text{tot}})$$

$$\sum m_i \hat{H}_i = \sum m_i \hat{H}_i + Q + \dot{W} = M \frac{d\hat{u}}{dt}$$

in mixture ⇒ $\hat{H}_{\text{mixture}} = f(x_i, T, P)$

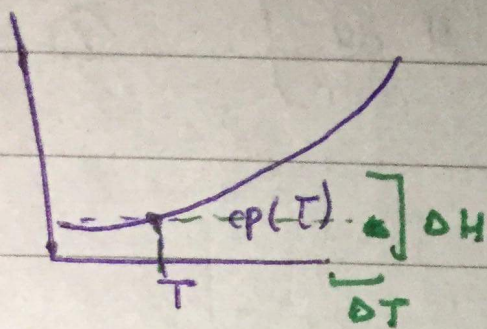
in pure component ⇒ $\hat{H}_{\text{pure comp}} = f(T, P) = \hat{H}_j$

$x_i \rightarrow$ is mass fraction of i

$$\sum x_i = 1$$

$$\hat{H}_{\text{mix}} = \sum x_j \hat{H}_j \quad \text{أو صيغة بـ } m_j$$

$$\begin{aligned} m \hat{H}_{\text{mix}} &= m \left(\sum x_j \hat{H}_j \right) = \sum \dot{m}_j x_j \hat{H}_j = \sum \dot{m}_j \hat{H}_j \\ &= \sum \dot{m}_j \hat{H}_j = \dot{m}_1 \hat{H}_1 + \dot{m}_2 \hat{H}_2 + \dots \end{aligned}$$



$$\text{slope} = \frac{\Delta \hat{H}}{\Delta T} = c_p(T) = \frac{d\hat{H}}{dT}$$

* separate and integrate.

$$\int_{T_1}^{T_2} d\hat{H} = \int_{T_1}^{T_2} c_p(T) dT$$

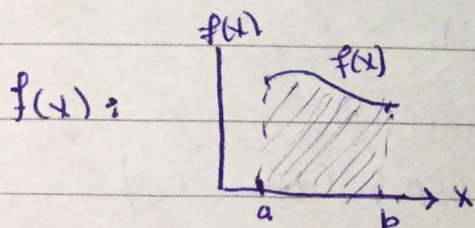
Temps Here, w/ reference.

$$\Delta \hat{H} = \hat{H}_2 - \hat{H}_1 = \int_{T_1}^{T_2} c_p(T) dT$$

$$\Delta \hat{H} = \hat{H}_2(T_2) - \hat{H}_1(T_{\text{ref}}) = \int_{T_{\text{ref}}}^{T_2} c_p(T) dT$$

$$\hat{H} = \Delta \hat{H} = \int_{T_{\text{ref}}}^T c_p(T) dT$$

mean value thm of $\int$ "integral"s



$$\text{area} = \int_a^b f(x) dx$$

$$\bar{f}(b-a) = \text{Area}$$

$$\bar{f} = \frac{\int_a^b f(x) dx}{(b-a)} \quad \bar{f}(b-a) = \int_a^b f(x) dx$$

so $\Downarrow$

$$\bar{c}_p = \frac{\int_{T_{\text{ref}}}^T c_p dT}{(T - T_{\text{ref}})} \quad \int_{T_{\text{ref}}}^T c_p dT = \bar{c}_p (T - T_{\text{ref}})$$

$$\left[\sum_{\text{in}} m_i \hat{H}_i - \sum_{\text{out}} m_i \hat{H}_i + \dot{Q} + \dot{W} = M \frac{d\hat{u}}{dt} \right] \text{--- ①}$$

$$\hat{H}_i = \int_{T_{\text{ref}}}^T c_p(T) dt$$

$$\left[\hat{H} = \bar{c}_p (T - T_{\text{ref}}) \right] \text{--- ②}$$

$$\begin{aligned} \hat{H}_{\text{mix}} &= \sum x_i \hat{H}_i = \sum x_j \bar{c}_{p,i} (T - T_{\text{ref}}) \\ &= (T - T_{\text{ref}}) \sum_j x_j \bar{c}_{p,i} \end{aligned}$$

$$\bar{c}_{p,\text{mix}} = \frac{\sum x_i \bar{c}_{p,i}}{\sum x_i}$$

$$\bar{c}_{p,m} = \sum x_i \bar{c}_p$$

$$\text{so, } \hat{H}_{\text{mix}} = \bar{c}_{p,\text{mix}} (T - T_{\text{ref}})$$

$$\begin{aligned} \sum_{\text{in}} m_i c_{p,i} (T_i - T_{\text{ref}}) &= \sum_{\text{out}} m_i (c_{p,i}) (T_{\text{ref}} - T_{\text{ref}}) \\ + \dot{Q} + \dot{W} &= M \frac{d\hat{u}}{dt} \end{aligned}$$

