

Practice Problems - Solution

Questions

Question 1

A large well-mixed tank used to allow settling of large particles from brine usually operates at steady-state with constant input (10 kg/min of 0.20 mass fraction salt in water) and output flowrates (10 kg/min, at the salt concentration in the tank). Due to operator error, a valve is opened and an additional 10 kg/min of pure water is introduced to the tank. Material balances on the total mass (M , in kg) and mass of salt (S , in kg) in the tank yield the following pair of equations:

$$\begin{aligned}\frac{dM}{dt} &= 10 \\ \frac{dS}{dt} &= 10 \times 0.2 - 10 \left(\frac{S}{M} \right)\end{aligned}$$

Where S/M represents the mass fraction of salt in the tank.

At $t = 0$, the mass of brine $M = 1000$ kg at 0.20 mass fraction, so $S = (0.20/M) = 200$ kg.

- Using `solve_ivp` and the initial conditions provided, solve the system above for a time long enough that tank overflow occurs, estimated to be at $M = 2000$ kg.
- Plot the total mass and the mass fraction of salt in the tank as a function of time.

Solution

This problem should be relatively straightforward – just a straight use of the builtin solvers. Remember that you need to solve the problem simultaneous, so the dependent variable is a vector.

Let $x = [M, S]$ then

$$\frac{dx}{dt} = \begin{bmatrix} \frac{dM}{dt} \\ \frac{dS}{dt} \end{bmatrix} = \begin{bmatrix} 10 \\ 2 - \frac{10S}{M} \end{bmatrix}$$

With the IC $x(0) = [M(0), S(0)] = [1000, 200]$.

Question 2

An irreversible first-order reaction $A \rightarrow B$ occurs in a catalyst of thickness $L = 0.001$ m; assume that the catalyst is wide in the other directions. At steady state, diffusion and reaction in the slab are described by,

$$D \frac{d^2 C_A}{dx^2} = k C_A$$

Where the diffusivity $D = 1.2 \times 10^{-9} \text{ m}^2/\text{s}$, and the rate constant $k = 0.001 \text{ s}^{-1}$.

The reactant at the surface of the catalyst ($x = 0$) is at concentration $C_{A0} = 0.2 \text{ mol/L}$. The catalyst is supported by an impermeable wall, so there is no flux of either species through the lower surface of the catalyst:

$$\left. \frac{dC_A}{dx} \right|_{x=L} = 0$$

- a) Use the shooting method (with `solve_ivp`) to obtain a solution for the concentration profile $C_A(x)$.
- b) Use `solve_bvp` to obtain the same solution.
- c) Present your results.

Solution

This problem is again setting up an ode, but here it is a boundary value problem. There are some choices to make when shooting: first, you can elect to solve in either direction (so your IVP starts either at $x = 0$ or at $x = L$), and, second, you can either do linear interpolation to get the unknown initial condition (since this is a linear ode) or you can rely on in-built solvers.

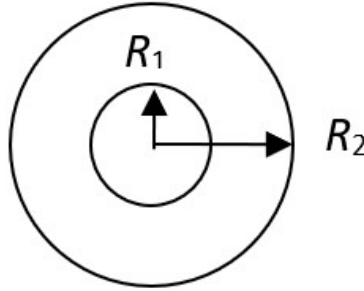
For `solve_bvp`, the main thing is understanding how to set up the initial conditions and express the boundary conditions as a residual. First, express system as a pair of first-order equations.

Let $u = \frac{dC_A}{dx}$ then $\frac{du}{dx} = \frac{d^2 C_A}{dx^2}$ and the ode becomes $D \frac{du}{dx} = k C_A$.

Hence $\frac{d}{dx} \begin{bmatrix} C_A \\ u \end{bmatrix} = \begin{bmatrix} u \\ \frac{k}{D} C_A \end{bmatrix}$ subject to $C_A(x = 0) = 0.2$ and $u(x = L) = 0$. Now we write the code!

