

CM 3310 Process Control

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Lecture 8

Modeling and Simulation

- **Motivation:** need to use other tools including computer simulation to analyze and improve performance of controlled process

Types of Mathematical Models:

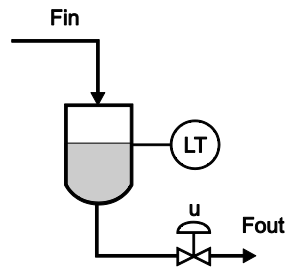
- i) Empirical models : use direct data to fit parameters of ODEs
- ii) Knowledge-based models: use physics, chemistry, etc. to obtain models
- iii) Mixed

Some Purpose of Mathematical Models:

- i) Better understand the role of various process parameters on the dynamic and steady-state behavior of the process
- ii) Allow for prediction of process outcomes, specially for prevention of undesirable outcomes such as onset of instability or potential violation of constraints

- iii) Provide equations needed for simulation runs and optimal tuning (and operator training)
- iv) Basis for testing different control strategies or process retrofits
- v) Used in feedforward-feedback control, as well as in advanced control strategies such as “model-predictive control”

Examples of Knowledge-based models: Liquid level of a tank



rate of liquid accumulation in tank = mass rate in – mass rate out

$$\frac{d(\rho Ah)}{dt} = \rho_{in} F_{in} - \rho_{out} F_{out}$$

where F_{in} and F_{out} are volumetric flow rates in and out, respectively.

Assume $\rho = \rho_{in} = \rho_{out} = \text{constant}$ and A is constant. Using Toricelli's law:

$$F_{out} = k_v u \sqrt{h}$$

$$\rightarrow A \frac{dh}{dt} = F_{in} - k_v u \sqrt{h} \quad (1)$$

Remarks:

1. Due to the term $u\sqrt{h}$, equation is no longer a linear ODE. Thus, the previous analysis methods do not apply immediately.
2. Generally, analytical solutions for nonlinear models are difficult to obtain. Instead, simulations are used.
3. However, for “local analysis”, a linear approximation can be used. This process which is known as “linearization” will replace the original nonlinear equation such as (1) by a linear equation.
4. The linear equation can then be analyzed for local stability and dynamic behavior using our previous methods (as long as the variables continue to reside in the small neighborhood of the chosen operating point).

Linearization of nonlinear functions

Given: nonlinear function $f(x, y, z)$ and “nominal/operating” point (x_o, y_o, z_o)

Linearized approximation:

$$f(x, y, z) \approx \alpha_0 + \alpha_1(x - x_o) + \alpha_2(y - y_o) + \alpha_3(z - z_o) \quad (2)$$

where

$$\alpha_0 = f(x_o, y_o, z_o)$$

$$\alpha_1 = \left. \frac{\partial f}{\partial x} \right|_{(x_o, y_o, z_o)}$$

$$\alpha_2 = \left. \frac{\partial f}{\partial y} \right|_{(x_o, y_o, z_o)}$$

$$\alpha_3 = \left. \frac{\partial f}{\partial z} \right|_{(x_o, y_o, z_o)}$$

Remarks:

1. Linear approximation is often valid in a “small” region around the operating conditions only.
2. Link to <http://pages.mtu.edu/~tbco/cm416/Linearization.pdf> for a short derivation

Returning to the tank level model in (1) and divide it by A

$$\frac{dh}{dt} = \frac{F_{in} - k_v u \sqrt{h}}{A} \quad (3)$$

with

- h as the process variable,
- u as the valve opening
- F_{in} as the disturbance variable.

(The valve coefficient k_v will be considered as a “parameter”, i.e. it is expected not to change during the process but is a fixed number that is associated with manufacture of the valve. Likewise, A is the cross-sectional area of the cylindrical tank which is fixed by design, and thus treated as a parameter.)

