

Special Modeling Techniques

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Summary of Topics

There are two special topics that are useful and possibly required to use Laplace transform techniques to solve our process dynamics problems:

- Deviation variables.
- Linearization of ODEs.

Deviation Variables

It may be convenient to use deviation variables when modeling a problem. Deviation variables are simply the difference of the actual variable to the original value.

Mathematically:

$$y'(t) \equiv y(t) - y(0) = y(t) - y^*$$

when our initial condition corresponds to an initial steady state ($y(0) = y^*$). This is convenient because it greatly simplifies the application of the Laplace transform. Transforming an n-th order derivative to Laplace space requires the first (n-1) derivatives at $t = 0$. If we use deviation variables, these will all be zero. So, an n-th order ODE in the form of:

$$a_n \frac{d^n y'}{dt^n} + a_{n-1} \frac{d^{n-1} y'}{dt^{n-1}} + \dots + a_2 \frac{d^2 y'}{dt^2} + a_1 \frac{dy'}{dt} + a_0 y' = f'(t)$$

simply becomes an n-th order polynomial in s :

$$(a_n s^n + a_{n-1} s^{n-1} + \dots + a_2 s^2 + a_1 s + a_0) \bar{y}' = \bar{f}'(t).$$

How do we convert our original ODE to be in terms of deviation variables? Substitute in & separate out the terms involving the initial conditions. If we start from a steady state condition then the combination of terms involving the initial condition will be equal to zero & disappear. For the n-th order ODE let's insert the sum of the deviation variable & the steady state value in for the variables:

$$a_n \frac{d^n y}{dt^n} + a_{n-1} \frac{d^{n-1} y}{dt^{n-1}} + \dots + a_1 \frac{dy}{dt} + a_0 y = f(t)$$
$$a_n \frac{d^n (y' + y^*)}{dt^n} + a_{n-1} \frac{d^{n-1} (y' + y^*)}{dt^{n-1}} + \dots + a_1 \frac{d(y' + y^*)}{dt} + a_0 (y' + y^*) = (f' + f^*)$$

Since the time derivative of steady state variables are zero:

$$a_n \frac{d^n y'}{dt^n} + a_{n-1} \frac{d^{n-1} y'}{dt^{n-1}} + \dots + a_1 \frac{dy'}{dt} + a_0 (y' + y^*) = (f' + f^*)$$

Let's group the steady state variables together:

$$a_n \frac{d^n y'}{dt^n} + a_{n-1} \frac{d^{n-1} y'}{dt^{n-1}} + \dots + a_1 \frac{dy'}{dt} + a_0 y' = f' + (f^* - a_0 y^*)$$

But since at the steady state variables are related by $f^* - a_0 y^* = 0$:

$$a_n \frac{d^n y'}{dt^n} + a_{n-1} \frac{d^{n-1} y'}{dt^{n-1}} + \dots + a_1 \frac{dy'}{dt} + a_0 y' = f' .$$

It appears that all we've done is change the original variables directly to the deviation variables, but we've really done more than just that.

As an example, let's look at the equation that comes from the mass balance on an upright cylindrical tank with a liquid of constant density. This equation will be:

$$A \frac{dh}{dt} = F_0 - F_1$$

where h , F_0 , and F_1 can all be functions of time. Since it is an ODE, we also need a **boundary condition**. If the condition is set at $t = 0$, then it is an **initial condition**. If we consider that we are modeling a perturbation to the steady state condition, then the initial condition is for steady state, or:

$$\text{IC: } \frac{dh}{dt} = 0 \Rightarrow F_0^* = F_1^*.$$

If we relate the outlet flow to the tank level, then we can get our steady state level, h^* . Let's assume the outlet flow is proportional to the level, or $F_1 = C_1 h$. Then:

$$A \frac{dh}{dt} = F_0 - C_1 h$$
$$\text{IC: } F_0^* = C_1 h_1^* \Rightarrow h^* = \frac{F_0^*}{C_1}.$$

Let's define the deviation variables:

$$h'(t) \equiv h(t) - h^*$$
$$F_0'(t) \equiv F_0(t) - F_0^*$$

Now the ODE & IC are:

$$A \frac{d}{dt}(h' + h^*) = (F_0' + F_0^*) - C_1(h' + h^*)$$
$$A \frac{dh'}{dt} + A \frac{dh^*}{dt} = (F_0' - C_1 h') + (F_0^* - C_1 h^*)$$

and: $A \frac{dh'}{dt} = F_0' - C_1 h'$

with: $h'(0) = 0$.

With deviation variables, the initial conditions will always be zeros, which may be easier to work with to solve the ODEs (especially when using Laplace transforms).