15/2/2018

$$\sum_{\text{stream } i} \dot{m}_i c_{p,i} (T_i - T_{ref}) - \sum_{\text{stream } out} \dot{m} \bar{c}_p (T_{ic} - T_{ref}) + Q + W$$

$$= \frac{d}{dt} (U) = \frac{d}{dt} (m \hat{u})$$

$$\frac{d(m)}{dt} = \sum_{in} \dot{m}_i - \sum_j \dot{m}_{ic}$$

$$\sum_i \dot{m}_i = \sum_{ic} \dot{m}_{ic} \Rightarrow \dot{m}_{in} = \dot{m}_{out} = \dot{m}$$

$$\rightarrow \frac{d}{dt} (M_{sys} \hat{u}), \hat{u}(T, p)$$

$$H = \hat{u} + p\hat{v} \Rightarrow \hat{u} = \hat{H} - p\hat{v}$$

$$\frac{d\hat{u}}{dt} = \frac{d}{dt} (H - p\hat{v})$$

$$\frac{dH}{dt} - \frac{d}{dt} (p\hat{v})$$

$$\frac{dH}{dt} - p \frac{d\hat{v}}{dt} - \hat{v} \frac{dp}{dt}$$

$\hat{v} \text{ constant}$

$$= \frac{dH}{dt} - \hat{v} \frac{dp}{dt}$$

$$= \frac{dH}{dt}$$

$p \text{ constant}$ * good approximation for liquid!

$$\frac{d\hat{u}}{dt} = \frac{dH}{dt} = \frac{d}{dt} (M_{system} \hat{H})$$

$$\text{if } M_{sys} \text{ constant} = M_{sys} \frac{d\hat{H}}{dt} = p\hat{v} \frac{d\hat{H}}{dt}$$

$$M_{sys} = p\hat{v}$$

$$p_{in} = p = \text{constant}$$

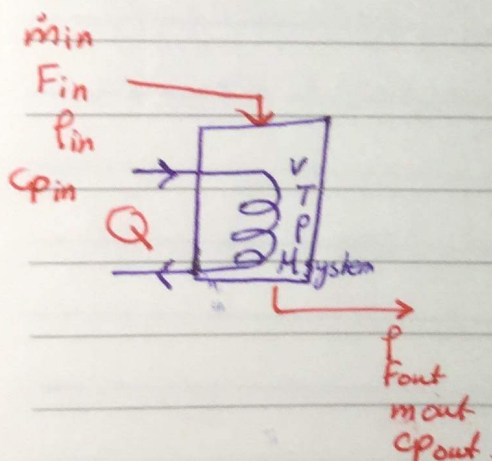
$$c_p(T) = \frac{d\hat{H}}{dT} \rightarrow d\hat{H} = c_p dT$$

$$\rho V \frac{d\hat{H}}{dt} = \rho V c_p \frac{dT}{dt}$$

$$\sum_{\text{stream in}} \dot{m}_i \bar{c}_{p,i} (T_i - T_{ref}) - \sum_{\text{stream is out}} \dot{m}_{ic} \bar{c}_{p,ic} (T_{ic} - T_{ref})$$

$$+ Q + W = \rho V c_p \frac{dT}{dt} \quad \text{"Temp. state variable"}$$

Ex.: Stirred Tank Heater



① MB:

$$\frac{dH_{system}}{dt} = \dot{m}_{in} - \dot{m}_{out}$$

$$\dot{m}_{in} = \dot{m}_{out} = \dot{m}$$

* physical properties:-

$$P_{in} = P$$

$$c_{p,in} = c_p$$

change in avg $c_p \approx$ negligible.

