CHE302 LECTURE VII
DYNAMIC BEHAVIORS OF REPRESENTATIVE PROCESSES (II)

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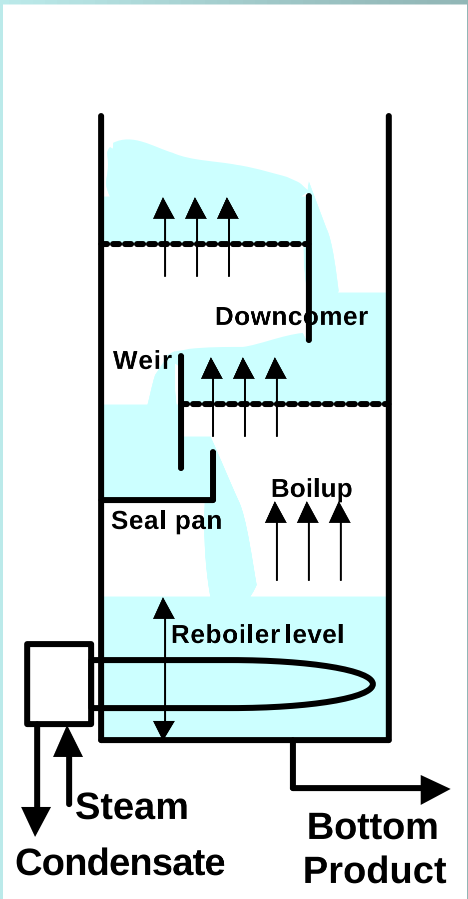
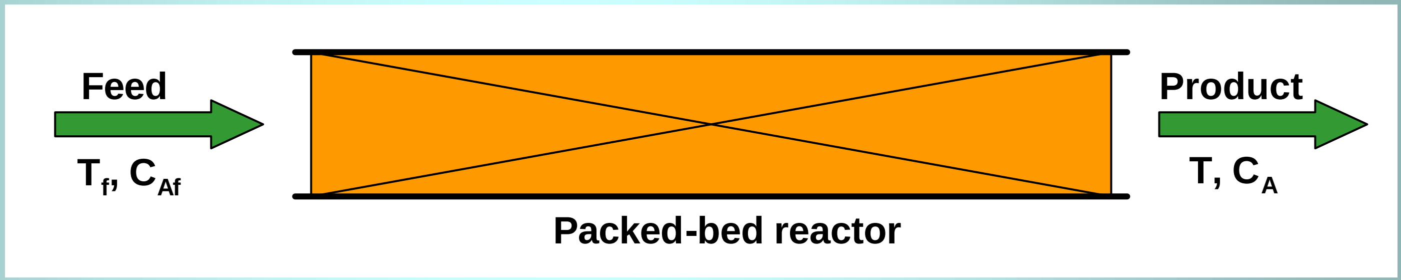
INVERSE RESPONSE IN CHEMICAL PROCESSES

- **Reboiler level to the change in boilup rate**
  - If boilup rate is increase, more liquid will vaporized and the inventory in the reboiler will be reduced and the level will be decreased.
  - However, at the beginning of the boilup rate increase, more vapor is generated and the vapor will flow upward to the stage above. In that stage, more vapor will pass through the liquid and the density of liquid will decrease so that the more liquid will spill over the weir. This results a temporary increase in the level of reboiler.
  - Eventually, the density of liquid settles down and overflow will reach at another steady state. Then the reboiler level will be decreased.



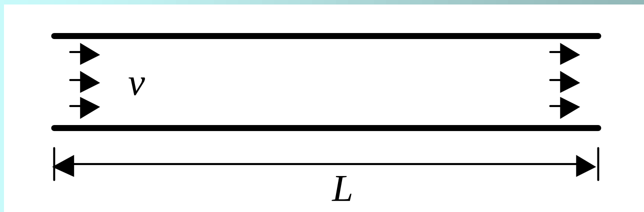
- **Outlet Temp of the exothermic packed bed reactor to feed temp change**
  - An increase in feed temp will speed up the reaction rate and the reactor outlet temp will increase due to the increased reaction heat generated.
  - However, at the beginning of the feed temp increase, more reaction occurs in the inlet part of the reactor and more reactants are consumed. This causes a decrease of reactant concentration in the outlet part of the reactor, and the outlet temp will decrease due to temporary drop in reactant concentration.
  - Eventually, increase in feed temp will enhance the reaction and generate more reaction heat and the outlet temp will increase slowly.



TIME DELAYS

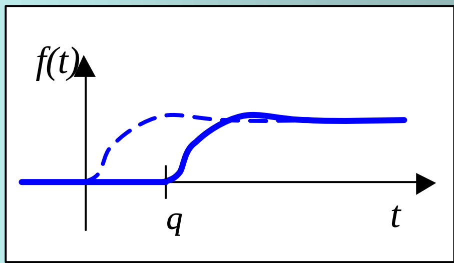
- **Fluid transportation through a pipe**
  - **Also, called distance-velocity lag, transportation lag, dead time**

$$q = \frac{\text{length of pipe}}{\text{fluidvelocity}} = \frac{\text{volume of pipe}}{\text{volumetric flowrate}}$$



- **Transfer function**

$$y(t) = \begin{cases} 0 & \text{for } t < q \\ x(t-q) & \text{for } t \geq q \end{cases} \quad \Rightarrow \quad \frac{Y(s)}{X(s)} = G(s) = e^{-qs}$$



- **Many high-order system can be approximated by a first-order plus dead-time model (FOPDT)**

$$G(s) = \frac{Ke^{-qs}}{ts+1}$$

But this transfer function cannot tell what the zeros are and what the poles are if it appears in denominator.