Question 3

You wish to solve for the steady-state temperature distribution in a long annular cylinder:



With $R_1 = 5$ cm and $R_2 = 10$ cm. In cylindrical coordinates, the governing equation is:

$$\frac{d^2T}{dr^2} + \frac{1}{r} \frac{dT}{dr} = 0$$

The temperature of the inside wall is constant, $T(R_1) = 120^\circ\text{C}$. The heat loss through the outside wall has been measured as $\dot{Q} = 1$ kW per m of pipe length (along the axis), so

$$-k \left. \frac{dT}{dr} \right|_{r=R_2} = \frac{\dot{Q}}{2\pi R_2}$$

The pipe is steel, with $k = 14 \text{ W m}^{-1}\text{K}^{-1}$.

- Write code to implement the finite difference approach for this problem; clearly state the finite difference approximation you are using as a comment within the code. Make n configurable (i.e., there is a line $n = \dots$ near the top of the file; you can decide whether n represents internal nodes or all nodes as convenient).
- Note: You need to consider the boundary nodes separately to the interior nodes. You can use in-built methods to solve the resulting matrix equation.
- Make suitable plot(s) to illustrate your results. What is the temperature at R_2 and the temperature gradient at R_1 ?

Solution

See hand-written notes.

Question 4

The governing equation for the steady-state temperature distribution in a pin fin (pictured below) is:

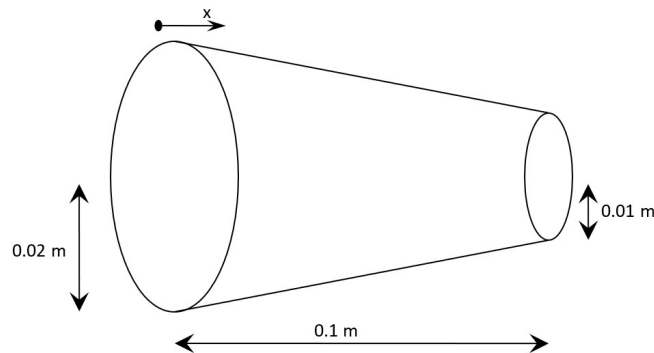
$$\frac{d}{dx} \left([r(x)]^2 \frac{dT}{dx} \right) - \frac{2h}{k} r(x) (T - T_{\text{air}}) = 0$$

Where the boundary conditions are given by:

$$T(0) = 100^\circ\text{C} \qquad -k \frac{dT}{dx} \Big|_{x=L} = h(T(L) - T_{\text{air}})$$

The radius r of the fin varies with distance according to $r(x) = 0.02 - 0.1x$ [in m] and the length $L = 0.10$ m. The air temperature $T_{\text{air}} = 20^\circ\text{C}$ and the pin is steel, with $h = 20\text{Wm}^{-2}\text{K}^{-1}$ and $k = 14\text{Wm}^{-1}\text{K}^{-1}$.

- Convert the system into a pair of first-order differential equations. Please write your system of first-order equations as a comment in your ode file, together with the boundary conditions you are using.
- Solve the system as a boundary-value problem with `solve_bvp`. [If you prefer, you can solve the problem via shooting with `solve_ivp`].
- Make suitable plot(s) to illustrate your results.



Solution

Again, a second-order bvp. First, convert to a pair of first-order equations. There are two choices that should give the same result.

Let $u = r^2 \frac{dT}{dx}$ then the ode becomes :

$$\frac{du}{dx} - \frac{2h}{k} r(x)(T - T_{\text{air}}) = 0$$

Giving a pair of equations,

$$\frac{d}{dx} \begin{bmatrix} T \\ u \end{bmatrix} = \begin{bmatrix} \frac{u}{r^2} \\ \frac{2h}{k} r (T - T_{\text{air}}) \end{bmatrix}$$

subject to boundary conditions $T(0) = 100$ and $-k \frac{dT}{dx} \Big|_{x=L} = h(T(L) - T_{\text{air}})$.

We need to re-express the second condition in terms of u :

$$-k \frac{u(L)}{r(L)^2} = h(T(L) - T_{\text{air}})$$

Alternative,

Note, we could have defined u differently. For clarity, I will call it v .

