Lecture Notes II

Example 6   Continuous Stirred-Tank Reactor (CSTR)

Chemical reactors together with mass transfer processes constitute an important part of chemical technologies. From a control point of view, reactors belong to the most difficult processes. This is especially true for fast exothermal processes.

We consider CSTR with a simple exothermal reaction A □ B. For the development of a mathematical model of the CSTR, the following assumptions are made,

1. neglected heat capacity of inner walls of the reactor, constant density and specific heat capacity of liquid,
2. constant reactor volume, constant overall heat transfer coefficient, and
3. constant and equal input and output volumetric flow rates.

As the reactor is well-mixed, the outlet stream concentration and temperature are identical with those in the tank.

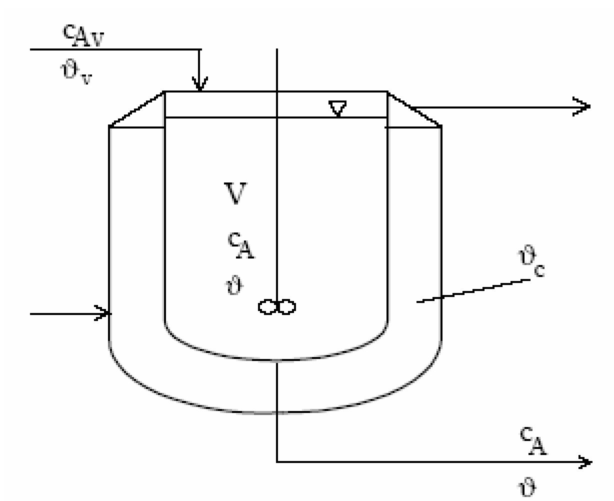


Figure 1.   A nonisothermal CSTR.

Mass balance of the component A can be expressed as

$$V\frac{dc_A}{dt} = qc_{Av} - qc_A - Vr(c_A, \vartheta) \tag{1}$$

where

t - time variable,
c_A - molar concentration of A (mole/volume) in the outlet stream,
c_{Av} - molar concentration of A (mole/volume) in the inlet stream,
V - reactor volume,
q - volumetric flow rate,
$r(c_A, \vartheta)$ - rate of reaction per unit volume,
ϑ- temperature of reaction mixture.

The rate of reaction is a strong function of concentration and temperature (Arrhenius law)

$$r(c_A, \vartheta) = kc_A = k_0 e^{\frac{E}{R\vartheta}} c_A \qquad 2$$

where k_0 is the frequency factor, E is the activation energy, and R is the gas constant.
Heat balance gives

$$V\rho\, c_p \frac{d\vartheta}{dt} = q\rho\, c_p \vartheta_v - q\rho\, c_p \vartheta - \alpha F(\vartheta - \vartheta_c) + V(-\Delta H) r(c_A, \vartheta) \qquad 3$$

where

ϑv - temperature in the inlet stream,

ϑc - cooling temperature,

ρ - liquid density,

c_p - liquid specific heat capacity,

α - overall heat transfer coefficient,

F - heat transfer area,

$(-\Delta H)$ - heat of reaction.

Initial conditions are

$c_A(0) = c_A^0$

$\vartheta(0) = \vartheta^0$

The process state variables are concentration c_A and temperature ϑ. The input variables are ϑ_c, c_{Av}, ϑ_v and among them, the cooling temperature can be used as a manipulated variable. The reactor is in the steady-state if derivatives with respect to time in equations (1), (3) are zero. Consider the steady-state input variables $\vartheta_c^s, c_{Av}^s, \vartheta_v^s$

The steady-state concentration and temperature can be calculated from the equations

$$0 = qc_{Av}^s - qc_A^s - Vr(c_A^s, \vartheta^s) \qquad 4$$

$$0 = q\rho\, c_p \vartheta_v^s - q\rho\, c_p \vartheta^s - \alpha F(\vartheta^s - \vartheta_c^s) + V(-\Delta H) r(c_A^s, \vartheta^s) \qquad 5$$

Please finish the rest as homework.

Example 7 Mathematical model of a thermocouple

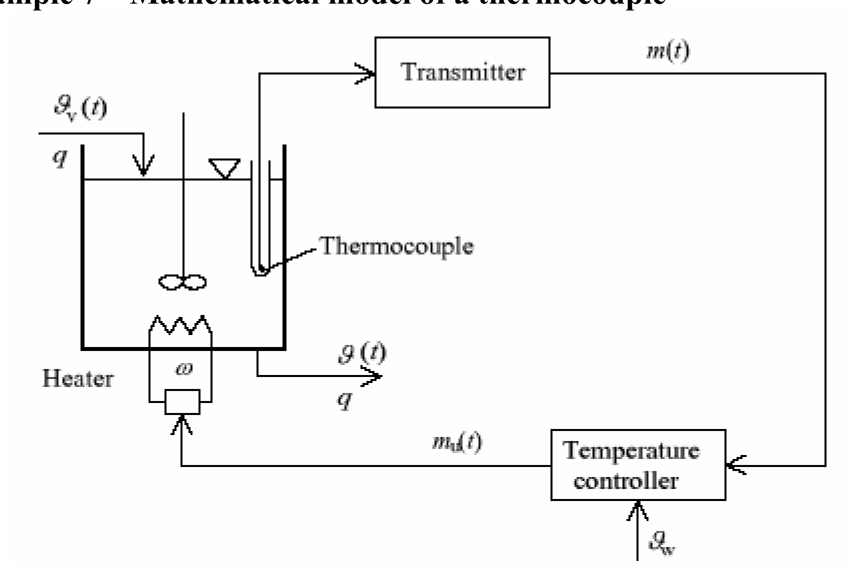
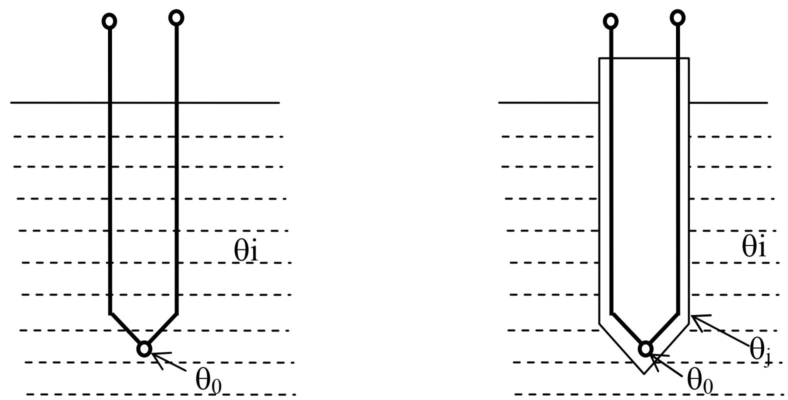