- **Polynomial approximations to $e^{-\theta s}$**
  - **Taylor series approximation**

$$e^{-\theta s} = 1 - \theta s + \frac{\theta^2 s^2}{2!} - \frac{\theta^3 s^3}{3!} + \frac{\theta^4 s^4}{4!} - \frac{\theta^5 s^5}{5!} + \cdots$$

  - **1/1 Pade approximation**

$$e^{-\theta s} = 1 - \theta s + \frac{\theta^2 s^2}{2!} - \frac{\theta^3 s^3}{3!} + \cdots \approx \frac{1+bs}{1+as}$$

$$1 + (a-\theta)s + (0.5\theta^2 - a\theta)s^2 + \cdots \approx 1 + bs$$

$$a - \theta = b, \quad (0.5\theta^2 - a\theta) = 0$$

$$\Rightarrow a = \theta/2, \quad b = -\theta/2$$

$$G_1(s) = \frac{1-(\theta/2)s}{1+(\theta/2)s}$$

  - **2/2 Pade approximation**

$$e^{-\theta s} = 1 - \theta s + \frac{\theta^2 s^2}{2!} - \frac{\theta^3 s^3}{3!} + \frac{\theta^4 s^4}{4!} - \cdots \approx \frac{1+bs+ds^2}{1+as+cs^2}$$

$$1 + (a-\theta)s + (0.5\theta^2 - a\theta + c)s^2 + (a\theta^2/2 - \theta^3/6 - c\theta) + \cdots \approx 1 + bs + ds^2$$

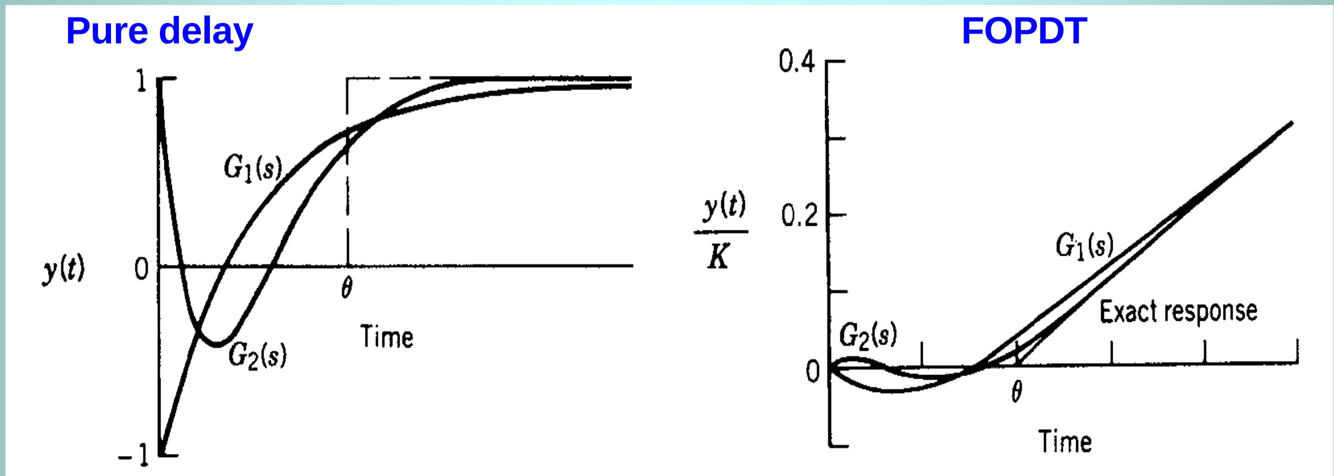
$$a - \theta = b, \quad (0.5\theta^2 - a\theta + c) = d,$$

$$(a\theta^2/2 - \theta^3/6 - c\theta) = 0, \ (\theta^4/24 - a\theta^3/6 + c\theta^2/2) = 0$$

$$\Rightarrow a = \theta/2, \ b = -\theta/2, \ c = d = \theta^2/12$$

$$G_2(s) = \frac{1-(\theta/2)s+(\theta^2/12)s^2}{1+(\theta/2)s+(\theta^2/12)s^2}$$

- **Taylor series approximation**
  - Increase the order of numerator (physical realizability)
  - AR and phase angle are different from the exact
  - Low accuracy
- **Pade approximation**
  - Does not change the order of transfer function
  - Only phase angle is different
  - Higher accuracy
  - Oscillatory behavior (complex poles and zeros)



APPROXIMATION OF HIGHER-ORDER SYSTEMS

- **Approximation by FOPDT or SOPDT models**

$$G(s) = \frac{K}{(t_1 s+1)(t_2 s+1)\cdots(t_n s+1)}$$

If $t_1 \gg (t_2,\cdots,t_n)$, (t_1 is the "dominant time constant")

