Case Study 1 - One-Dimensional Mass Balance of a Reactor

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1 Background

Chemical engineers make extensive use of idealized reactors in their design work. We focus on single or coupled well-mixed reactors. These are examples of lumped-parameter systems.

Figure 1 depicts an elongated reactor with a single entry and exit point. This reactor can be characterized as a distributed-parameter system. If it is assumed that the chemical being modeled is subject to first-order decay [1] and the tank is well-mixed vertically and laterally, a mass balance can be performed on a finite segment of length Δx, as in

$$V\frac{\Delta c}{\Delta t} = \underbrace{Qc(x)}_{\text{Flow in}} - \underbrace{Q\left[c(x) + \frac{\partial c(x)}{\partial x}\Delta x\right]}_{\text{Flow out}} - \underbrace{DA_c\frac{\partial c(x)}{\partial x}}_{\text{Dispersion in}} + \underbrace{DA_c\left[\frac{\partial c(x)}{\partial x} + \frac{\partial}{\partial x}\frac{\partial c(x)}{\partial x}\Delta x\right]}_{\text{Dispersion out}} - \underbrace{kVc}_{\text{Decay reaction}} \tag{1}$$

where V = volume (m^3), Q = flow rate (m^3/h), c is concentration (moles/m^3), D is a dispersion coefficient (m^2/h), A_c is the tank's cross-sectional area (m^2), and k is the first-order decay coefficient (h^{-1}). Note that the dispersion terms are based on Fick's first law,

$$Flux = -D\frac{\partial c}{\partial x} \tag{2}$$

It specifies that turbulent mixing tends to move mass from regions of high to low concentration. The parameter D, therefore, reflects the magnitude of turbulent mixing.

1.1 Tasks

1. Briefly explain what the terms in Eq. (1) are in relation to the diagram in Fig. (1)

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[1] That is, the chemical decays at a rate that is linearly proportional to how much chemical is present.
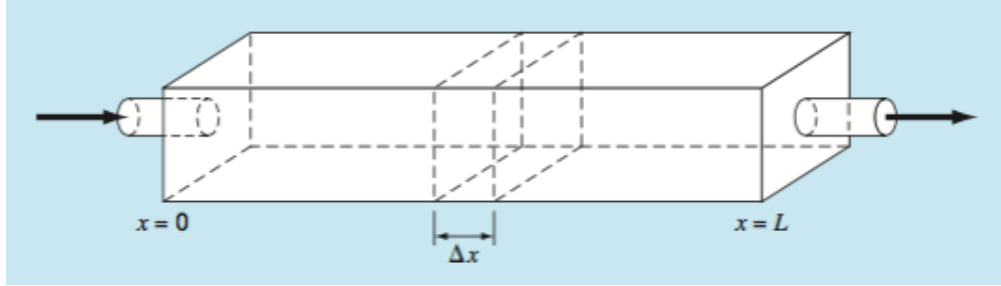
Figure 1: An elongated reactor with a single entry and exit point. A mass balance is developed around a finite segment along the tank's longitudinal axis in order to derive a differential equation for the concentration

2. Briefly compare the effects of a large dispersion coefficient (D) does to the system against a small D

3. Briefly define first order decay

4. Briefly explain Fick's first law

5. Briefly explain turbulent mixing

1.2 Problem Reduction

If Δx and Δt are allowed to approach zero, Eq. (1) becomes

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - U\frac{\partial c}{\partial x} - kc \tag{3}$$

where U = Q/A_c is the velocity of the water flowing through the tank. The mass balance for Fig. (1) is, therefore, now expressed as a parabolic partial differential equation. Equation (3) is sometimes referred to as the advection-dispersion equation with first- order reaction. At steady state, it is reduced to a second-order ODE,

$$0 = D\frac{d^2 c}{dx^2} - U\frac{dc}{dx} - kc \tag{4}$$

Prior to t = 0, the tank is filled with water that is devoid of the chemical. At t = 0, the chemical is injected into the reactor's inflow at a constant level of c_{in}. Thus, the following boundary conditions hold:

$$Qc_{in} = Qc_0 - DA_c\frac{dc}{dx} \tag{5}$$

and

$$c'(L, t) = 0 \tag{6}$$

2

The second condition specifies that the chemical leaves the reactor purely as a function of flow through the outlet pipe. That is, it is assumed that dispersion in the reactor does not affect the exit rate.

1.3 Tasks

1. Briefly explain what a parabolic partial differential equation is

2. Briefly point out what makes an advection-dispersion equation and relate it to our problem.

2 Problem Proper

Use numerical methods to solve Eq. (4) for the steady-state levels in the reactor. Note that this is an ODE boundary-value problem.