Linearizing the right-hand side of equation at operating point $(h_0, u_0, F_{in,0})$:

$$\begin{aligned} f(h, u, F_{in}) &= \frac{F_{in} - k_v u \sqrt{h}}{A} \\ &\approx \alpha_0 + \alpha_1(h - h_0) + \alpha_2(u - u_0) + \alpha_3(F_{in} - F_{in,0}) \end{aligned}$$

Where

$$\begin{aligned} \alpha_0 &= \frac{F_{in,0} - k_v u_0 \sqrt{h_0}}{A} \\ \alpha_1 &= \left. \frac{\partial f}{\partial h} \right|_{h_0, u_0, F_{in,0}} = \frac{-k_v u_0}{2A\sqrt{h_0}} \\ \alpha_2 &= \left. \frac{\partial f}{\partial u} \right|_{h_0, u_0, F_{in,0}} = \frac{-k_v \sqrt{h_0}}{A} \\ \alpha_3 &= \left. \frac{\partial f}{\partial F_{in}} \right|_{h_0, u_0, F_{in,0}} = \frac{1}{A} \end{aligned}$$

Note: Although the forms of the various coefficients appear to be complicated, they simply attain a numerical value at the chosen operating points and should be treated as such.

Substituting back to (3),

$$\frac{dh}{dt} = \alpha_0 + \alpha_1(h - h_0) + \alpha_2(u - u_0) + \alpha_3(F_{in} - F_{in0})$$

Or

$$\frac{dh}{dt} - \alpha_1 h = \alpha_2 u + \alpha_3 F_{in} + \left[\alpha_0 - \alpha_1 h_0 - \alpha_2 u_0 - \alpha_3 F_{in0} \right]$$

$$\left(\frac{2A\sqrt{h_0}}{k_v u_0} \right) \frac{dh}{dt} + h = \left(-\frac{2h_0}{u_0} \right) u + \left(\frac{2\sqrt{h_0}}{k_v u_0} \right) F_{in} + \beta$$

$$\text{where } \beta = h_0 \left(\frac{3A+2}{A} \right) + \frac{2F_{in0}\sqrt{h_0}}{k_v u_0} \left(\frac{A-1}{A} \right)$$

The time constant and process gain of the linearized system are thus

$$\tau = \frac{2A\sqrt{h_0}}{k_v u_0} \quad K_p = -\frac{2h_0}{u_0}$$

Caution: It appears like both these terms are not affected by the disturbance. However, since operating point are often to be at a chosen steady state $\rightarrow$ both u_0 and h_0 will both depend on F_{in0} . Thus τ and K_p will ultimately be affected by F_{in0} .

Numerical approach to obtaining Linearized Models:

- In some cases, obtaining the coefficients in a set of linearized models may require complex partial differentiations
- If the numerical values of the process parameters as well as the operating points are already given, then one can use the numerical (finite difference) approximation of the partial derivatives

Given: $f(x, y, z)$ and (x_0, y_0, z_0)

Linearized approximation:

$$f(x, y, z) \approx \alpha_0 + \alpha_1(x - x_0) + \alpha_2(y - y_0) + \alpha_3(z - z_0)$$

where,

$$\begin{aligned} \alpha_0 &= f(x_0, y_0, z_0) \\ \alpha_1 &= \left. \frac{\partial f}{\partial x} \right|_{x_0, y_0, z_0} \approx \frac{f(x_0 + \Delta x, y_0, z_0) - f(x_0, y_0, z_0)}{\Delta x} \\ \alpha_2 &= \left. \frac{\partial f}{\partial y} \right|_{x_0, y_0, z_0} \approx \frac{f(x_0, y_0 + \Delta y, z_0) - f(x_0, y_0, z_0)}{\Delta y} \end{aligned}$$

$$\alpha_3 = \left. \frac{\partial f}{\partial z} \right|_{x_0, y_0, z_0} \approx \frac{f(x_0, y_0, z_0 + \Delta z) - f(x_0, y_0, z_0)}{\Delta z}$$

Note: with $\Delta x = \varepsilon \cdot x_0, \Delta y = \varepsilon \cdot y_0, \Delta z = \varepsilon \cdot z_0$, often choose $10^{-4} < \varepsilon < 0.01$

Example:

Obtain a linearization of the following coupled set of ODEs:

$$\begin{aligned} \frac{dx}{dt} &= -kx^2y + \beta e^{-(y/x)} \\ \frac{dy}{dt} &= -\sqrt{x^2 + \sigma y} \end{aligned}$$

around the operating point $(x_o, y_o) = (1, 0.5)$ for parameter values of $k = 2, \beta = 0.75$ and $\sigma = 2.2$.

