

This is the process that we will use to write and solve dynamic process models.

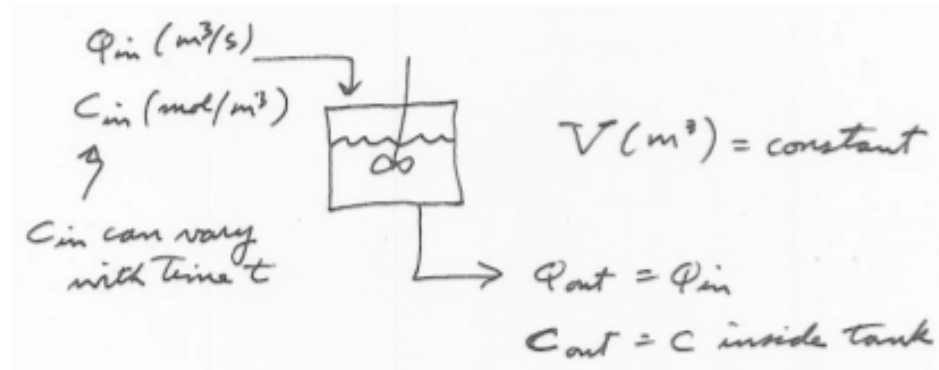
- 1) Write unsteady-state balance equation. In this class, we will write material and energy balances. This step will result in one or more differential equations.
- 2) Linearize the differential equation if necessary. In this class, we only consider linear differential equations. Linearization is accomplished by applying the first-order Taylor approximation (Taylor expansion) to nonlinear terms. Linearized equations are approximate for small deviations from an initial state.
- 3) Define deviation variables. We will consider how the process deviates from an initial steady-condition that we specify.
- 4) Apply the Laplace transform. In most cases, we can lookup the transform terms in a table of Laplace transforms, e.g., on p. 10 of Chau's textbook.
- 5) Solve the resulting algebraic equation for the transform of the output variable in terms of the "transfer function" of the process times the transform of the input variable. Specify the input variable as a function of time and apply the Laplace transform.
- 6) Apply the inverse transform in order to transform the solution from the frequency domain, or Laplace transform domain, back into the time domain. We may need to separate the equation into a sum of simple terms by doing a "partial-fraction expansion." After partial-fraction expansion, we can lookup the terms in a table of Laplace transforms.

Here is a simple process, a tank containing a constant volume of liquid and with constant inlet and outlet flow rates of liquid.

A chemical component is present in the inlet flow to the tank. The concentration of this component can change with time without changing the flow rates of liquid.

As the inlet concentration changes, the concentration in the tank will change.

The tank is well-mixed such that the concentration in the outlet pipe is the same as that everywhere inside the tank.



Now write a component balance around the volume of liquid in the tank:

COMPONENT BALANCE

$$\text{ACCUM} = \text{IN} - \text{OUT} + \text{GEN}$$

$$V \frac{dC}{dt} = \phi C_{in} - \phi C_{out} + 0 \text{ (NO RXN)}$$

$\frac{\text{m}^3 \text{ mol}}{\text{m}^3 \cdot \text{s}} \quad \frac{\text{m}^3 \text{ mol}}{\text{s} \text{ m}^3}$

Rearranging,

$$\tau \frac{dC}{dt} + C = \overset{\substack{\uparrow \\ \text{FORCING FUNCTION, INPUT}}}{C_{in}(t)}$$

where  $\tau \equiv \frac{V}{\phi}$  &  $\tau$  has units of sec.

where we have defined the space time  $\tau$ . The right hand side of the equation is the forcing function or input.

This equation is a linear equation, so we don't have to linearize it.

Now define deviation variables. The initial steady-state conditions are denoted by a subscript s.

$$C(0) = C_s$$

$$C_{IN}(0) = C_{IN,s}$$

The deviation variables are denoted by a superscript delta. Chau's book uses an apostrophe, but an apostrophe is also used to signify a derivative, so I prefer to use a delta.

$$C^{\Delta} = C - C_s \quad \Rightarrow \quad C = C^{\Delta} + C_s$$

$$C_{IN}^{\Delta} = C_{IN} - C_{IN,s} \quad \Rightarrow \quad C_{IN} = C_{IN}^{\Delta} + C_{IN,s}$$

Now substitute the deviation variables into the system equation:

$$\tau \frac{dC^{\Delta}}{dt} + \tau \frac{dC_s}{dt} + C^{\Delta} + C_s = C_{IN}^{\Delta} + C_{IN,s}$$

$$\tau \frac{dC^A}{dt} + \tau \frac{dC_S}{dt} + C^A + C_S = C_{IN}^A + C_{IN,S}$$

AT INITIAL STEADY STATE

$$\tau \frac{dC_S}{dt} + C_S = C_{IN,S}$$

↓  
@ SS

$$\tau \frac{dC^A}{dt} + C^A = C_{IN}^A$$

Now we have our system equation in terms of the deviation variables.