$$\dot{m}_{in} c_{p,in} (T_{in} - T_{ref}) - \dot{m}_{out} \bar{c}_{p,out} (T_{out} - T_{ref}) + Q + W$$

$$= \rho V c_p \left(\frac{dT}{dt} \right) \quad T_{out} = T$$

$$\dot{m} c_p (T_{in} - T_{ref}) - \dot{m} c_p (T - T_{ref}) + Q + W$$

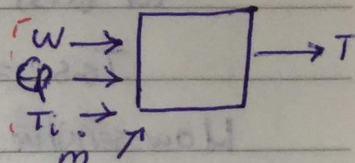
$$= \rho V c_p \frac{dT}{dt}$$

$$\dot{m} c_p (T_{in} - T) - \dot{m} c_p T_{ref} + \dot{m} c_p T_{ref} + Q + W$$

$$= \rho V c_p \frac{dT}{dt}$$

$$\left(\frac{\rho V c_p}{\dot{m} c_p} \right) \frac{dT}{dt} = (T_{in} - T) + \frac{Q}{\dot{m} c_p} + \frac{W}{\dot{m} c_p}$$

$$\left[\left(\frac{\rho V c_p}{\dot{m} c_p} \right) \frac{dT}{dt} + T = T_{in} + \frac{Q}{\dot{m} c_p} + \frac{W}{\dot{m} c_p} \right]$$



if the system :

- ① isolated $\rightarrow \frac{\rho V c_p}{\dot{m} c_p} \frac{dT}{dt} + T = T_{in} + \frac{Q}{\dot{m} c_p}$ $Q=0$
- ② no viscous material $\rightarrow \frac{\rho V c_p}{\dot{m} c_p} \frac{dT}{dt} + T = T_{in}$ $W=0$

$$\left[\frac{\rho V c_p}{\dot{m} c_p} \right] \dot{m} = \rho F$$

$$\dot{m}_{in} = \dot{m}_{out}, \quad \dot{m}_{in} = \rho F$$

$$\Rightarrow F_{in} = F_{out} = F$$

$$\left[\frac{\rho V c_p}{\rho F c_p} \right] = \left[\frac{V}{F} \right] \left[\frac{\frac{m^3}{m^3}}{\frac{m^3}{m^3}} \right] = [hr]$$

$$\left[\frac{\rho V c_p}{\dot{m} c_p} \right] \Rightarrow [\tau] \Rightarrow \text{time constant.}$$

$$\frac{dT}{dt} + \underbrace{\left(\frac{F}{V} \right)}_{K_1} T = \underbrace{\left(\frac{F}{V} \right)}_{K_1} T_{in} + \frac{Q}{\rho V c_p}$$

$$\tau \left(\frac{V}{F} \right) \frac{dT}{dt} + T = T_{in} + K_2 \frac{Q}{F}$$

اضرب الطرفين بـ $\left(\frac{V}{F} \right)$ ←

$$K_1 = 1$$

$$K_2 = \frac{V/F}{\rho V c_p} = \frac{1}{\rho F c_p} = \frac{1}{\dot{m} c_p}$$

$$\Rightarrow \tau \frac{dT}{dt} + T = K_1 T_{in} + K_2 Q$$

at [s.s]

$$T_{s.s} = K_1 (T_{in})_{s.s} + K_2 (Q)_{s.s}$$

How sensitive is ?

هتے نفیرے تاثرے

$$K_1 = \frac{T_{s.s}}{(T_{in})_{s.s}}, \quad K_2 = \frac{T_{s.s}}{Q_{s.s}}$$

* الیکٹرک ریفرنس آئی

$$\begin{bmatrix} \frac{v}{T} \end{bmatrix} = \begin{bmatrix} \frac{v}{T} \end{bmatrix} = \begin{bmatrix} \frac{v}{T} \end{bmatrix}$$

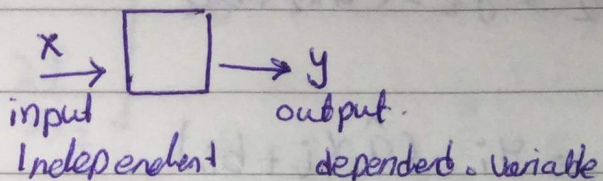
$$\begin{bmatrix} \frac{v}{T} \end{bmatrix} = \begin{bmatrix} \frac{v}{T} \end{bmatrix}$$

$$\frac{v}{T} + \tau \left(\frac{v}{T} \right) = T \left(\frac{v}{T} \right) + T_b$$

$$\Rightarrow \frac{v}{T} + \tau \left(\frac{v}{T} \right) = T \left(\frac{v}{T} \right) + T_b$$

18/2/2018.

