CM3310 Spring 2008

(Dr. Tom Co, 1/25/2008)

Lecture 5. Empirical Models

Linear First Order Process:

Standard form: $\tau \frac{dx}{dt} + x = K \qquad x(0) = x_0$

Model Parameter: τ is known as the "time constant"

Solution: $x = (x_0 - K)e^{-t/\tau} + K$

Empirical Relationships:

1. Steady state: $x_{ss} = K$
2. Time Constant: let $x(\tau) = x_\tau$, then

$$\frac{x_\tau - x_0}{K - x_0} = 1 - e^{-1} = 0.632$$

Example: (Isothermal CSTR with first order reaction, page 41, equation 2.29)

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{Ain} - C_A) - kC_A$$

Let C_{Ain} be constant. Rearrange to "fit" standard form:

$$\left(\frac{V/F}{1 + Da}\right)\frac{dC_A}{dt} + C_A = \left(\frac{1}{1 + Da}\right)C_{Ain}$$

Where Da is the "Damkohler number" defined as

$$Da = \frac{V/F}{1/k} = \text{ratio of residence time to reaction time}$$

Then the steady state is given by

$$C_{Ass} = \frac{1}{1 + Da}C_{Ain}$$

And the time constant is given by

$$\tau = \left(\frac{V/_F}{1 + Da} \right)$$

Drill: Suppose the residence time (*V/F*) is 10 hr., what is the reaction rate constant (hr^{-1}) based on Figure 1?

Ans: 2.0 hr^{-1}

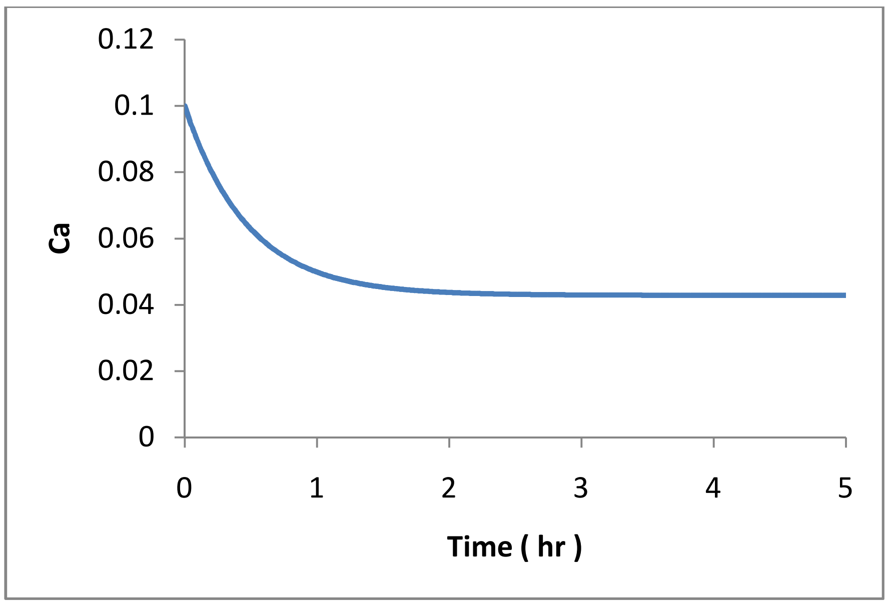

Figure 1.

Linear Second Order Process:

Standard form: $\tau_n{}^2 \frac{d^2x}{dt^2} + 2\zeta\tau_n \frac{dx}{dt} + x = K \qquad x(0) = x_0;\ \frac{dx}{dt}(0) = 0$

Parameters: ζ is known as the "damping coefficient" and
τ_n is known as the "time constant"

Solution: $x = (x_0 - K)g(t) + K$

Where

$$g(t) = \begin{cases} \left(\frac{-r_2}{r_1 - r_2}\right) e^{r_1 t} + \left(\frac{r_1}{r_1 - r_2}\right) e^{r_2 t} & \text{if } \zeta > 1 \text{ (overdamped)} \\ \left(1 + \frac{t}{\tau_n}\right) e^{-t/\tau_n} & \text{if } \zeta = 1 \text{ (critically damped)} \\ \left(\frac{1}{\sqrt{1-\zeta^2}}\right) \sin(\beta t + \phi)\ exp\left(-\zeta \frac{t}{\tau_n}\right) & \text{if } \zeta < 1 \text{ (underdamped)} \end{cases}$$

$$r_1 = \frac{-\zeta + \sqrt{\zeta^2 - 1}}{\tau_n} \qquad r_2 = \frac{-\zeta - \sqrt{\zeta^2 - 1}}{\tau_n}$$

$$\beta = \frac{\sqrt{1-\zeta^2}}{\tau_n} \qquad \phi = \tan^{-1}\left(\frac{\sqrt{1-\zeta^2}}{\zeta}\right)$$