Figure 2. Control loop for the Stirred Heating Tank



a) bare thermocouple   b) thermocouple with protect jacket

Figure 3. Temperature sensor (thermocouple)

a) Mathematical model of a bare thermocouple

The energy balance for the bare thermocouple is,

$$C_1 \frac{d\theta_0}{dt} = Q_i - Q_0 \qquad 6$$

where C_1 is the molar specific heat capacity of the thermocouple, Q_i is the heat flow from the media to the thermocouple, and Q_0 is the heat lost by the thermocouple. And,

$$Q_i = \alpha_1 A_1(\theta_i - \theta_0) = \frac{\theta_i - \theta_0}{R_1} \qquad 7$$

where R_1 is the heat resistor, $R_1 = \dfrac{1}{\alpha_1 A_1}$, A_1 surface area of the tip of the thermocouple, α_1 is the heat transfer coefficient of the heat transfer between the media and the thermocouple.

Assume $Q_0 = 0$, substitute Eq.7 into Eq.6,

$$R_1 C_1 \frac{d\theta_0}{dt} + \theta_0 = \theta_i \qquad 8$$

Follow the steps used in the early examples,

$$R_1 C_1 \frac{d\theta_0}{dt} + \Delta\theta_0 = \Delta\theta_i \qquad 9$$

Therefore it is a first order system.

b) Mathematical model of a thermocouple with protect jacket

1. The energy balance for the thermocouple with protect jacket is,

$$C_2 \frac{d\theta_j}{dt} = Q_{ij} - Q_{j0} - Q_j - Q_0 \qquad 10$$

where C_2 is the molar specific heat capacity of the thermocouple protect jacket, Q_{ij} is the heat flow from the media to the thermocouple protect jacket, Q_{j0} is the heat flow from the thermocouple protect jacket to the thermocouple, and Q_j, Q_0 are the heat lost by the thermocouple jacket and the thermocouple itself respectively.

2. Assume Q_j, Q_0 are equal zero,

$$C_2 \frac{d\theta_j}{dt} = \alpha_2 A_2 (\theta_i - \theta_j) - \alpha_1 A_1 (\theta_j - \theta_0) \qquad 11$$

where A_2 is the heat transfer surface area of the thermocouple protect jacket, A_1 is the heat transfer surface area of the thermocouple tip, α_2 is the heat transfer coefficient of the heat transfer between the media and the thermocouple protect jacket, α_1 is the heat transfer coefficient of the heat transfer between the thermocouple protect jacket and the thermocouple.

Since $A_2 >> A_1$,

$$C_2 \frac{d\theta_j}{dt} = \alpha_2 A_2 (\theta_i - \theta_j) \qquad 12$$

we can also arrive at

$$R_2 C_2 \frac{d\Delta\theta_j}{dt} + \Delta\theta_j = \Delta\theta_i \qquad 13$$

where $R_2 = \frac{1}{\alpha_2 A_2}$.

3. The accumulation of the heat in the thermocouple tip is,

$$C_1 \frac{d\theta_0}{dt} = \alpha_1 A_1 (\theta_j - \theta_0) \qquad 14$$

Similarly we can arrive,

$$R_1 C_1 \frac{d\Delta\theta_0}{dt} + \Delta\theta_0 = \Delta\theta_j . \qquad 15$$

4. Now differentiate both sides of Eq.15 with respect to t,

$$R_1 C_1 \frac{d^2\Delta\theta_0}{dt^2} + \frac{d\Delta\theta_0}{dt} = \frac{d\Delta\theta_j}{dt} . \qquad 16$$

Substitute Eqs.13 and 15 into 16, and let $\tau_1 = R_1C_1$, $\tau_2 = R_2C_2$,

$$\tau_1 \tau_2 \frac{d^2\Delta\theta_0}{dt^2} + (\tau_1 + \tau_2) \frac{d\Delta\theta_0}{dt} + \Delta\theta_0 = \Delta\theta_i . \qquad 17$$

It is a second order system.