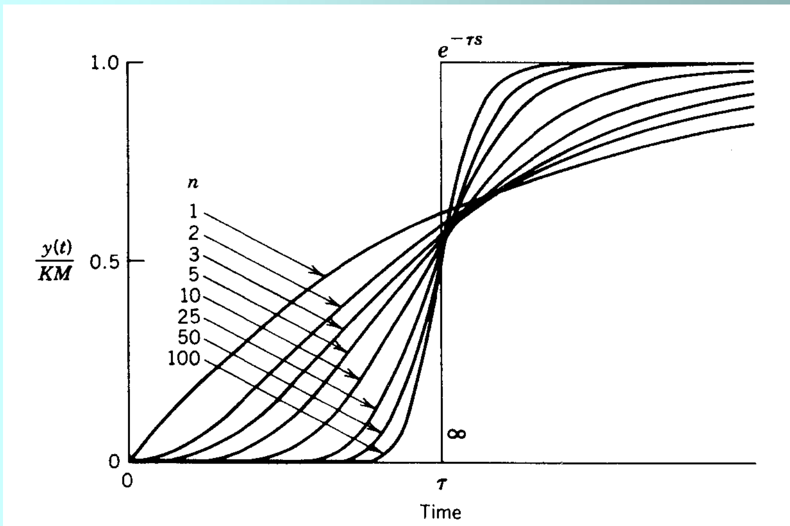
$$G(s) \approx \frac{Ke^{-qs}}{(t_1 s+1)} \quad \text{where } q = t_2+\cdots+t_n$$

If $t_1, t_2 \gg (t_3,\cdots,t_n)$, ($t_1$ and t_2 are the "dominant time constants")

$$G(s) \approx \frac{Ke^{-qs}}{(t_1 s+1)(t_2 s+1)} \quad \text{where } q = t_3+\cdots+t_n$$

- **nth-order system with equal time constants**

$$G_n(s) = \frac{K}{\left(\dfrac{t}{n}s+1\right)^n}$$



– **Step response**

$$y(t) = KM\left[1 - e^{-nt/t}\sum_{i=0}^{n-1}\frac{(nt/t)^i}{i!}\right]$$

By deinition, $e \triangleq \lim_{x\to 0}(1+x)^{1/x} = 2.7182818285...$

$$\lim_{n\to\infty} G_n(s) = \lim_{n\to\infty}\frac{K}{(\dfrac{t}{n}s+1)^n} = \lim_{n\to\infty}\frac{K}{\left[(\dfrac{ts}{n}+1)^{n/ts}\right]^{ts}} = \frac{K}{\left[\lim_{x\to 0}(1+x)^{1/x}\right]^{ts}} = Ke^{-ts}$$

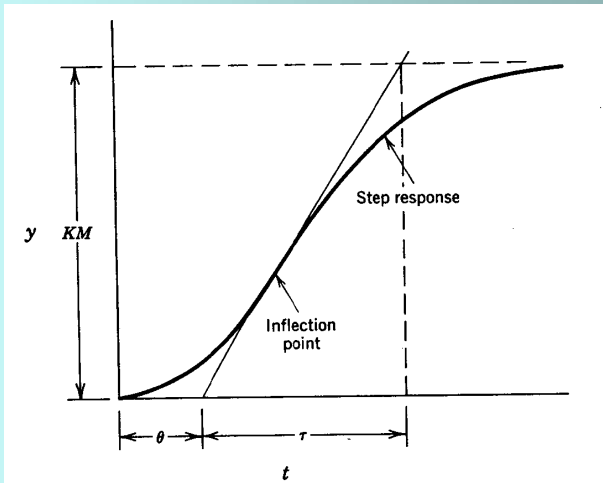
FITTING DATA TO EMPIRICAL MODELS

- **Fitting FOPDT model using step test**
  - **With a step response**

1. Obtain gain $K = \dfrac{y(\infty) - y(0)}{u(\infty) - u(0)}$

2. Estimated time delay by inspection

- **Visual inspection**
- **Use of tangent line at inflection point**



3. Find time constant

- **Graphical method** $y'(0) = KM / t$
- **Rearrange data: the slope is the reciprocal of time constant**

$$e^{-(t-q)t} = \frac{KM - (y(t) - y(0))}{KM} \Rightarrow \ln\left[\frac{y(\infty) - y_i}{y(\infty) - y(0)}\right] = -\frac{t_i - q}{t}$$

- **Sundaresan and Krishnaswamy (1977)**

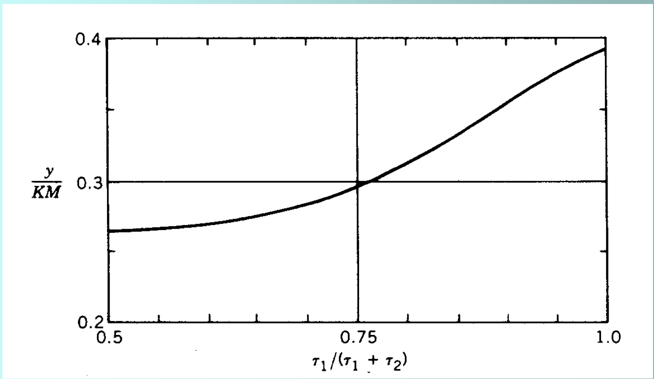
$$q = 1.3t_{35.3\%} - 0.29t_{85.3\%} \qquad t = 0.67(t_{85.3\%} - t_{35.3\%})$$

- **Fitting SOPDT model using step test**
  - **Harriot's Method for overdamped systems**