Non-Linear Differential Equations

Non-linear ODEs are ones with at least one non-linear term (other than those involving t). So, the following ODE is non-linear:

$$\frac{dy}{dt} + y^2 = t^2$$

whereas the following is still linear:

$$\frac{dy}{dt} + y = t^2.$$

Deviation variables are not necessarily easier to work with when dealing with non-linear ODEs. For example, for the tank problem with a non-linear valve:

$$A \frac{dh}{dt} = F_0 - C_1 \sqrt{h}$$

when we apply deviation variables we get:

$$A \frac{dh'}{dt} = F_0' + F_0^* - C_1 \sqrt{h' + h^*}.$$

In this case we cannot factor out & eliminate the steady state values.

Linearization of ODEs for Approximate Solutions

There are more methods for solving linear ODEs than for solving non-linear ODEs. Sometimes the solution to the **linearized** ODE may be close enough to the solution of the original non-linear ODE that it may be of use. This is especially true when the driving function is a disturbance around the steady-state value. Presumably, the changes to the state variable are fairly small.

Make use of Taylor series expansion to expand the function $f(x)$ around $x = x_0$:

$$f(x) = f(x_0) + \left. \frac{df}{dx} \right|_{x=x_0} (x - x_0) + \frac{1}{2!} \left. \frac{d^2 f}{dx^2} \right|_{x=x_0} (x - x_0)^2 + \dots + \frac{1}{n!} \left. \frac{d^n f}{dx^n} \right|_{x=x_0} (x - x_0)^n + \dots$$

We can linearize by dropping all of the 2nd order terms and higher. So:

$$f(x) \approx f(x_0) + \left. \frac{df}{dx} \right|_{x=x_0} (x - x_0).$$

As an example, let's look at flow through a tank with non-linear valve characteristics:

$$A_1 \frac{dh_1}{dt} = F_0 - F_1 = F_0 - C_v \sqrt{h_1} \Rightarrow A_1 \frac{dh_1}{dt} + C_v \sqrt{h_1} = F_0.$$

The $\sqrt{h_1}$ term makes the ODE non-linear. However, let's do a Taylor series expansion of terms around the steady state value h_1^* :

$$F_1(h_1) = F_1(h_1^*) + \left. \frac{dF_1}{dh_1} \right|_{h_1=h_1^*} (h_1 - h_1^*) + \frac{1}{2} \left. \frac{d^2F_1}{dh_1^2} \right|_{h_1=h_1^*} (h_1 - h_1^*)^2 + \frac{1}{6} \left. \frac{d^3F_1}{dh_1^3} \right|_{h_1=h_1^*} (h_1 - h_1^*)^3 + \dots$$

We will denote $F_1(h_1^*) \equiv F_1^* = F_0^*$ (since, at steady state, the flows in & out are equal). We also know that:

$$F_1 = C_v \sqrt{h_1} \Rightarrow \frac{dF_1}{dh_1} = \frac{C_v}{2\sqrt{h_1}} \Rightarrow \left. \frac{dF_1}{dh_1} \right|_{h_1=h_1^*} = \frac{C_v}{2\sqrt{h_1^*}}$$

So, keeping only the first or linear term from the expansion:

$$A_1 \frac{dh_1}{dt} = F_0 - F_1 \approx F_0 - F_0^* - \frac{C_v (h_1 - h_1^*)}{2\sqrt{h_1^*}}$$

$$A_1 \frac{dh_1}{dt} + \frac{C_v (h_1 - h_1^*)}{2\sqrt{h_1^*}} = F_0 - F_0^*$$

Using deviation variables $h_1' \equiv h_1 - h_1^*$ and $F_0' = F_0 - F_0^*$, then:

$$A_1 \frac{dh_1'}{dt} + \left(\frac{C_v}{2\sqrt{h_1^*}} \right) h_1' = F_0'$$

Even though there is still a non-linear term in the expression, $\sqrt{h_1^*}$, it is a constant so does not affect the linear/non-linear nature of the ODE.

There are other terms that may be need to be linearized:

- Effect of geometry: horizontal cylinder volume vs. liquid level.
- Effect of temperature on reaction rate: $k_A = k_{A,0} e^{-E_A/RT}$.
- Effect of non-linear reaction rate kinetics: $r_A = k_A C_A^2$.

Conversion to Deviation Variables & Linearization of ODEs in a Combined Operation

We can linearize the ODE & insert deviation variables directly in a single combined operation that works just as well for linear and non-linear ODES. The procedure is:

- Consider the ODE to have the form of:

$$C \frac{dy}{dt} = F(x_1, x_2, \dots, x_N, y)$$

where C is a constant.