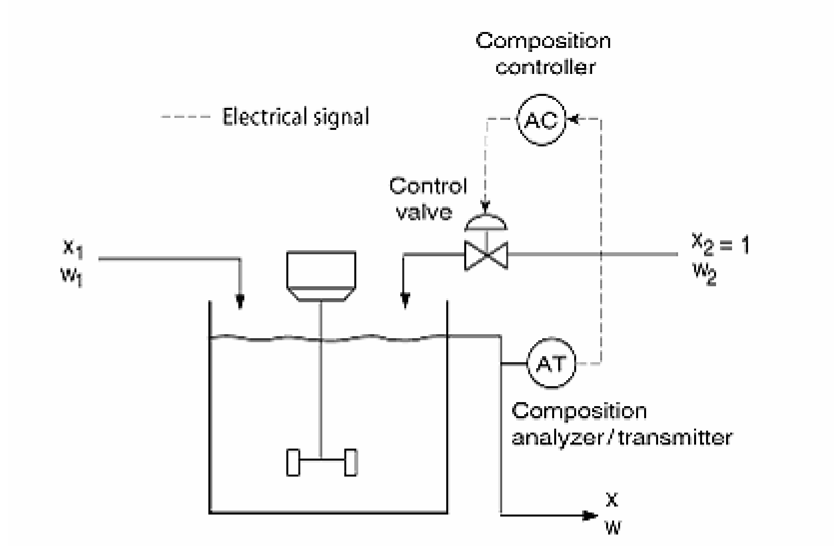


Figure 4. Blending system and Control Method 1, measure x and adjust w_2

Example 8 The pneumatic control valve

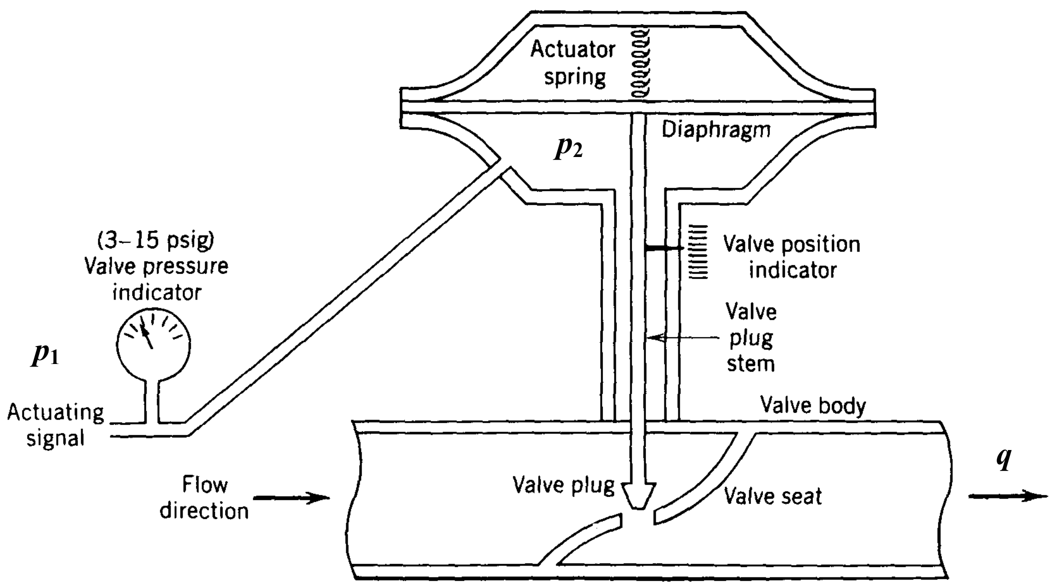


Figure 5. The schematic diagram of a pneumatic control valve

Mass balance of compress air (signal),

$$F_i - F_0 = C\frac{dp_2}{dt} \qquad 18$$

where C is the capacitor, p_2 is the pressure in the diaphragm chamber, F_i, F_0, are the in and out compress air flow rates.

Since the diaphragm chamber is sealed, $F_0 = 0, F_i = \dfrac{p_1 - p_2}{R}$, R is the resistance of the compress air line, therefore,

$$RC\frac{dp_2}{dt} + p_2 = p_1 \quad 19$$
and
$$RC\frac{d(p_2^0 + \Delta p_2)}{dt} + (p_2^0 + \Delta p_2) = (p_1^0 + \Delta p_1) \quad 20$$
when there is no action,
$$p_2^0 = p_1^0 . \quad 21$$
Let $T_v = RC$,
$$T_v \frac{d\Delta p_2}{dt} + \Delta p_2 = \Delta p_1 \quad 22$$
Assume the effective area of the diaphragm is A_0, and let c_s be the rigidity coefficient of the spring, according the Hooke's law,
$$A_0 \Delta p_2 = c_s \Delta l \quad 23$$
where Δl is the displacement of the diaphragm caused by the force acted on by p_2. Substitute into Eq.22,
$$T_v \frac{d\Delta l}{dt} + \Delta l = \frac{A_0}{c_s}\Delta p_1 \quad 24$$
Assume a linear relationship between the change of the fluid flow rate Δq and the displacement of the diaphragm Δl,
$$\Delta q = K\Delta l \quad 25$$
Substitute Eq.25 into 24,
$$T_v \frac{d\Delta q}{dt} + \Delta q = \frac{A_0}{c_s} K\Delta p_1 \quad 26$$
or,
$$T_v \frac{d\Delta q}{dt} + \Delta q = K_v \Delta p_1 \quad 27$$
where

$K_v = \frac{A_0}{c_s} K$ is the gain of the pneumatic control valve and,

$T_v = RC$ is the time constant of the pneumatic control valve.

This is a first order system.

If the time constant of the pneumatic control valve is much smaller than the time constant of the process it is controlling, $T_v \to 0$，
$$\Delta q = K_v \Delta p_1. \quad 28$$
It is a proportional system.