The next step is to apply the Laplace Transform. The values of the deviation variables are zero at time zero.

$$\mathcal{L}\left[\frac{dC^A}{dt}\right] = sG(s) - C^A(t=0) = sG(s) \quad \mathcal{L}[C^A(t)] = G(s)$$

Time domain differential equation:

$$\tau \frac{dC^A}{dt} + C^A = C_{in}^A$$

Frequency domain algebraic equation:

$$\tau s G(s) + G(s) = G_{in}(s)$$

Now solve the transform equation for the transform of the output variable.

$$G(s) = \left( \frac{1}{\tau s + 1} \right) G_{in}(s)$$

$$G(s) = G_p(s) G_{in}(s)$$

The transform of the output variable equals the "transfer function" of the process,  $G_p(s)$ , times the transform of the input variable. For this process,

$$G_p(s) = \left( \frac{1}{\tau s + 1} \right)$$

Now we are ready to specify our forcing function, the deviation in the inlet concentration as a function of time.

As an example, consider a Dirac delta input, also termed a unit impulse input.

$$\delta(t - t_j) = 0 \quad \text{for } t < t_j \quad \text{where } t_j \text{ is the time at which the input occurs}$$

$$\delta(t - t_j) = 0 \quad \text{for } t > t_j$$

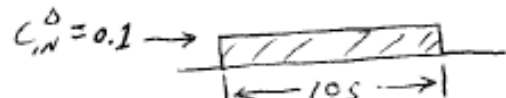
$$\int_{-\infty}^{+\infty} \delta(t - t_j) dt = 1$$

$$C_{IN}^{\Delta}(t) = \delta(t) \quad \text{WITH UNITS } \left( \frac{\text{mol}}{\text{m}^3} \right)$$

$$\int_{-\infty}^{+\infty} C_{IN}^{\Delta}(t) dt = \int_{-\infty}^{+\infty} \delta(t) dt = 1 \left( \frac{\text{mol} \cdot \text{s}}{\text{m}^3} \right)$$

In reality, we can't create a perfect impulse input. But we can approximate one by adding our component to the inlet over a time period that is short with respect to the space time:

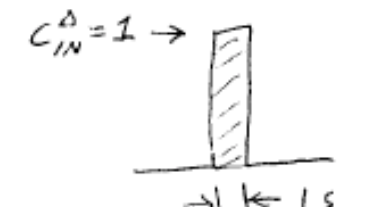
$$\text{FOR } \Delta t = 10s \ll \tau(s)$$



A horizontal line with a rectangular pulse of height 0.1 and width 10s. The pulse is shaded with diagonal lines. An arrow points to the height with the label  $C_{IN}^0 = 0.1$ . Below the pulse, a double-headed arrow indicates the width is 10s.

$$AREA = 1 \left( \frac{\text{mol} \cdot s}{m^3} \right)$$

OR



A horizontal line with a narrow rectangular pulse of height 1 and width 1s. The pulse is shaded with diagonal lines. An arrow points to the height with the label  $C_{IN}^0 = 1$ . Below the pulse, a double-headed arrow indicates the width is 1s.

$$AREA = 1 \left( \frac{\text{mol} \cdot s}{m^3} \right)$$

The product of the flow rate  $Q$  and the integral of the input equals the number of moles in the input:

$$Q \left( \frac{\text{m}^3}{\text{s}} \right) \int_{-\infty}^{+\infty} C_{IN}^{\Delta}(t) dt = \Phi (\text{mol})$$

↑ NUMERICAL VALUE IS  $\Phi$   
BUT UNITS ARE (mol)

With this unit impulse input, the concentration in the tank will jump to this level:

$$C^{\Delta}(t=0+) = \frac{\Phi (\text{mol})}{V (\text{m}^3)} = \frac{1}{2} \left( \frac{\text{mol}}{\text{m}^3} \right)$$

↑  
NUMERICAL VALUE  
IS  $\left( \frac{1}{2} \right)$  BUT UNITS ARE  
(mol/m<sup>3</sup>)

$$C(s) = \left( \frac{1}{s+1} \right) C_{IN}(s)$$

The Laplace transform of a unit impulse = 1.