- Find the total differential of the right-hand-side function:

$$dF = \left(\frac{\partial F}{\partial x_1} \right) dx_1 + \left(\frac{\partial F}{\partial x_2} \right) dx_2 + \dots + \left(\frac{\partial F}{\partial x_N} \right) dx_N + \left(\frac{\partial F}{\partial y} \right) dy$$

where the partial derivatives are found by holding all other variables constant.

- Approximate the total differential as the finite difference from the initial steady state, i.e., as the finite deviation variable:

$$dF \approx \Delta F = F - F^* = F'$$

$$dx_1 \approx \Delta x_1 = x_1 - x_1^* = x'_1 \quad \text{and so on.}$$

Any partial derivative that is not a constant is to be set equal to its value at the initial steady state:

$$dF \approx F' = \left(\frac{\partial F}{\partial x_1} \right)^* x'_1 + \left(\frac{\partial F}{\partial x_2} \right)^* x'_2 + \dots + \left(\frac{\partial F}{\partial x_1} \right)^* x'_2 + \left(\frac{\partial F}{\partial y} \right)^* y'$$

- Change the ODE from terms of the original variable to that of the deviation variable. Insert the approximate form of the total differential:

$$C \frac{dy'}{dt} = \left(\frac{\partial F}{\partial x_1} \right)^* x'_1 + \left(\frac{\partial F}{\partial x_2} \right)^* x'_2 + \dots + \left(\frac{\partial F}{\partial x_1} \right)^* x'_2 + \left(\frac{\partial F}{\partial y} \right)^* y'$$

This procedure will work whether the ODE is linear or non-linear.

Linear Example: Heated Stirred Tank with Constant Inlet Flow

The heat balance equation for a stirred tank with a steam heating coil is:

$$\rho V \hat{C}_p \frac{dT_1}{dt} = \rho F_0 \hat{C}_p (T_0 - T_1) + UA(T_s - T_1)$$

If the inlet flow rate F_0 is a constant then the only variables besides T_1 are T_0 and T_s . The total differential to the right-hand-side function is:

$$d[\rho F_0 \hat{C}_p (T_0 - T_1) + UA(T_s - T_1)] = [\rho F_0 \hat{C}_p] dT_0 + [UA] dT_s - [\rho F_0 \hat{C}_p + UA] dT_1.$$

Since all of the terms in the brackets are constants they can be inserted into the original ODE without any real change to the accuracy of the original ODE:

$$\rho V \hat{C}_p \frac{dT_1'}{dt} = [\rho F_0 \hat{C}_p] T_0' + [UA] T_s' - [\rho F_0 \hat{C}_p + UA] T_1'.$$

Non-Linear Example: Heated Stirred Tank with Variable Inlet Flow

This heat balance equation is the same:

$$\rho V \hat{C}_p \frac{dT_1}{dt} = \rho F_0 \hat{C}_p (T_0 - T_1) + UA(T_s - T_1)$$

but now the inlet flow rate F_0 is also a variable. The total differential to the right-hand-side function is:

$$d[\rho F_0 \hat{C}_p (T_0 - T_1) + UA(T_s - T_1)] = [\rho \hat{C}_p (T_0 - T_1)] dF_0 + [\rho F_0 \hat{C}_p] dT_0 + [UA] dT_s - [\rho F_0 \hat{C}_p + UA] dT_1$$

Now the only bracketed term that is constant is the one in front of the dT_s differential – all other bracketed terms have some variable term in them. The terms involving T_0 , T_1 , or F_0 evaluated at the original steady state condition and then inserted into the original ODE:

$$\rho V \hat{C}_p \frac{dT_1'}{dt} = [\rho \hat{C}_p (T_0^* - T_1^*)] F_0' + [\rho F_0^* \hat{C}_p] T_0' + [UA] T_s' - [\rho F_0^* \hat{C}_p + UA] T_1'.$$

Now the original ODE has been modified – the effect of the flow rate has been linearized.

Non-Linear Example: Flow Through Valve with Non-Linear Characteristics

Let's look at our flow through a tank with non-linear valve characteristics again:

$$A_1 \frac{dh_1}{dt} = F_0 - F_1 = F_0 - C_v \sqrt{h_1}.$$

We know that h_1 is a variable – the inlet flow F_0 is the other possible variable. The total differential to the right-hand-side variable is:

$$d[F_0 - C_v \sqrt{h_1}] = dF_0 - \left[\frac{C_v}{2\sqrt{h_1}} \right] dh_1.$$

The bracketed term in front of dh_1 is a variable so we will use its constant value evaluated at h_1^* . Inserting into the original ODE & converting differentials to deviation variables:

$$A_1 \frac{dh_1'}{dt} = F_0' - \left[\frac{C_v}{2\sqrt{h_1^*}} \right] h_1'.$$

Since we are holding the coefficient on h_1' constant we have approximated the original non-linear ODE with a linearized version.