Transfer-Function Representation and time domain response of Control-System Element

1. The general form of the first order element,
$$\tau \frac{dy(t)}{dt} + y(t) = Kx(t) \quad 29$$
Its transfer function,

$$G(s) = \frac{Y(s)}{X(s)} = \frac{K}{\tau s + 1} \qquad 30$$

Step input $x(t) = MU(t)$,

$$Y(s) = G(s)X(s) = \frac{K}{\tau s + 1} \cdot \frac{M}{s} \qquad 31$$

$$y(t) = \mathcal{L}^{-1}\left[\frac{K}{\tau s + 1} \cdot \frac{M}{s}\right] = KM\left(1 - e^{-\frac{t}{\tau}}\right) \qquad 32$$

When M =1 (unit step input),

$$y(t) = K\left(1 - e^{-\frac{t}{\tau}}\right)_{t=\tau} = 0.632\,. \qquad 33$$

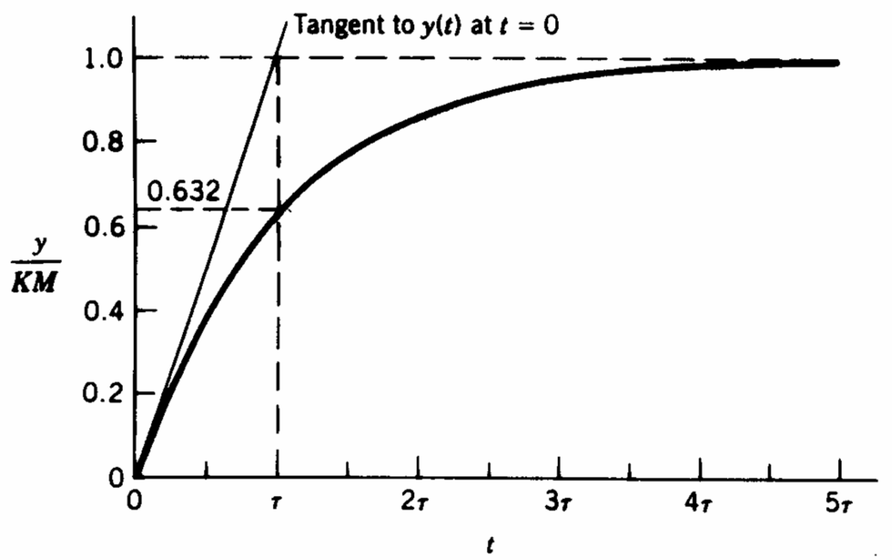


Figure 6. Step response of a first order system

2. The general form of a second order element,

$$\tau_m^2 \frac{d^2 y(t)}{dt^2} + 2\zeta\tau_m \frac{dy(t)}{dt} + y(t) = x(t) \qquad 34$$

Transfer function,

$$G(s) = \frac{Y(s)}{X(s)} = \frac{1}{\tau_m^2 s^2 + 2\zeta\tau_m s + 1} \qquad 35$$

$$= \frac{\omega_0^2}{s^2 + 2\zeta\omega_0 s + \omega_0^2} \qquad 36$$

where $\omega_0 = \dfrac{1}{\tau_m}$ is the undamped natural frequency and ζ is the damping ratio of the system.

Given a step input $x(t) = MU(t)$,

$$Y(s) = G(s)X(s) = \frac{1}{\tau^2 s^2 + 2\zeta\tau\, s + 1} \cdot \frac{M}{s} \qquad 37$$

$$y(t) = \mathcal{L}^{-1}\left[\frac{1}{\tau^2 s^2 + 2\zeta\tau\, s + 1} \cdot \frac{M}{s}\right] \qquad 38$$

We will discuss this system in great detail in later chapters.