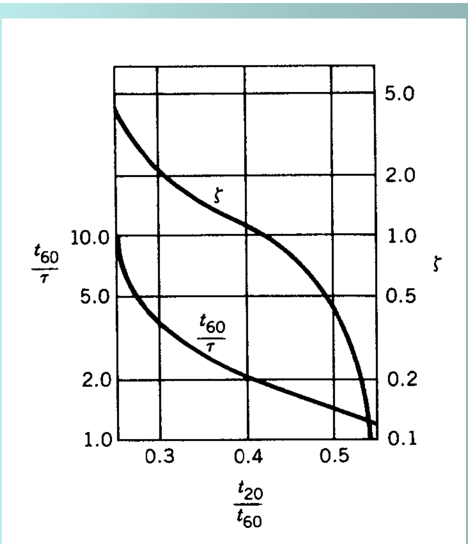
    Calculate $y_{t_{73\%}/2.6}$ and read $t_1/(t_1+t_2)$ from graph

    $$t_1 + t_2 = t_{73\%}/1.3$$

    If graph is out of range, it is not applicable and possibly higher-order or underdamped.



  - **Smith's method**
    - **Use $t_{20\%}$ and $t_{60\%}$.**
    - **Read parameters from graph**



- **Nonlinear/Linear Regression**

  Use of optimization to minimize the error between the data and calculated model value.

$$\min_{K,t,z,q} \sum_{i=1}^{N} (y(t_i) - y_i)^2 \quad \text{where } y(t_i) = f(t_i, K, t, z, q)$$

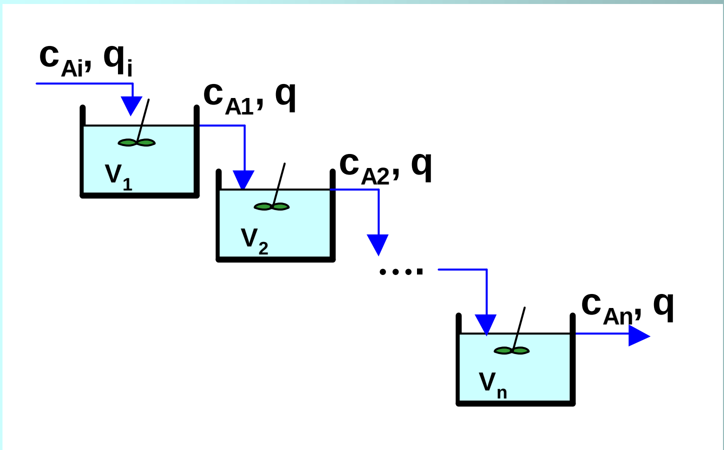
INTERACTING AND NONINTERACTING PROCESSES

- **Non interacting process**
  - **The first tank affects the second tank but second tank does not affect the first tank and so on. This is called "noninteracting".**
  - **Each tank can be modeled as**

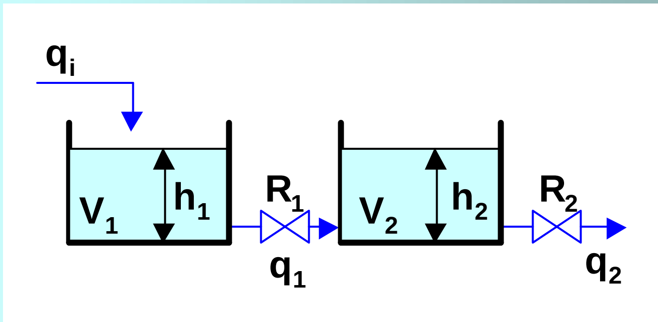
$$\frac{C_{Aj}(s)}{C_{A(j-1)}(s)} = \frac{K_j}{t_j s + 1}$$

  - **For the whole system**

$$\frac{C_{An}(s)}{C_{Ai}(s)} = \prod_{j=1}^{n} \frac{K_j}{(t_j s + 1)}$$



- **Interacting process**
  - **Many chemical processes exhibit interacting nature.**



$$A_1\frac{dh_1}{dt}=q_i-q_1 \qquad A_2\frac{dh_2}{dt}=q_1-q_2$$

$$q_1=\frac{1}{R_1}(h_1-h_2) \qquad q_2=\frac{1}{R_2}h_2$$

$$A_1\frac{dh_1}{dt}=q_i-\frac{1}{R_1}(h_1-h_2) \qquad A_2\frac{dh_2}{dt}=\frac{1}{R_1}(h_1-h_2)-\frac{1}{R_2}h_2$$

$$A_1R_1s\tilde{H}_1(s)+\tilde{H}_1(s)-\tilde{H}_2(s)=R_1\tilde{Q}_i(s)$$

$$\frac{A_2R_1R_2}{R_1+R_2}s\tilde{H}_2(s)+\tilde{H}_2(s)=\frac{R_2}{R_1+R_2}\tilde{H}_1(s)\Rightarrow\frac{\tilde{H}_2(s)}{\tilde{H}_1(s)}=\frac{R_2/(R_1+R_2)}{A_2R_1R_2/(R_1+R_2)s+1}$$

$$\frac{\tilde{H}_2(s)}{\tilde{Q}_i(s)}=\frac{R_2}{A_1A_2R_1R_2s^2+(A_1R_1+A_2R_2+A_1R_2)s+1}$$

$$\boxed{\frac{\tilde{H}_2(s)}{\tilde{Q}_i(s)}=\frac{R_2}{t^2s^2+2zt\,s+1}} \quad \text{where } t=\sqrt{A_1A_2R_1R_2}\,,\ z=\frac{(A_1R_1+A_2R_2+A_1R_2)}{2\sqrt{A_1A_2R_1R_2}}$$