Fittings $\left[\begin{array}{l} \rightarrow \text{linear} \\ \rightarrow \text{non-linear} \end{array} \right] \rightarrow \text{optimization problem}$



"black box"

"Don't care about the process"

x	y
x_1	y_1
x_2	y_2
x_n	y_n

by experiment

measure y

(x_i, y_i)

$i = 1, n$

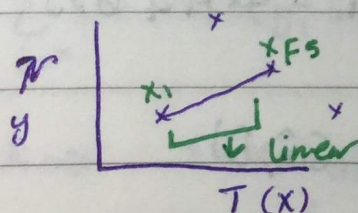
ex 8

$$\mu = f(T)$$

"viscosity"

T	μ
25°	μ_1
40°	μ_2

$\downarrow$ plot



$$y = f(x)$$

$$y = ax + b$$

$x[y_1, x_{15}]$

$$y - \hat{y} = \text{error}$$

data model

$$y_i - \hat{y}_i = e_i$$

$$\hat{y}_i = a\hat{x}_i + b$$

$$y_i - (a\hat{x}_i + b) = e_i$$

$\leftarrow$ error

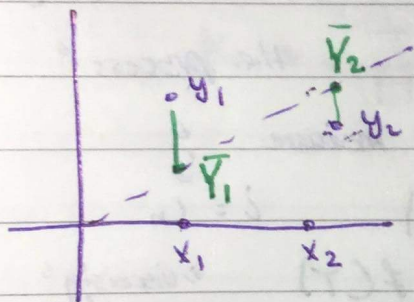
$$y_i = \hat{a}x_i + \hat{b} + e_i$$

$$e_i = y_i - (\hat{a}x_i + \hat{b})$$

$$i_1 \quad (x_1, y_1) \rightarrow e_1 = y_1 - (\hat{a}x_1 + \hat{b})$$

$$i_2 \quad (x_2, y_2) \rightarrow e_2 = y_2 - (\hat{a}x_2 + \hat{b})$$

$$e_i = y_i - (\hat{a}x_i + \hat{b})$$



$$y_2 = \bar{y}_2 = e_2 \quad (-ve)$$

$$e_1 = y_1 - \bar{y}_1 \quad (+ve)$$

total error is the sum of squares

$$\sum e_i^2 = \sum_{i=1}^n [y_i - (\hat{a}x_i + \hat{b})]^2$$

$$E(\hat{a}, \hat{b}) = \sum_{i=1}^n [y_i - (\hat{a}x_i + \hat{b})]^2$$

→ minimize $E(\hat{a}, \hat{b})$

Remark 3

$$y = f(x_1, x_2)$$

$$\underset{x_1, x_2}{\text{minimize}} \quad f(x_1, x_2)$$

$$y = f(x_1)$$

minimize $f(x_1)$ How?? by derivation.

$$f(x) = x^2 \rightarrow \min x^2$$

$$\frac{\partial f}{\partial x} = 2x = 0$$

$$\frac{\partial f}{\partial x} = -ve \rightarrow \max.$$

$$\frac{\partial f}{\partial x} = +ve \rightarrow \min.$$

$$y = f(x_1, x_2)$$

$$\begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix} = 0 \Rightarrow \Delta f = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$E(\hat{a}, \hat{b}) = \sum_{i=1}^n [y_i - (\hat{a}x_i + \hat{b})]^2$$

$$\Delta E \begin{bmatrix} \frac{\partial E}{\partial \hat{a}} \\ \frac{\partial E}{\partial \hat{b}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

① $\hat{a}$ بالمتجه $\frac{\partial E}{\partial \hat{a}}$
 البديل يعتمد على $\hat{a}$ و $\hat{b}$
 ② $\hat{b}$ بالمتجه $\frac{\partial E}{\partial \hat{b}}$

$$\frac{\partial E}{\partial \hat{a}} = \sum_{i=1}^n -2(y_i - \hat{a} - \hat{b}x_i) = 0$$

$$\frac{\partial E}{\partial \hat{b}} = \sum_{i=1}^n -2x_i(y_i - \hat{a} - \hat{b}x_i) = 0$$

* Remark $\Rightarrow \sum (x_i + y_i) = \sum x_i + \sum y_i$

* Summation ($\sum$) is a linear operator.