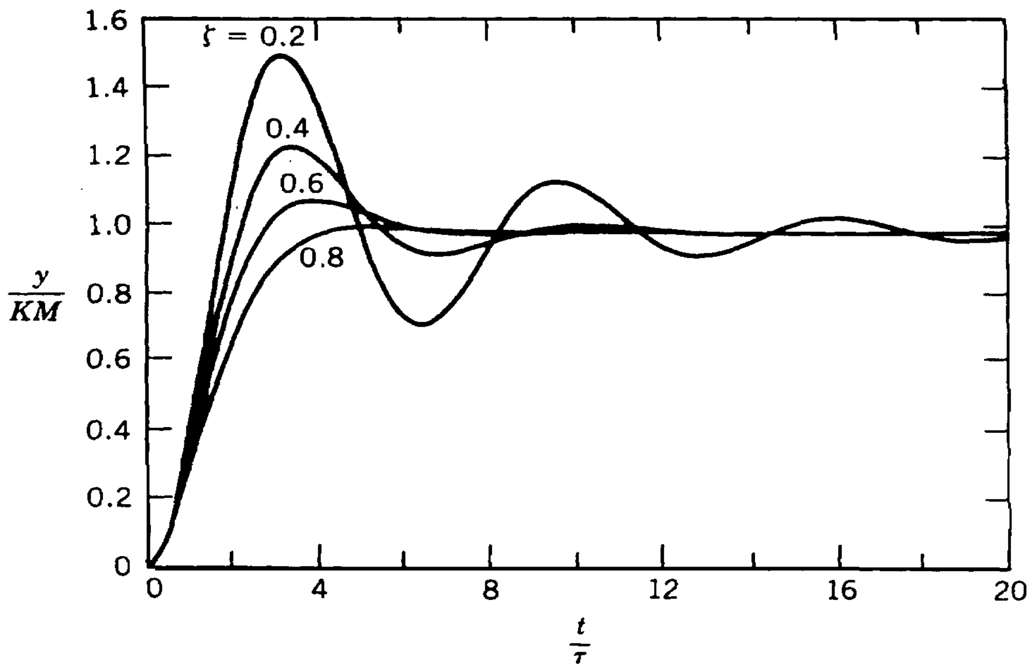


Figure 7. Step response of a second order system

3. The general form of the proportional element,

$$y(t) = Kx(t). \qquad 39$$

Its transfer function is,

$$G(s) = \frac{Y(s)}{X(s)} = K \qquad 40$$

Given a step input $x(t) = MU(t)$,

$$Y(s) = G(s)X(s) = K\frac{M}{s} \qquad 41$$

$$y(t) = \mathcal{L}^{-1}\left[K\frac{M}{s}\right] = KMU(t) \qquad 42$$

It is a step with KM as its magnitude.

4. The general form of the integral element,

$$\tau_i \frac{dy(t)}{dt} = Kx(t) \qquad 43$$

Its transfer function is,

$$G(s) = \frac{Y(s)}{X(s)} = \frac{K}{\tau_i s} \qquad 44$$

Given a step input $x(t) = MU(t)$,

$$Y(s) = G(s)X(s) = \frac{K}{\tau_i s}\frac{M}{s} \qquad 45$$

$$y(t) = \mathcal{L}^{-1}\left[\frac{KM}{\tau_i s^2}\right] = \frac{KM}{\tau_i} t \qquad 46$$

It is a ramp at the slop of KM/τ_i.

5. The general form of the differential element,

$$y(t) = \tau_d \frac{dy(t)}{dt} \qquad 47$$

Its transfer function is,

$$G(s) = \frac{Y(s)}{X(s)} = \tau_d s \qquad 48$$

Given a step input $x(t) = MU(t)$,

$$Y(s) = G(s)X(s) = \tau_d s \frac{M}{s} = \tau_d M \qquad 49$$

$$y(t) = \mathcal{L}^{-1}\left[\tau_d M\right] = \tau_d M\delta(t) \qquad 50$$

It is a impulse.

6. The general form of delay element

$$y(t) = x(t - \tau) \qquad 51$$

Its transfer function is,

$$G(s) = \frac{Y(s)}{X(s)} = e^{-\tau s} \qquad 52$$

Given a step input $x(t) = MU(t)$,

$$Y(s) = G(s)X(s) = e^{-\tau s}\frac{M}{s} \qquad 53$$

$$y(t) = \mathcal{L}^{-1}\left[e^{-\tau s}\frac{M}{s}\right] = M(t - \tau) \qquad 54$$

It is a step after a time delay of τ.

Development of Empirical Dynamic Models from Step Response Data

Higher order system and dead time

Connecting many tanks makes the system correspondingly higher order. Thus by a series of first order systems, we can get an infinite number of higher order systems. Suppose we have a well-mixed overflow tank of time constant τ. If we introduce a step increase in the inlet temperature or concentration, we will (by the well-mixed assumption) immediately detect a rise in the outlet stream – the familiar first-order lag response as in the Figure 6. If we have instead two tanks in series, each half the volume of the original, we will detect a second-order, sigmoid response at the outlet as in the Figure 7. If we continue to increase the number of tanks in the series, always maintaining the total volume, we observe a slower initial response with a faster rise around the time constant. This behavior is shown in Figure 9.

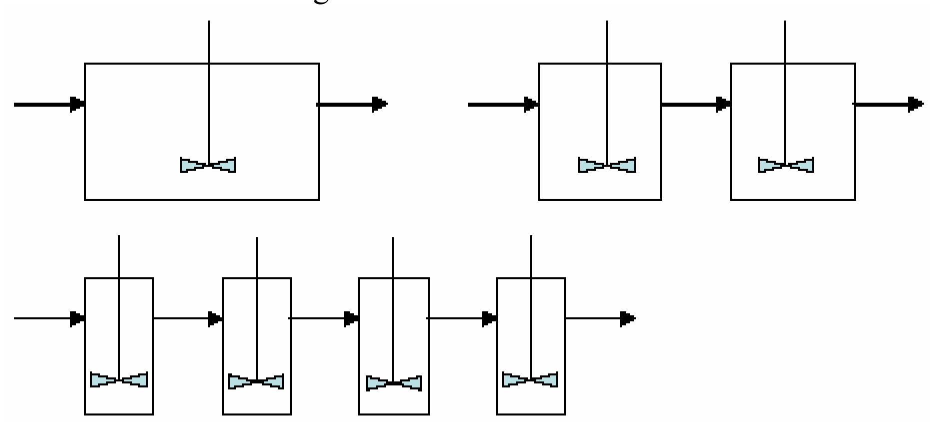


Figure 8. Well mixed tanks in series.