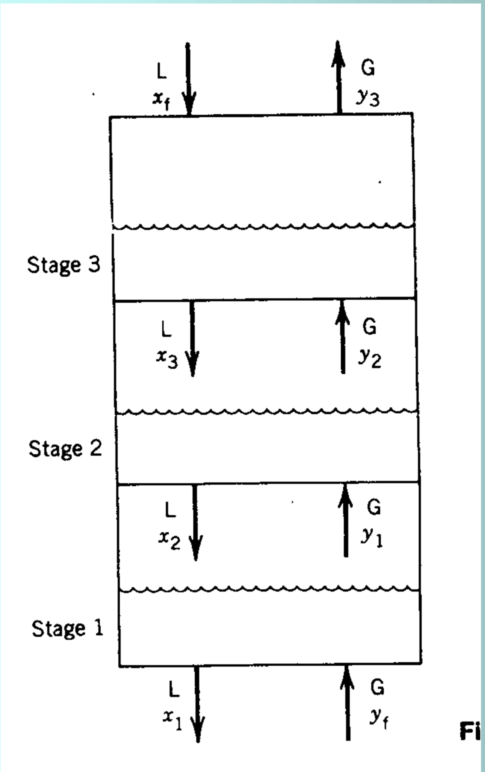
Since arithmetic mean $\geq$ geometric mean, $z>1$ (overdamped)

STAGED SYSTEM

- **Three-stage absorber**
  - **Assumptions**
    - **Constant liquid holdup (*H*)**
    - **Perfect mixing on each stage**
    - **Neglecting holdup of gas**
    - **Equilibrium:** $y_i = ax_i + b$

$$H\frac{dx_i}{dt} = G(y_{i-1} - y_i) + L(x_{i-1} - x_i)$$

$$H\frac{dx_i}{dt} = aGx_{i-1} - (L + aG)x_i + Lx_{i+1}$$



  - **Definition:**
    - **The stage liquid residence time** $t = H / L$
    - **The stripping factor** $s = aG / L$
    - **The gas-to-liquid ratio** $K = G / L$

$$t\frac{dx_1}{dt} = K(y_f - b) - (1+s)x_1 + x_2 \qquad t\frac{d\tilde{x}_1}{dt} = K\tilde{y}_f - (1+s)\tilde{x}_1 + \tilde{x}_2$$

$$t\frac{dx_2}{dt} = s\,x_1 - (1+s)x_2 + x_3 \qquad t\frac{d\tilde{x}_2}{dt} = s\,\tilde{x}_1 - (1+s)\tilde{x}_2 + \tilde{x}_3$$

$$t\frac{dx_3}{dt} = s\,x_2 - (1+s)x_3 + x_f \qquad t\frac{d\tilde{x}_3}{dt} = s\,\tilde{x}_2 - (1+s)\tilde{x}_3 + \tilde{x}_f$$

$$\begin{aligned} 0 &= K(\bar{y}_f - b) - (1+s)\bar{x}_1 + \bar{x}_2 \\ 0 &= s\,\bar{x}_1 - (1+s)\bar{x}_2 + \bar{x}_3 \\ 0 &= s\,\bar{x}_2 - (1+s)\bar{x}_3 + \bar{x}_f \end{aligned} \quad \Longrightarrow \quad \begin{aligned} \bar{x}_1 &= \left(\bar{x}_f + s\,K(\bar{y}_f - b)\right)/(1+s^2) \\ \bar{x}_2 &= \left(\bar{x}_f + (1+s+s^2)K(\bar{y}_f - b)\right)/(1+s+s^2) \\ \bar{x}_3 &= \left((1-s)\bar{x}_f + (1+s)K(\bar{y}_f - b)\right)/(1+s^2) \\ \bar{y}_i &= a\bar{x}_i + b \end{aligned}$$

$$(ts + 1 + s)X_1(s) - X_2(s) = KY_f(s)$$

$$(ts + 1 + s)X_2(s) - s\,X_1(s) - X_3(s) = 0$$

$$(ts + 1 + s)X_3(s) - s\,X_2(s) = X_f(s)$$

$$Y_i(s) = aX_i(s)$$

– **With** $\tilde{X}_f(s) = 0$

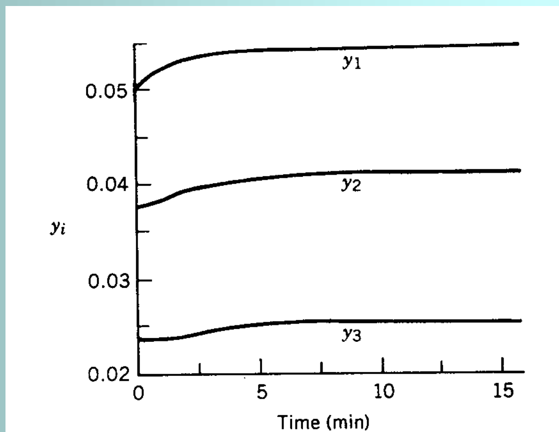
$$X_1(s) = K\frac{1+s+s^2}{1+s+s^2+s^3}\,\frac{\left(\dfrac{t^2}{1+s+s^2}s^2 + \dfrac{2t(1+s)}{1+s+s^2}s + 1\right)}{\left(\dfrac{t}{1+s}s+1\right)\left(\dfrac{t^2}{1+s^2}s^2 + \dfrac{2t(1+s)}{1+s^2}s + 1\right)}Y_f(s)$$