$\Rightarrow$ Eq. ①

$$\sum_{i=1}^n (y_i - \hat{a} - \hat{b}x_i) = 0 \Rightarrow \sum_{i=1}^n y_i - \sum_{i=1}^n \hat{a} - \sum_{i=1}^n \hat{b}x_i = 0$$

$$\Rightarrow \sum_{i=1}^n y_i - n\hat{a} - \hat{b} \sum_{i=1}^n x_i = 0$$

~~$$\sum_{i=1}^n (y_i - \hat{a} - \hat{b}x_i) = 0$$~~

$$\Rightarrow \sum_{i=1}^n y_i = n\hat{a} + \hat{b} \sum_{i=1}^n x_i \quad \text{Linear}$$

$$\text{Eq. (2)} \quad \sum_{i=1}^n x_i (y_i - \hat{a} - \hat{b}x_i) = 0$$

$$\sum x_i y_i - \hat{a} \sum x_i - \sum \hat{b} x_i^2 = 0$$

$$\hat{a} \sum x_i + \hat{b} \sum x_i^2 = \sum x_i y_i$$

$$n \hat{a} + \hat{b} (\sum x_i) = \sum y_i \quad \text{--- (3)}$$

$$(\sum x_i) \hat{a} + \hat{b} (\sum x_i^2) = \sum x_i y_i \quad \text{linear in } \hat{a} + \hat{b} \quad \text{--- (4)}$$

$$\rightarrow Ax = b$$

$$\sum x_i \begin{bmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix} \begin{bmatrix} \hat{a} \\ \hat{b} \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum x_i y_i \end{bmatrix}$$

$$\hat{b} = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{n \sum x_i^2 - (\sum x_i)^2}$$

get $\hat{a}$ from eq (3)

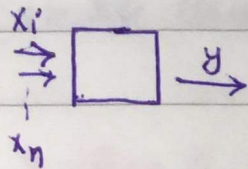
$$\hat{a} = \frac{\sum y_i - \hat{b} (\sum x_i)}{n}$$

$$\hat{a} = \underbrace{\frac{\sum y_i}{n}}_{\bar{y}} - \hat{b} \underbrace{\left(\frac{\sum x_i}{n}\right)}_{\bar{x}}$$

$$\boxed{\hat{a} = \bar{y} - \hat{b} \bar{x}}$$

20/2/2018.

Tues.



$$y = \alpha + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_i x_i + \dots + \beta_n x_n$$

$$y = \alpha + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_i x_i^n + \dots + \beta_n x_n^n$$

(y_i, x_i) "polynomial, linear in α and β "

$$y = \alpha + \tilde{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_3 x_3 + \dots + \epsilon \rightarrow \text{error}$$

true value

$$y = \bar{x} \hat{\beta} + \epsilon$$

$P = \text{number of variables variable.}$

$$\bar{x} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1P} \\ x_{21} & x_{22} & \dots & x_{2P} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nP} \end{bmatrix}$$

$n = \text{number of data points.}$

$(y_i, x_{i1}, x_{i2}, \dots, x_{iP})$

let $i=1 \rightarrow (y_1, x_{11}, x_{12}, \dots, x_{1P})$

$$y_1 = \alpha + \hat{\beta}_1 x_{11} + \hat{\beta}_2 x_{12} + \dots + \hat{\beta}_P x_{1P}$$

$$\hat{\beta} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_P \end{bmatrix}$$

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_P \end{bmatrix}$$

$$\epsilon = y - \bar{x} \hat{\beta}$$

$$\text{minimum } \epsilon^T \epsilon = (y - \hat{\beta} \bar{x}) (y - \bar{x} \hat{\beta})$$