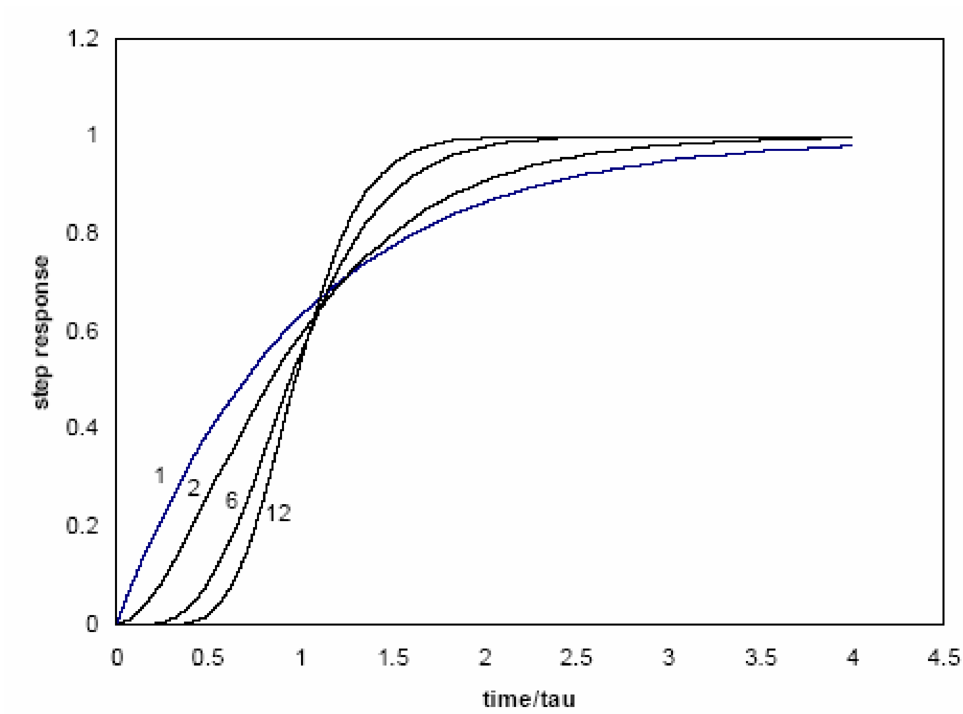


Figure 9. Time response of well mixed tanks in series.

If taken to the limit of an infinite number of tanks, we finally obtain a pure delay, in which the full step disturbance is not seen at the outlet until time τ has passed. This is the dead time, or transmission delay; it is familiar to anyone who has waited at the faucet for the hot water to arrive. That lead us to consider a simple model of the first-order-plus-time-delay.

Approximate using first-order-plus-time-delay model

The transfer function of the first-order-plus-time-delay,

$$G(s) = \frac{Ke^{-\theta}s}{\tau s + 1} \qquad 55$$

Step response,

$$y(t) = KM\left(1 - e^{-\frac{t-\theta}{\tau}}\right) \qquad 56$$

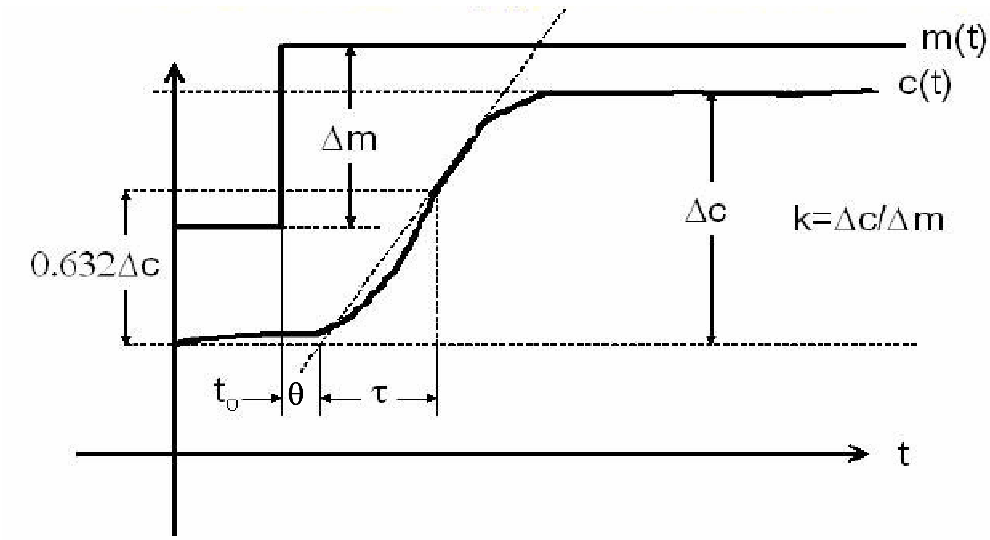


Figure 10. The time response of first-order-plus-time-delay system

For a first-order-plus-time-delay order model, we note the following characteristics (step response)

a. The response attains 63.2% of its final response at one time constant ($t = \tau + \theta$).
b. The line drawn tangent to the response at maximum slope ($t = \theta$) intersects the 100% line at ($t = \tau + \theta$). [see Fig. 10]
c. K is found from the steady state response for an input change magnitude M. The step response is essentially complete at $t = 5\tau$. In other words, the settling time is $t_s = 5\tau$.

There are two generally accepted graphical techniques for determining model parameters τ, θ, and K.

Method 1. Slope-intercept method: First, a slope is drawn through the inflection point of the process reaction curve in Figure 10. Then t and θ are determined by inspection. Alternatively, τ can be found from the time that the normalized response is 63.2% complete or from determination of the settling time, τ_s. Then set $\tau = \tau_s / 5$.

Method 2. Sundaresan and Krishnaswamy's Method: This method avoids use of the point of inflection construction entirely to estimate the time delay. They proposed that two times, t_1 and t_2, be estimated from a step response curve, corresponding to the 35.3%

and 85.3% response times, respectively. The time delay and time constant are then estimated from the following equations,

$$\theta = 1.3t_1 - 0.29t_2 \qquad 57$$

$$\tau = 0.67(t_2 - t_1) \qquad 58$$

These values of θ and τ approximately minimize the difference between the measured response and the model, based on a correlation for many data sets.