Then solve Eq. (3) to characterize the transient response—that is, how the levels change in time as the system approaches the steady state. This application involves a PDE.

Use the following values: D=2, U=1, Δx=2.5, k=0.2, and c_{in} =100.

2.1 Tasks

1. what ODE numerical methods do you plan to use ?

2. what PDE numerical methods do you plan to use ?

3. which methods have versions existing in our Java git repo?

4. which methods are you contributing to our Java git repo?

5. show a flow chart for your plan of solution.

3 Solution Strategy

A steady-state solution can be developed by substituting centered finite differences for the first and the second derivatives in Eq. (4) to give

$$0 = D\frac{c_{i+1} - 2c_i + c_{i-1}}{\Delta x^2} - U\frac{c_{i+1} - c_{i-1}}{2\Delta x} - kc_i \tag{7}$$

Collecting terms gives

$$-\left(\frac{D}{U\Delta x} + \frac{1}{2}\right)c_{i-1} + \left(\frac{2D}{U\Delta x} + \frac{k\Delta x}{U}\right)c_i - \left(\frac{D}{U\Delta x} - \frac{1}{2}\right)c_{i+1} = 0 \tag{8}$$

This equation can be written for each of the system's nodes. At the reactor's ends, this process introduces nodes that lie outside the system. For example, at the inlet node (i=0),

$$-\left(\frac{D}{U\Delta x}+\frac{1}{2}\right)c_{-1}+\left(\frac{2D}{U\Delta x}+\frac{k\Delta x}{U}\right)c_0-\left(\frac{D}{U\Delta x}-\frac{1}{2}\right)c_1=0 \qquad (9)$$

The c_{-1} can be removed by invoking the first boundary condition. At the inlet, the following mass balance must hold:

$$Qc_{in}=Qc_0-DA_c\frac{\partial c_0}{\partial x}$$

where c_0 = concentration at x = 0.

Thus, this boundary condition specifies that the amount of chemical carried into the tank by advection through the pipe must be equal to the amount carried away from the inlet by both advection and turbulent dispersion in the tank. A finite divided difference can be substituted for the derivative

$$Qc_{in}=Qc_0-DA_c\frac{c_1-c_{-1}}{2\Delta x}$$

which can be solved for

$$c_{-1}=c_1+\frac{2\Delta xU}{D}c_{in}-\frac{2\Delta xU}{D}c_0$$

which can be substituted into Eq. (9) to give

$$\left(\frac{2D}{U\Delta x}+\frac{k\Delta x}{U}+2+\frac{\Delta xU}{D}\right)c_0-\left(\frac{2D}{U\Delta x}\right)c_1=\left(2+\frac{\Delta xU}{D}\right)c_{in} \qquad (10)$$

A similar exercise can be performed for the outlet, where the original difference equation is

$$-\left(\frac{D}{U\Delta x}+\frac{1}{2}\right)c_{n-1}+\left(\frac{2D}{U\Delta x}+\frac{k\Delta x}{U}\right)c_n-\left(\frac{D}{U\Delta x}-\frac{1}{2}\right)c_{n+1}=0 \qquad (11)$$

The boundary condition at the outlet is

$$Qc_n-DA_c\frac{dc_n}{dx}=Qc_n$$

As with the inlet, a divided difference can be used to approximate the derivative.

$$Qc_n-DA_c\frac{c_{n+1}-c_{n-1}}{2\Delta x}=Qc_n \qquad (12)$$

Inspection of this equation leads us to conclude that $c_{n+1}=c_{n-1}$. In other words, the slope at the outlet must be zero for Eq. (12) to hold. Substituting this result into Eq. (11) and simplifying gives

$$-\left(\frac{2D}{U\Delta x}\right)c_{n-1} + \left(\frac{2D}{U\Delta x} + \frac{k\Delta x}{U}\right)c_n = 0 \tag{13}$$

Equations (8), (10), and (13) now form a system of n tridiagonal equations with n unknowns.

3.1 Tasks

1. Show how Eq. (8) was derived from the steady state Eq. (7)

2. Explain why the $c_{-1} = 0$ at the inlet

3. Explain why $c_{n+1} = c_{n-1}$ at the outlet

4. Define briefly what a tridiagonal matrix is

5. Do a quick research on what numerical method/ algorithm is efficient and effective in solving tridiagonal matrices

6. Demonstrate forming the tridiagonal matrix for solving our system

4 Expected Results

For example, if D=2,U=1, Δx=2.5, k=0.2, and c_{in} =100, the system is

$$\begin{bmatrix} 5.35 & -1.6 & & & \\ -1.3 & 2.1 & -0.3 & & \\ & -1.3 & 2.1 & -0.3 & \\ & & -1.3 & 2.1 & -0.3 \\ & & & -1.6 & 2.1 \end{bmatrix}\begin{Bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ c_4 \end{Bmatrix} = \begin{Bmatrix} 325 \\ 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix}$$

which can be solved for
$c_0 = 76.44 \quad c_1 = 52.47 \quad c_2 = 36.06$
$c_3 = 25.05 \quad c_4 = 19.09$

These results are plotted in Fig. 2. As expected, the concentration decreases due to the decay reaction as the chemical flows through the tank. In addition to the above computation, Fig. 2 shows another case with D = 4. Notice how increasing the turbulent mixing tends to flatten the curve.