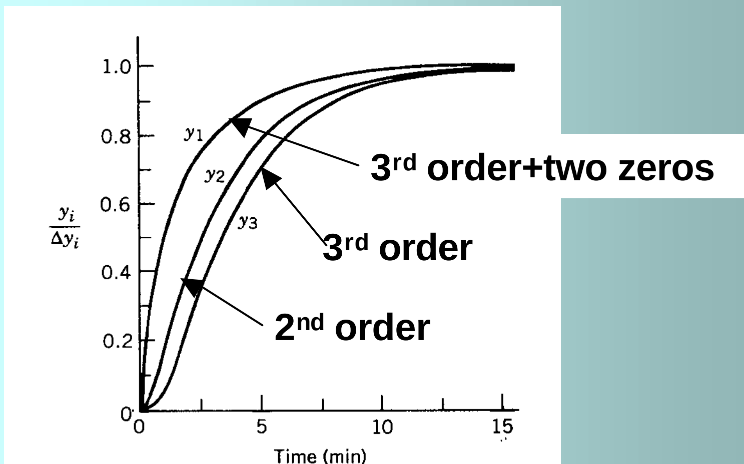
$$X_2(s) = K\frac{s}{1+s^2}\frac{1}{\left(\dfrac{t^2}{1+s^2}s^2+\dfrac{2t(1+s)}{1+s^2}s+1\right)}Y_f(s)$$

$$X_3(s) = K\frac{s^2}{1+s+s^2+s^3}\frac{1}{\left(\dfrac{t}{1+s}s+1\right)\left(\dfrac{t^2}{1+s^2}s^2+\dfrac{2t(1+s)}{1+s^2}s+1\right)}Y_f(s)$$

$$\frac{Y_1(s)}{Y_f(s)}=\frac{aX_1(s)}{Y_f(s)} \qquad \frac{Y_2(s)}{Y_f(s)}=\frac{aX_2(s)}{Y_f(s)} \qquad \frac{Y_3(s)}{Y_f(s)}=\frac{aX_3(s)}{Y_f(s)} \qquad (aK=s)$$

– **Step increase in gas feed composition**





- **Analysis using transfer function**
  - Easy to develop
  - Types of response can be recognized very conveniently
  - Parameter effects can be analyzed through lumped parameter

  - Linearization required when the system is nonlinear
    - If the effect of flow rate change, the previous example becomes nonlinear.
    - Due to linearization, new model has to be obtained when the operating condition changes widely.
  - For the nonlinear system analysis, numerical integration should be considered
    - Utilize differential equation solvers
      - Non-stiff case: explicit method
      - Stiff case: implicit methods
      - ODE
      - DAE
      - PDE

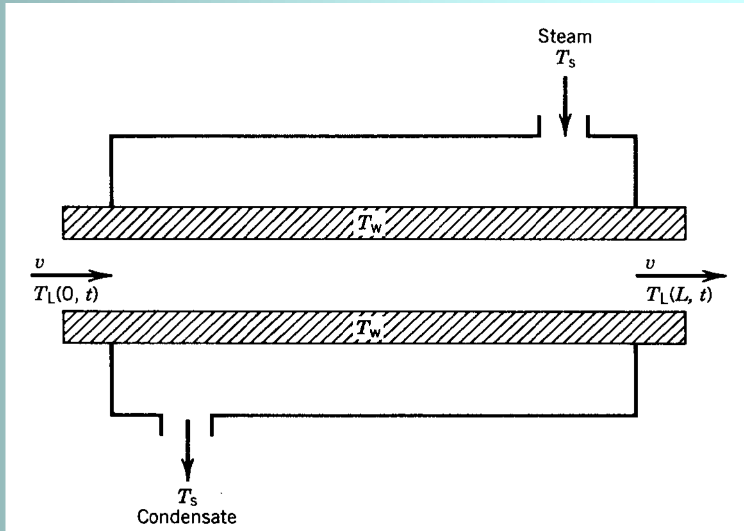
DISTRIBUTED PARAMETER SYSTEMS

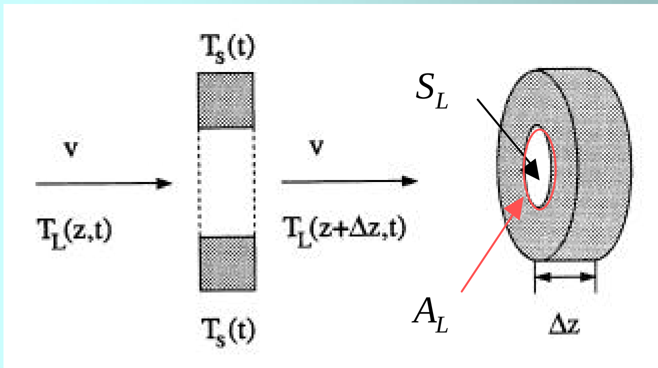
- **Lumped parameter system (ODE)**
  - **Dependent variables depend only on time, not on spatial location**
  - **Perfect mixing assumption eliminates the dependency on**
  - **spatial coordinates and the analysis will be conducted in averaging sense**
  - **All balances are valid around the boundary**

- **Distributed parameter system (PDE)**
  - **Dependent variables depend on time and also spatial location**
  - **Perfect mixing is not valid. (double pipe heat exchanger, packed bed reactor**