Example F-16XL Roll Mode Time Constant

In the early 1980s, two F-16 airplanes were modified to extend the fuselage length and incorporate a large area delta wing planform. These two airplanes, designated the F-16XL, were designed by the General Dynamics Corporation (now Lockheed Martin Tactical Aircraft Systems) (Fort Worth, Texas) and were prototypes for a derivative fighter evaluation program conducted by the United States Air Force.

In this method shown in figure 11, t_1 is defined as the time when the lateral stick input reaches 50 percent of maximum value. A line representing the maximum slope of the roll rate is plotted; the time at which this line intersects the x-axis is denoted as t_2. The roll rate reaches 63 percent of its maximum value at t_3. The τ_{eff} is the time difference between t_2 and t_1. The τ_r is the difference between t_2 and t_3.

A sample comparison is shown as figure 12. Although the flight data shows a higher order roll rate response, the model accurately reproduces the initial delay and roll rate onset.

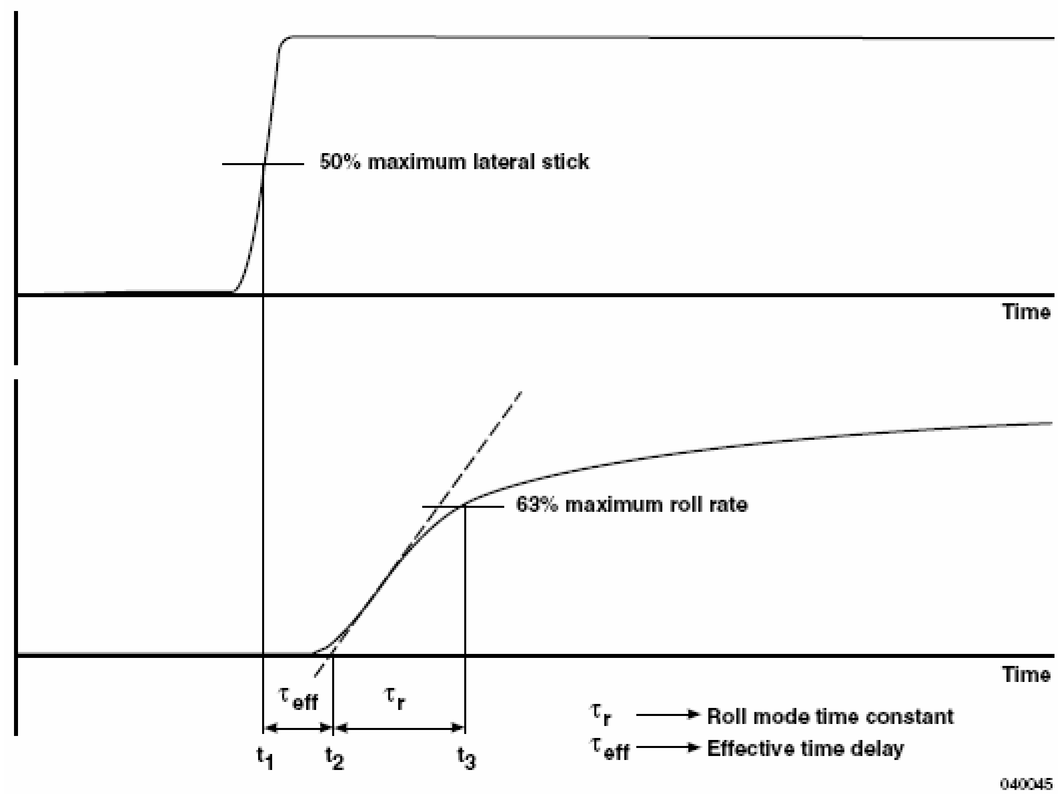


Figure 11. Time history method for τ_{eff} and τ_r calculation.

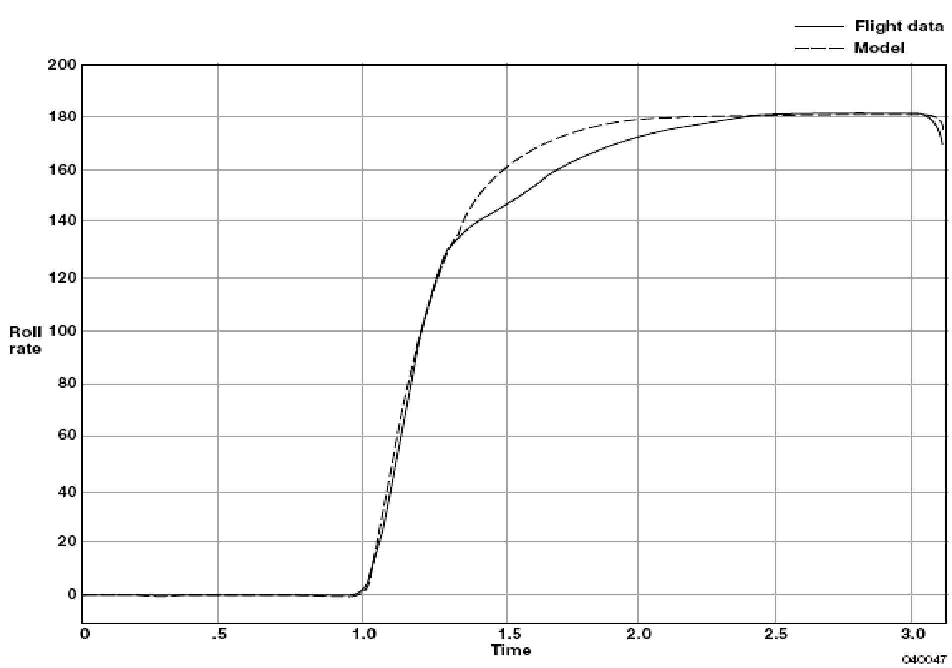


Figure 12. Sample result of comparison between model and F-16XL flight data.