Solution: The linearization can be obtained for each equation separately. Thus, with

$$\frac{dx}{dt} = f(x, y) \quad \text{and} \quad \frac{dy}{dt} = g(x, y)$$

we linearize $f(x, y)$ and $g(x, y)$ as follows:

$$f(x, y) \approx \alpha_0 + \alpha_1(x - x_0) + \alpha_2(y - y_0)$$

$$g(x, y) \approx \gamma_0 + \gamma_1(x - x_0) + \gamma_2(y - y_0)$$

with the coefficients evaluated as follows:

$$\alpha_0 = f(x_0, y_0) = -0.545$$

$$\alpha_1 = \frac{f(x_0 + \Delta x, y_0) - f(x_0, y_0)}{\Delta x} = -1.773$$

$$\alpha_2 = \frac{f(x_0, y_0 + \Delta y) - f(x_0, y_0)}{\Delta y} = -2.455$$

$$\gamma_0 = g(x_0, y_0) = -1.449$$

$$\gamma_1 = \frac{g(x_0 + \Delta x, y_0) - g(x_0, y_0)}{\Delta x} = -0.690$$

$$\gamma_2 = \frac{g(x_0, y_0 + \Delta y) - g(x_0, y_0)}{\Delta y} = -0.759$$

So finally, the linearized set of ODEs are:

$$\frac{dx}{dy} = -0.545 - 1.773(x - 1) - 2.455(y - 0.5)$$

$$\frac{dy}{dt} = -1.449 - 0.690(x - 1) - 0.759(y - 0.5)$$

Or after further rearrangement,

$$\frac{dx}{dt} = -1.773x - 2.455y + 2.455$$

$$\frac{dy}{dt} = -0.690x - 0.759y - 0.380$$

Question: How does one analyze behavior of processes having more than one process variables?

Example 2: A CSTR model after linearization might yield the following model

$$\frac{dC_A}{dt} = a_{11}C_A + a_{12}T + b_1u \quad (4)$$

$$\frac{dT}{dt} = a_{21}C_A + a_{22}T \quad (5)$$

Subject to: $C_A(0) = C_{Ao}$, $T(0) = T_o$

Answer: We could take derivatives and algebraic substitutions to reduce the problem to have a differential equation involving only one of the process variables.

Example 2 (continued):

- First take (d/dt) of ODE (4)

$$\frac{d^2C_A}{dt^2} = a_{11} \frac{dC_A}{dt} + a_{12} \frac{dT}{dt} + b_1 \frac{du}{dt} \quad (6)$$

- Next, substitute for (dT/dt) the right hand side of ODE (5),

$$\frac{d^2 C_A}{dt^2} = a_{11} \frac{dC_A}{dt} + a_{12}(a_{21}C_A + a_{22}T) + b_1 \frac{du}{dt} \quad (7)$$

or

$$\frac{d^2 C_A}{dt^2} - a_{11} \frac{dC_A}{dt} - a_{12}a_{21}C_A = a_{12}a_{22}T + b_1 \frac{du}{dt} \quad (8)$$

- Solve for T in ODE (4),

$$T = \frac{1}{a_{12}} \left(\frac{dC_A}{dt} - a_{11}C_A \right) - b_1 u \quad (9)$$