DPS EXAMPLE

- **Double pipe heat exchanger**





  - **Assumptions**
    - **Plug flow (no radial or angular variations in T_L)**
    - **Neglect axial conduction**
    - **Heat transfer resistance of the inside tube metal is neglected**
    - **Steam jacket is well mixed**

- **For a control volume, from the energy balance for the liquid**

$$r_L C_L S_L \Delta z \frac{dT_L(t,z)}{dt} = v r_L C_L S_L (T_L(t,z) - T_{ref}) - v r_L C_L S_L (T_L(t,z+\Delta z) - T_{ref})$$
$$+ h_L A_L \Delta z (T_W(t,z) - T_L(t,z))$$

$$\frac{dT_L(t,z)}{dt} = -\frac{v(T_L(t,z+\Delta z) - T_L(t,z))}{\Delta z} + \frac{h_L A_L}{r_L C_L S_L}(T_W(t,z) - T_L(t,z))$$

As $\Delta z \rightarrow 0$

$$\frac{dT_L}{dt} = -v\frac{\partial T_L}{\partial z} + \frac{1}{t_{HL}}(T_W - T_L) \quad \text{where } t_{HL} = \frac{r_L C_L S_L}{h_L A_L}$$

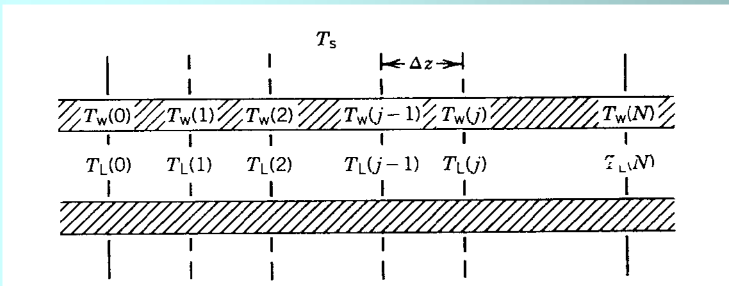
(A_L is a heat transfer area per unit length)

- **For a control volume, from the energy balance for the wall**

$$\frac{dT_W}{dt} = \frac{h_S A_S}{r_W C_W S_W}(T_S - T_W) - \frac{h_L A_L}{r_L C_L S_L}(T_W - T_L)$$

$$\frac{dT_W}{dt} = \frac{1}{t_{SW}}(T_S - T_W) - \frac{1}{t_{WL}}(T_W - T_L)$$

- **Discretization**
  - **PDE => ODE**
  - **Eliminate z-dependency**
  - **Replace**



$$T_L(t, z_j) = T_L^{\,j}(t) \quad \text{for } j = 0, \cdots, N$$

$$T_{LW}(t, z_j) = T_W^{\,j}(t) \quad \text{where } z(0) = 0, \cdots, z(N) = L$$

  - **Number of point *N* will decide the accuracy of solution**
  - **Finite difference approximation (FDM)**

$$\frac{\partial T_L}{\partial z} = \frac{T_L(t, z+\Delta z) - T_L(t, z)}{\Delta z} \quad \text{(forward difference approximation)}$$

$$\frac{\partial T_L}{\partial z} = \frac{T_L(t, z) - T_L(t, z-\Delta z)}{\Delta z} \quad \text{(backward difference approximation)}$$

$$\frac{\partial T_L}{\partial z} = \frac{T_L(t, z+\Delta z) - T_L(t, z-\Delta z)}{2\Delta z} \quad \text{(central difference approximation)}$$

  - **Other methods: method of characteristics, FEM, OC, etc.**

- **Using FDM with centered difference approx.**

$$\frac{dT_L^{\,1}}{dt} = -v\frac{T_L^{\,2}-T_L^{\,0}}{2\Delta z} + \frac{1}{t_{HL}}(T_W^{\,1}-T_L^{\,1}) \qquad \frac{dT_W^{\,1}}{dt} = \frac{1}{t_{SL}}(T_S - T_W^{\,1}) - \frac{1}{t_{HL}}(T_W^{\,1}-T_L^{\,1})$$

$$\frac{dT_L^{\,2}}{dt} = -v\frac{T_L^{\,3}-T_L^{\,1}}{2\Delta z} + \frac{1}{t_{HL}}(T_W^{\,2}-T_L^{\,2}) \qquad \frac{dT_W^{\,2}}{dt} = \frac{1}{t_{SL}}(T_S - T_W^{\,2}) - \frac{1}{t_{HL}}(T_W^{\,2}-T_L^{\,2})$$

$$\vdots \qquad\qquad\qquad\qquad \vdots$$

$$\frac{dT_L^{\,N}}{dt} = -v\frac{T_L^{\,N}-T_L^{\,N-1}}{\Delta z} + \frac{1}{t_{HL}}(T_W^{\,N}-T_L^{\,N}) \qquad \frac{dT_W^{\,N}}{dt} = \frac{1}{t_{SL}}(T_S - T_W^{\,N}) - \frac{1}{t_{HL}}(T_W^{\,N}-T_L^{\,N})$$