Empirical relationships for second order underdamped process:

1. Steady state:

$$x_{ss} = K$$

2. Overshoot ratio:

$$OvR = \frac{x_{over1} - x_{ss}}{x_{ss} - x_0} = \exp\left(-\frac{\pi\zeta}{\sqrt{1-\zeta^2}}\right)$$

3. Decay ratio:

$$DecR = \frac{x_{over2} - x_{ss}}{x_{over1} - x_{ss}} = \exp\left(-\frac{2\pi\zeta}{\sqrt{1-\zeta^2}}\right) = (OvR)^2$$

4. Period of Oscillation:

$$P = t_{over2} - t_{over1}$$
$$= \frac{2\pi\tau_n}{\sqrt{1-\zeta^2}}$$

5. Frequency of Oscillation:

$$\omega = \frac{1}{P} = \frac{\sqrt{1-\zeta^2}}{2\pi\tau_n} \quad \text{(in cycles per unit time)}$$
$$\omega = 2\pi\frac{1}{P} = \frac{\sqrt{1-\zeta^2}}{\tau_n} \quad \text{(in radians per unit time)}$$

(Note: 1 Hz = 1 cycle per second)

Example: Determine the damping coefficient, and time constant that matches the plot of the underdamped manometer height reading given in Figure 2.

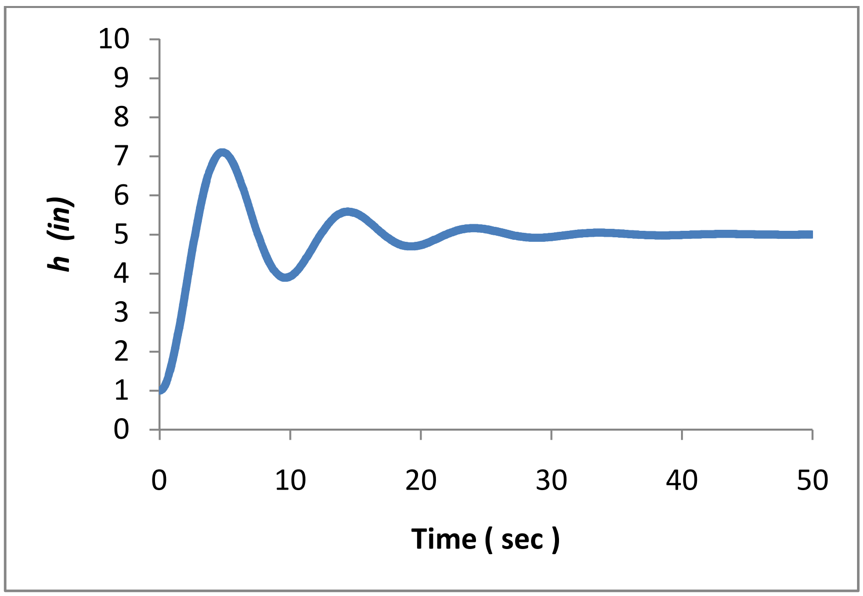

Figure 2.

From the plot we obtain the following values:

t_{over1}	5.1 sec
h_{over1}	7.07 in
t_{over2}	14.9 sec
h_{over2}	5.57 in
h_{ss}	5.0 in
h_0	1.0 in

Thus, we find

$$P = 14.9 - 5.1 = 9.8\ sec$$

$$OvR = \frac{7.07 - 5}{5 - 1} = 0.518$$

Solving for ζ and τ_n,

$$\exp\left(-\frac{\pi\zeta}{\sqrt{1-\zeta^2}}\right) = 0.518 \quad \rightarrow \quad \zeta = 0.20$$

$$\frac{2\pi\tau_n}{\sqrt{1-\zeta^2}} = 9.8 \quad \rightarrow \quad \tau_n = 1.53\ sec$$

Drill: What is the frequency in rad/sec?

Ans: 0.64 rad/sec