(T is Transpose)

$$\min E = (y - \hat{\beta} \bar{x})^T (y - \bar{x} \hat{\beta})$$

$$\begin{cases} \frac{\partial E}{\partial \hat{\beta}_L} = 0 \\ \frac{\partial E}{\partial \hat{\beta}_p} = 0 \end{cases}$$

$$\bar{x} \bar{x}^T \hat{\beta} = \bar{x}^T y$$

$$n \times p \quad p \times n \quad p \times 1 = p \times p \quad p \times 1$$

$$\bar{x}^T \bar{x} = C_{(p \times p)}$$

$$\hat{\beta}_{(p \times 1)}$$

$$[C_{(p \times p)}] [\hat{\beta}_{(p \times 1)}] \Rightarrow [p \times 1]$$

$$\bar{x}_{(p \times n)}^T y_{(n \times 1)} = b$$

$$x^T y \rightarrow C \hat{\beta} = b$$

$$A^{-1} Ax = b$$

$$\underline{A^{-1} A} x = A^{-1} b$$

$$I x = x = x^{-1} b$$

identity.

$A_{n \times n}$

$$[A] = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$A = LU$$

$$Ax = b$$

$$L U x = b$$

$$Lc = b \quad \text{solve for } c \rightarrow Ux = c$$

solve for x

* multiple Linear Regression.

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3$$

if $x_1 = 1$

$$y_i = (x_{1i}, x_{2i}, x_{3i}) \text{ (model)}$$

3 variable
3 point,

$i=1$

$$y_1 = \beta_1 x_{11} + \beta_2 x_{21} + \beta_3 x_{31}$$

True

$i=2$

$$y_2 = \beta_1 x_{21} + \beta_2 x_{22} + \beta_3 x_{23}$$

$i=3$

$$y_3 = \beta_1 x_{31} + \beta_2 x_{32} + \beta_3 x_{33}$$

$$E = \sum_{i=1}^3 (y_i - \sum_{j=1}^3 \beta_j x_{ij})^2$$

$$E = (y_1 - \beta_1 x_{11} - \beta_2 x_{12} - \beta_3 x_{13})^2 + (y_2 - \beta_1 x_{21} - \beta_2 x_{22} - \beta_3 x_{23})^2 + (y_3 - \beta_1 x_{31} - \beta_2 x_{32} - \beta_3 x_{33})^2$$

$$\frac{\partial E}{\partial \beta_1} = 0 \Rightarrow$$

$$\beta_1 x_{11} x_{11} + \beta_2 x_{11} x_{12} + \beta_3 x_{11} x_{13} + \beta_1 x_{21} x_{21} + \beta_2 x_{21} x_{22} + \beta_3 x_{21} x_{23}$$

$$+ \beta_1 x_{31} x_{31} + \beta_2 x_{31} x_{32} + \beta_3 x_{31} x_{33}$$

$$= y_1 x_{11} + y_2 x_{21} + y_3 x_{31}$$

$$\beta_1 (x_{11} x_{11} + x_{21} x_{21} + x_{31} x_{31}) + \beta_2 (x_{12} x_{12} + x_{22} x_{22} + x_{32} x_{32}) + \beta_3 (x_{13} x_{13} + x_{23} x_{23} + x_{33} x_{33}) = y_1 x_{11} + y_2 x_{21} + y_3 x_{31}$$

$$\Rightarrow \beta_1 \left(\sum_{i=1}^3 x_{i1} x_{i1} \right) + \beta_2 \left(\sum_{i=1}^3 x_{i2} x_{i2} \right) + \beta_3 \left(\sum_{i=1}^3 x_{i3} x_{i3} \right) = \sum_{i=1}^3 y_i x_{i1}$$

$$\begin{bmatrix} x_{11} & x_{21} & x_{31} \end{bmatrix} \begin{bmatrix} x_{11} \\ x_{21} \\ x_{31} \end{bmatrix} = x_{11} x_{11} + x_{21} x_{21} + x_{31} x_{31}$$

$$\underline{X}^T \underline{X} = \begin{bmatrix} x_{11} & x_{21} & x_{31} \\ x_{12} & x_{22} & x_{32} \\ x_{13} & x_{23} & x_{33} \end{bmatrix} \begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{bmatrix}$$

$$\underline{\beta} = (\underline{X}^T \underline{X})^{-1} \underline{X}^T$$

$$\underline{X}^T \underline{y} = \begin{bmatrix} x_{11} & x_{21} & x_{31} \\ x_{12} & x_{22} & x_{32} \\ x_{13} & x_{23} & x_{33} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

$$= y_1 x_{11} + y_2 x_{21} + y_3 x_{31}$$