In contrast, if dispersion is decreased, the curve would become steeper as mixing became less important relative to advection and decay. It should be noted that if dispersion is decreased too much, the computation will become subject to numerical errors. This type of error is referred to as static instability to contrast it with the dynamic instability due to too large a time step during a dynamic computation. The criterion to avoid this static instability is
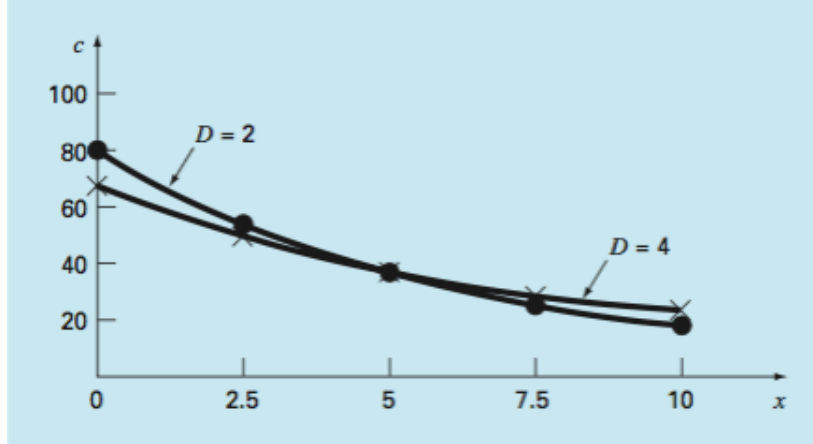
$$\Delta x \leq \frac{2D}{U}$$

Figure 2: Concentration versus s distance along the longitudinal axis of a rectangular reactor for a chemical that decays with first- order kinetics.

Thus, the criterion becomes more stringent (lower Δx) for cases where advection dominates over dispersion.

Aside from steady-state computations, numerical methods can be used to generate time-variable solutions of Eq. (3). Figure 3 shows results for $D = 2$, $U = 1$, $\Delta x = 2.5$, $k = 0.2$, and $c_{in} = 100$, where the concentration in the tank is 0 at time zero. As expected, the immediate impact is near the inlet. With time, the solution eventually approaches the steady-state level.

It should be noted that in such dynamic calculations, the time step is constrained by a stability criterion expressed as (Chapra, 1997)

$$\Delta t \leq \frac{(\Delta x)^2}{2D + k (\Delta x)^2}$$

Thus, the reaction term acts to make the time step smaller.

4.1 Tasks

1. discuss briefly how to use the methods in our Java lib

2. briefly review the code that you shall contribute to the Java lib

3. run your code and reconstruct the results in terms of Fig. 2 and Fig. 3 on the next page

References

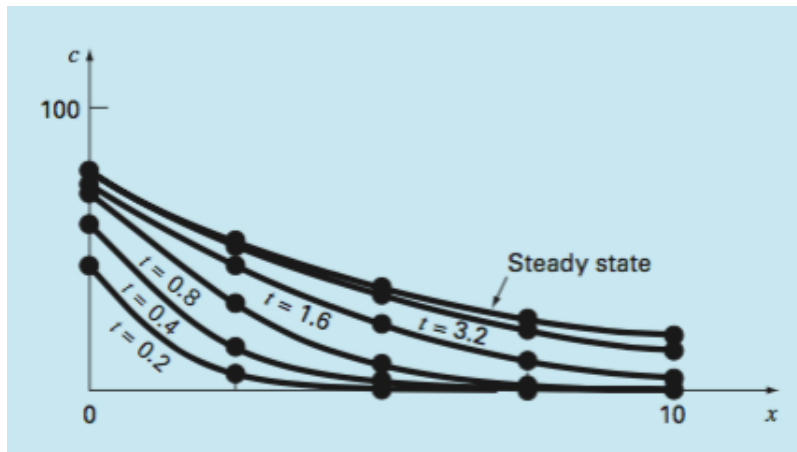[1] Chapra, S. C., Surface Water-Quality Modeling, McGraw-Hill, New York, 1997.

Figure 3: Concentration versus distance at different times during the buildup of chemical in a reactor.