Estimating Second-order Model Parameters Using Graphical Analysis

In general, a better approximation to an experimental step response can be obtained by fitting a second-order model to the data. Figure 13 shows the range of shapes that can occur for the step response model,

$$G(s) = \frac{K}{(\tau_1 s + 1)(\tau_2 s + 1)} \qquad 59$$

Figure 13 includes two limiting cases: $\tau_1/\tau_2 = 0$, where the system becomes first order, and, $\tau_1/\tau_2 = 1$, the critically damped case. The larger of the two time constants, τ_1, is called the dominant time constant. The assumed model is,

$$G(s) = \frac{Ke^{-\theta s}}{(\tau_1 s + 1)(\tau_2 s + 1)} \qquad 60$$

Parameters are estimated using so called Smith's Method,

1. Determine t_{20} and t_{60} from the step response.
2. Find ζ and t_{60}/τ from Figure 14.
3. Find t_{60}/τ from Figure 14 and then calculate τ (since t_{60} is known).

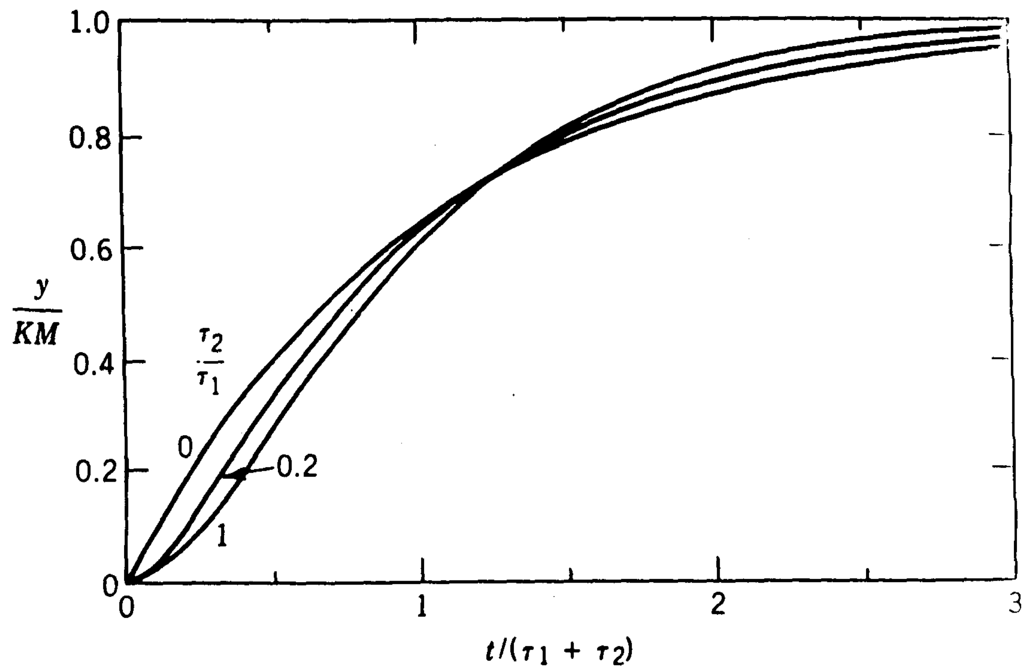


Figure 13. Step response for several overdamped second-order systems.

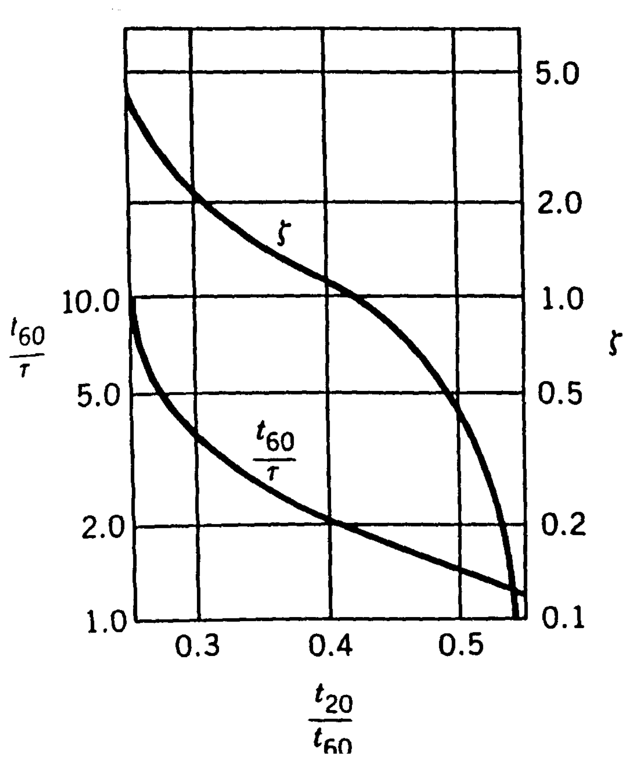


Figure 14. Relationship of ζ, τ, t_{20}, and t_{60} in Smith's method.