Thus, for a unit impulse input into our process,

$$C(s) = \left( \frac{1}{s+1} \right)$$

$$C(s) = G_p(s)$$

Note that the transform of the unit impulse response of a process,  $C(s)$ , equals the transfer function of the process,  $G_p(s)$ . This is a general result and is important to understand and to remember.

Now we are ready for the final step, apply the inverse transform:

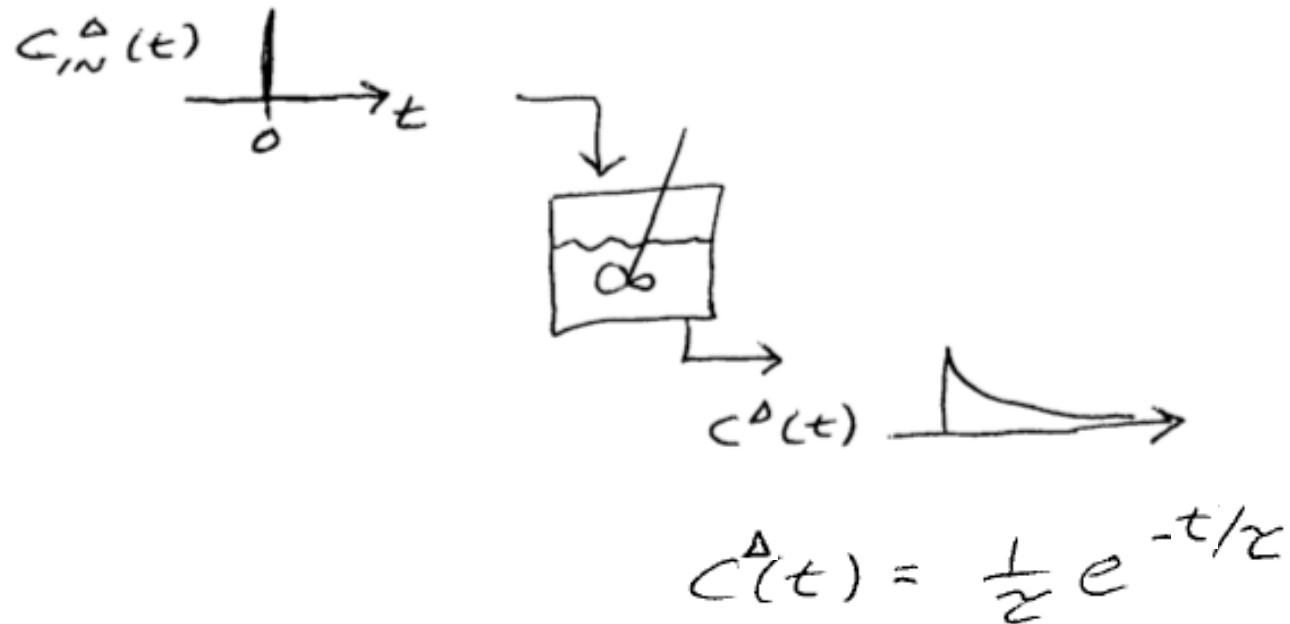
$$\mathcal{L}^{-1}[G(s)] = C^{\Delta}(t)$$

Our transfer function equation is simple such that we can look up the inverse transform in the table:

$$G(s) = \left( \frac{1}{\tau s + 1} \right)$$

$$C^{\Delta}(t) = \frac{1}{\tau} e^{-t/\tau}$$

Our solution is the response of the system to a unit impulse input. Of course, other inputs will result in other outputs.



The differential equation for this example can also be solved by using the "integrating factor" approach: integrate homogeneous equation (forcing function = 0) to obtain homogeneous solution, divide each term in full equation by homogeneous solution, integrate.

This approach can also be considered an integral transform. Its limitation is that it only works with first-order differential equations.

Laplace invented an integral transformation that can be applied to higher-order differential equations, e.g., those with second derivatives with respect to time.

The Laplace transform variable  $s$  is a marker of a first derivative with respect to time, and  $s^2$  is a marker of a second derivative.