CHE331 – Transport Phenomena I

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Introduction to Mathematical Modeling - I

(Please turn you cell-phones off)

Mathematical Modeling

- Mathematical modeling is a process in which an appropriately complete understanding of a …

  physical-chemical-biological-sociological-physiological

  … "(sub) system" is converted into a set of mathematical expressions.
- These mathematical expressions constitute the mathematical model.
- In engineering we most often use conservation laws (first principles) as a basis for mathematical models.
- Mathematical models are useful for the prediction of *future states* of the system or the description of *current and past states* of the system.

Mathematical Modeling

What are the physical properties/quantities that are conserved and are subject of conservation laws?

mass

~~volume~~

energy

momentum

electron spin

Are there other physical quantities that could be a subject of conservation laws?

YES!

Are we interested in them within the framework of this course?

NO!

Mathematical Modeling

We are interested only in mass, energy and momentum.

What is the simplest form of the conservation law that you have learned in previous courses?

Input - Output = Accumulation

Both Input and Output are essentially positive quantities. The minus sign appearing in the above equation indicates that the conserved quantity is “leaving” the system through the system boundary. It does not mean that the conserved quantity is negative by itself.

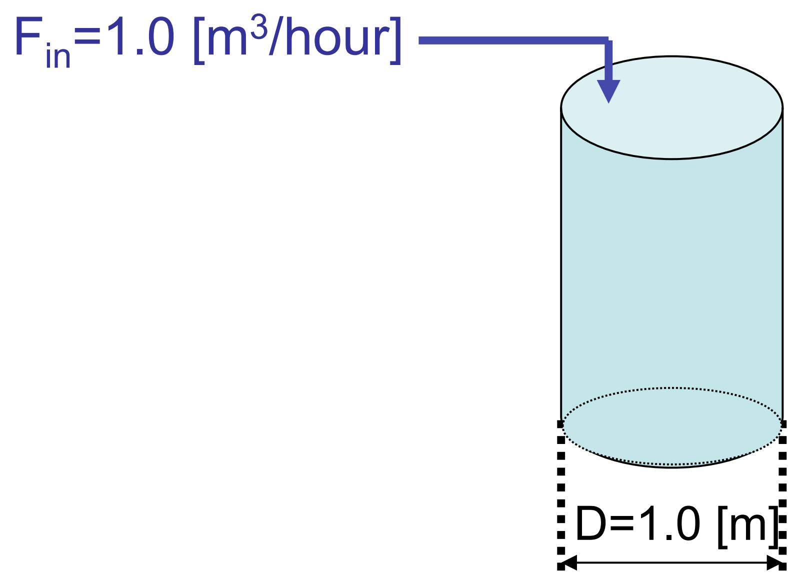
Mathematical Modeling

ACCUMULATION = Inventory of the system in **Position 2** − Inventory of the system in **Position 1**

ACCUMULATION = Inventory of the system at **Later Time** − Inventory of the system at **Earlier Time**

Mathematical Modeling

Let's consider a tank shown in illustration below, which is initially empty.



Question:

How is the level of the liquid in the tank changing with time?

Mathematical Modeling

Answer:

We will set up the mass balance of liquid in the tank.

<u>List of Variables:</u>

F_{in} (=) volumetric flow rate of liquid [m^3/hour]

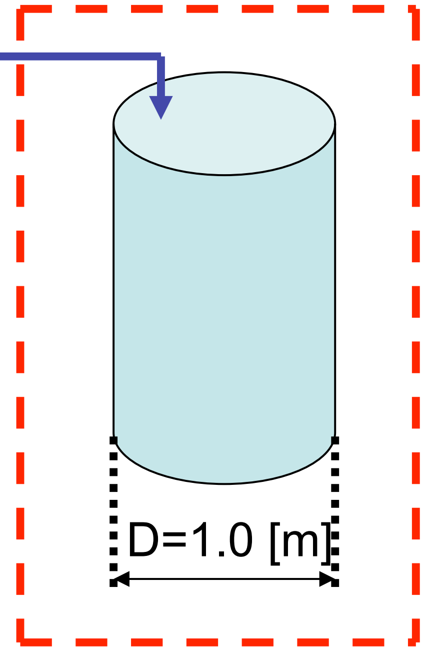
h (=) level of the liquid in the tank [m]

D (=) diameter of the tank [m]

ρ (=) density of the liquid [kg/m^3]

Next we will set the boundary of the system.