- Next, substitute the value of T from (9) into ODE (8),

$$\frac{d^2 C_A}{dt^2} - a_{11} \frac{dC_A}{dt} - a_{12}a_{21}C_A = a_{22} \left(\frac{dC_A}{dt} - a_{11}C_A \right) - a_{22}b_1 u + b_1 \frac{du}{dt} \quad (10)$$

Or,

$$\frac{d^2 C_A}{dt^2} - (a_{11} + a_{22}) \frac{dC_A}{dt} + (a_{11}a_{22} - a_{12}a_{21})C_A = -a_{22}b_1 u + b_1 \frac{du}{dt} \quad (11)$$

- If we had first taken (d/dt) of ODE (5) first, after a similar approach, we will arrive at

$$\frac{d^2 T}{dt^2} - (a_{11} + a_{22}) \frac{dT}{dt} + (a_{11}a_{22} - a_{12}a_{21})T = a_{21}b_1 u \quad (12)$$

In conclusion, for a set of n coupled linear 1st order ODEs involving the n variables given by

$$\frac{dy_1}{dt} = a_{11}y_1 + \dots + a_{1n}y_n + b_1 u$$

⋮

$$\frac{dy_n}{dt} = a_{n1}y_1 + \dots + a_{nn}y_n + b_n u$$

one can transform the problem to n decoupled ODEs for each variable given by

$$\gamma_n \frac{d^n y_1}{dt^n} + \dots + \gamma_1 \frac{dy_1}{dt} + \gamma_0 y_1 = k_{10}u + \dots + k_{1,n-1} \frac{d^{n-1}u}{dt^{n-1}}$$

⋮

$$\gamma_n \frac{d^n y_n}{dt^n} + \dots + \gamma_1 \frac{dy_n}{dt} + \gamma_0 y_n = k_{n0}u + \dots + k_{n,n-1} \frac{d^{n-1}u}{dt^{n-1}}$$

All are sharing the same characteristic equation:

$$\gamma_n \lambda^n + \dots + \gamma_1 \lambda + \gamma_0 = 0$$

and the same eigenvalues: $\lambda_1, \dots, \lambda_n$.

When analyzing the closed-loop behavior, one should first apply (i.e. substitute) the control laws, prior to reduction to the decoupled forms.

Example: Analyze the behavior of the following open-loop model using a proportional control law: $u = 1.5 (T_{set} - T)$

$$\begin{aligned}\frac{dT}{dt} &= -3T + C + 3u \\ \frac{dC}{dt} &= T - 4C\end{aligned}$$

Solution: First substitute control law

$$\begin{aligned}\frac{dT}{dt} &= -3T + C + 3 \left[1.5(T_{set} - T) \right] \\ \frac{dC}{dt} &= T - 4C\end{aligned}$$

then

$$\begin{aligned}\frac{dT}{dt} &= -7.5T + C + 4.5 T_{set} \\ \frac{dC}{dt} &= T - 4C\end{aligned}$$

and proceed as we did before to yield:

$$\begin{aligned}\frac{d^2T}{dt^2} + 11.5 \frac{dT}{dt} + 29T &= 4.5 \frac{dT_{set}}{dt} + 18 T_{set} \\ \frac{d^2C}{dt^2} + 11.5 \frac{dC}{dt} + 29C &= 4.5 T_{set}\end{aligned}$$

Thus, put in our standard forms and assuming T_{set} constant:

$$\begin{aligned}\left(\frac{1}{29}\right) \frac{d^2T}{dt^2} + \left(\frac{11.5}{29}\right) \frac{dT}{dt} + T &= \left(\frac{18}{29}\right) T_{set} \\ \left(\frac{1}{29}\right) \frac{d^2C}{dt^2} + \left(\frac{11.5}{29}\right) \frac{dC}{dt} + C &= \left(\frac{4.5}{29}\right) T_{set}\end{aligned}$$

From which we can evaluate $\tau_n = 0.185$ and $\zeta = 1.07$, i.e. both T and C will follow overdamped responses.

Note: An alternative approach to the substitution approach used above will be to use matrix methods (to be discussed in later lectures)