- **Initial conditions and boundary conditions**

$$T_L(0,z) = T_{L,t_0}(z) \Rightarrow T_L^{\,0}(0) = T_{L,t_0}(0), \cdots, T_L^{\,N}(0) = T_{L,t_0}(z_N) \quad \text{(I.C. for } T_L\text{)}$$

$$T_W(0,z) = T_{W,t_0}(z) \Rightarrow T_W^{\,0}(0) = T_{W,t_0}(0), \cdots, T_W^{\,N}(0) = T_{W,t_0}(z_N) \quad \text{(I.C. for } T_W\text{)}$$

$$T_L(t,0) = T_F(t) \Rightarrow T_L^{\,0}(t) = T_F(t) \quad \text{(B.C. for } T_L\text{)}$$

$$T_W(t,0) = T_A(t) \Rightarrow T_W^{\,0}(t) = T_A(t) \quad \text{(B.C. for } T_W\text{)}$$

- **Inputs: Steam T ($T_S(t)$) and Feed T ($T_F(t)$)**
- **Outputs: $T_L(t)$ and $T_W(t)$ at each location in z**
- **2 PDE's become 2N ODE's**

- **Transfer function**

Tri-diagonal matrix

$$\begin{bmatrix} t_{L1}s+1 & b_1 & 0 & \cdots & 0 \\ c_1 & t_{L1}s+1 & b_2 & \ddots & \vdots \\ 0 & c_2 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & b_{N-1} \\ 0 & \cdots & 0 & c_{N-1} & t_{L1}s+1 \end{bmatrix} \begin{bmatrix} T_L^{\ 1} \\ T_L^{\ 2} \\ \vdots \\ T_L^{\ N} \end{bmatrix} = K_W \begin{bmatrix} T_W^{\ 1} \\ T_W^{\ 2} \\ \vdots \\ T_W^{\ N} \end{bmatrix} + \begin{bmatrix} K_F \\ 0 \\ \vdots \\ 0 \end{bmatrix} T_F(t)$$

$$\begin{bmatrix} t_{W1}s+1 & 0 & \cdots & 0 \\ 0 & t_{W2}s+1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & t_{WN}s+1 \end{bmatrix} \begin{bmatrix} T_W^{\ 1} \\ T_W^{\ 2} \\ \vdots \\ T_W^{\ N} \end{bmatrix} = K_L \begin{bmatrix} T_L^{\ 1} \\ T_L^{\ 2} \\ \vdots \\ T_L^{\ N} \end{bmatrix} + \begin{bmatrix} K_S \\ K_S \\ \vdots \\ K_S \end{bmatrix} T_S(t)$$

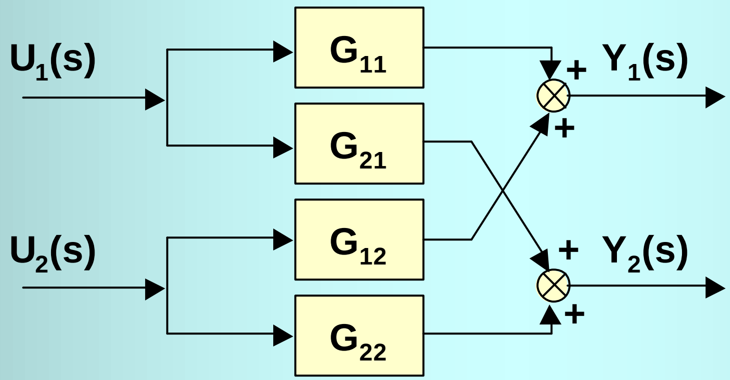
  - **FDM usually generates tri-diagonal matrix.**
  - **Quite high order system if N is big.**
  - **May not be convenient to analyze.**

MIMO systems

- **Multi-Input Multi-Output System**

$$\begin{bmatrix} Y_1(s) \\ Y_2(s) \\ \vdots \\ Y_n(s) \end{bmatrix} = \underbrace{\begin{bmatrix} G_{11}(s) & G_{12}(s) & \cdots & G_{1m}(s) \\ G_{21}(s) & G_{22}(s) & & G_{2m}(s) \\ \vdots & & \ddots & \vdots \\ G_{n1}(s) & G_{n2}(s) & \cdots & G_{nm}(s) \end{bmatrix}}_{\text{Transfer function matrix}} \begin{bmatrix} U_1(s) \\ U_2(s) \\ \vdots \\ U_m(s) \end{bmatrix}$$

  - **MISO (n=1) and SIMO (m=1) are possible.**
  - **2x2 system**



- **From SS model to TF model for MIMO system**
  - **With deviation variables after linearization**

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \mathbf{A}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \mathbf{B}\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \quad \Rightarrow \quad \dot{\mathbf{x}} = \mathbf{Ax} + \mathbf{Bu}$$

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \mathbf{C}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \mathbf{D}\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \quad \Rightarrow \quad \mathbf{y} = \mathbf{Cx} + \mathbf{Du}$$

$$s\mathbf{X}(s) = \mathbf{AX}(s) + \mathbf{BU}(s) \quad \Rightarrow \quad (s\mathbf{I} - \mathbf{A})\mathbf{X}(s) = \mathbf{BU}(s)$$

$$\mathbf{Y}(s) = \mathbf{CX}(s) + \mathbf{DU}(s) \quad \Rightarrow \quad \mathbf{Y}(s) = \left[\mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{B} + \mathbf{D}\right]\mathbf{U}(s)$$

$$\therefore \ \mathbf{G}(s) = \left[\mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{B} + \mathbf{D}\right]$$

  - **Generally for (pxm) system, A is (nxn), B is (nxm), C is (pxn) and D is (pxm) matrices, respectively.**
  - **Then, G(s) is (pxm) transfer function matrix.**