Mathematical Modeling



Apply the mass conservation law:

Input - Output = Accumulation [kg]

$$F_{in}\rho \cdot \Delta t \quad - \quad 0 \quad = \quad V\rho\Big|_{t+\Delta t} \quad - \quad V\rho\Big|_{t}$$

Mathematical Modeling

$$F_{in} \cdot \rho \cdot \Delta t = V \cdot \rho\Big|_{t=t+\Delta t} - V \cdot \rho\Big|_{t=t}$$

$$\left(\frac{m^3}{s}\right)\left(\frac{kg}{m^3}\right)(s) = \quad (m^3)\left(\frac{kg}{m^3}\right)$$

$$F_{in} \cdot \rho = \frac{V \cdot \rho\Big|_{t=t+\Delta t} - V \cdot \rho\Big|_{t=t}}{\Delta t}$$

$$\lim_{\Delta t \to 0}\left[F_{in} \cdot \rho\right] = \lim_{\Delta t \to 0}\left[\frac{V \cdot \rho\Big|_{t=t+\Delta t} - V \cdot \rho\Big|_{t=t}}{\Delta t}\right]$$

Mathematical Modeling

$$F_{in} \cdot \rho = \frac{d(V \cdot \rho)}{dt} = \rho \frac{dV}{dt} \quad \Rightarrow \quad F_{in} = \frac{dV}{dt}$$

… and if density is constant,

$$F_{in} = \frac{dV}{dt} \quad \rightarrow \quad F_{in} = \frac{d\left(\frac{\pi D^2}{4} h\right)}{dt}$$

Mathematical Modeling

$$\rightarrow F_{in} = \frac{\pi D^2}{4}\frac{dh}{dt} \quad \rightarrow \quad \frac{dh}{dt} = \frac{4F_{in}}{\pi D^2}$$

$$\rightarrow dh = \frac{4F_{in}}{\pi D^2}\,dt \quad \rightarrow \quad \int dh = \frac{4F_{in}}{\pi D^2}\int dt$$

$$\rightarrow \int_{h=0}^{h=h} dh = \frac{4F_{in}}{\pi D^2}\int_{t=0}^{t=t} dt \quad \rightarrow \quad h = \frac{4F_{in}}{\pi D^2}\,t$$

Mathematical Modeling

The mathematical model in differential form is:

$$F_{in} = \frac{\pi D^2}{4}\frac{dh}{dt}$$

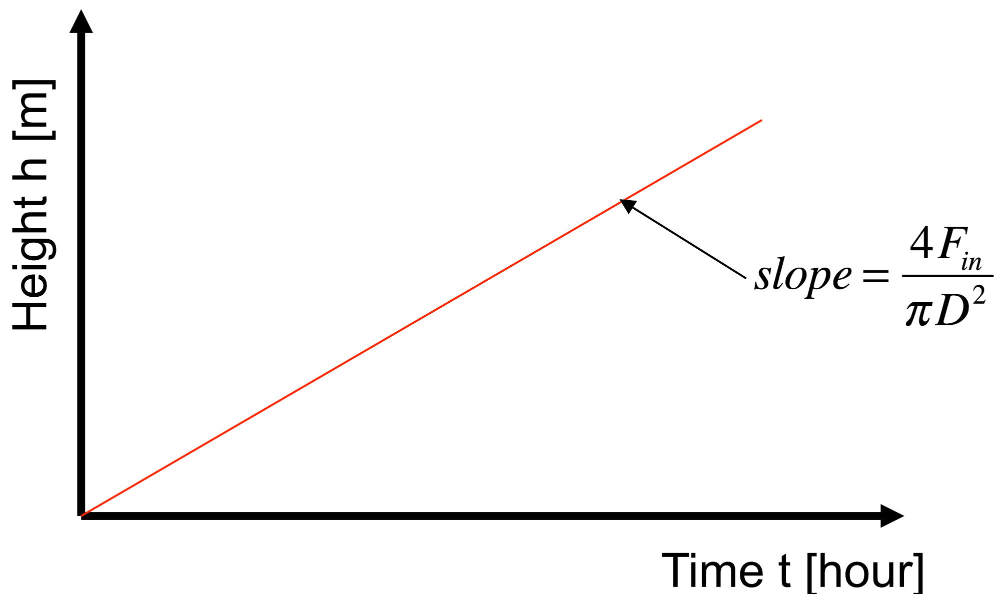
With the initial condition:

$$at \quad t = 0 \quad h = 0$$

Mathematical Modeling

The mathematical model in integral form is:

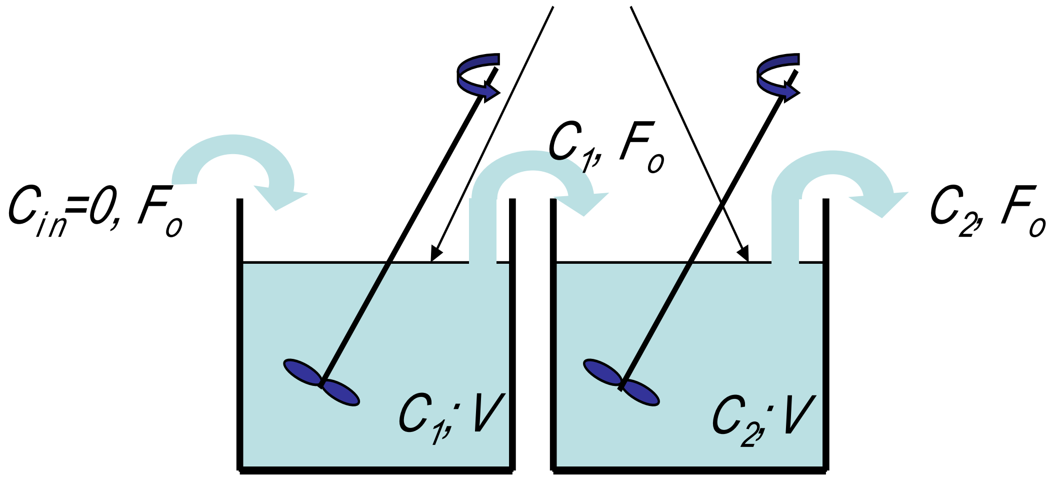
$$h = \frac{4F_{in}}{\pi D^2}\, t$$



Two tanks are connected, as shown in the illustration below. Initially, the first tank is filled with salty water at concentration C_1, $t = 0 = C_o$, while the second tank (initially) does not contain any salt, i.e., C_2, $t = 0 = 0$.

At time $t = 0$, *a* constant volumetric flow rate of freshwater, F_o, starts flowing into the first tank. The constant liquid level in each vessel is maintained by withdrawing liquid from the tank. The liquid in each vessel is well mixed; therefore, a uniform (but not constant) concentration of salt is maintained throughout the tank's volume.

$$At \quad t = 0 \quad C_1 = C_o \quad and \quad C_2 = 0$$



a) Develop a mathematical model to predict the concentration of salt in the stream leaving the first tank as a function of time. Develop an algebraic expression that would allow you to calculate how long it would take for salt concentration in the first tank to reach 10% of the initial concentration.

b) Develop a mathematical model to predict salt concentration in the second tank at any time after t=0..

c) Make a Graph [C vs. time t], which will show C_1 and C_2 as a function of time (assume practical and realistic values for C_o, F_o, and V).

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Thank you for your attention!