Let $v = \frac{dT}{dx}$ then the ode becomes :

$$\frac{d}{dx} (r^2 v) - \frac{2h}{k} r(x)(T - T_{\text{air}}) = 0$$

This definition forces us to do a little more work :

$$\begin{aligned} v \frac{d}{dx} (r^2) + r^2 \frac{dv}{dx} - \frac{2h}{k} r(x)(T - T_{\text{air}}) &= 0 \\ v 2r \frac{dr}{dx} + r^2 \frac{dv}{dx} - \frac{2h}{k} r(x)(T - T_{\text{air}}) &= 0 \\ -0.2rv + r^2 \frac{dv}{dx} - \frac{2h}{k} r(x)(T - T_{\text{air}}) &= 0 \end{aligned}$$

Hence,

$$\frac{d}{dx} \begin{bmatrix} T \\ v \end{bmatrix} = \begin{bmatrix} v \\ \frac{2h}{kr^2} r (T - T_{\text{air}}) + \frac{0.2rv}{r^2} \end{bmatrix} = \begin{bmatrix} v \\ \frac{2h}{kr} (T - T_{\text{air}}) + \frac{0.2v}{r} \end{bmatrix}$$

subject to boundary conditions $T(0) = 100$ and $-kv(L) = h(T(L) - T_{\text{air}})$. Now we write the code and either method should give the same result.

Question 5

Carbon dioxide is being absorbed into the surface of an alkaline solution containing a catalyst. The concentration, $C(t,x)$, of CO_2 in solution is described by the following equation,

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - kC$$

Where t is time, x is the distance from the surface, D is the diffusivity of CO_2 in the alkaline solution and k is a reaction rate constant.

Initially, there is no CO_2 dissolved in the solution. At time 0, the partial pressure of CO_2 in the gas at the solution's surface is suddenly increased to 1 atm, which gives a concentration at the surface of $C(t,0) = 0.030$ mol/L. Assume that the solution is deep, so that the dissolved CO_2 concentration far from the surface is 0. Take $D = 1.5 \times 10^{-9}$ m²/s and $k = 35$ s⁻¹.

- State suitable boundary and initial conditions for this problem.
- Solve this PDE at steady state first. So set $\frac{\partial C}{\partial t} = 0$ and solve the resulting ODE.
- Establish a set of equations to solve the PDE using the method of lines; include equations to implement the boundary conditions. Use second-order approximations wherever difference equations are required.
- Implement the solution; you should obtain a solution that approaches steady-state (start using a 0.01 s timeframe). The boundary layer is quite thin; try using a depth of 10^{-5} m and node spacing of 10^{-6} m. Does the steady state solution match the one you first obtained?
- Check that your solution is reasonable by halving the step size Δx .
- Make suitable plots to illustrate the solution.

Solution

- We want to solve for the concentration $C(t,x)$

$$\text{IC : } C(0, x) = 0 \text{ mol/L}$$

$$\text{BCs : } C(t, 0) = 0.030 \text{ mol/L}$$

$$C(t, L) = 0 \text{ mol/L or we could try } \left. \frac{\partial C}{\partial x} \right|_{x=L} = 0$$

where L is “deep enough” to be equivalent to infinity; here, it is suggested that 10^{-5} m will do! In fact, we really expect both of these BCs to be satisfied and one check on our numerical solution should be to test the one we don't implement.

- Please see file. Note that this is a shooting method problem.
- We want to apply finite difference approximations in the x -direction only. This will leave us with a set of ode IVPs (one per node) in place of a PDE. See notes in PDF.
- This is a case of implementing the equation and then playing a little with the values to get what you expect. I solved it using `solve_ivp` and then looked at the graph.

If you increase the time frame to 0.1 s then it looks like steady-state has been reached. You need a bit more depth to get to 0 concentration, maybe 50 μm rather than 10 μm .

The second interesting plot is concentration vs. depth at a given time. The solution shows this changing with time.

Question 6

Heat transfer, at unsteady state and in one-dimension, is governed by the equation:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

You wish to model the temperature $T(t,x)$ at various depths in soil. Assume that the temperature at the soil surface $T(t,0)$ varies over the year according to:

$$T(t, 0) = 10 - 14 \cos \left[\frac{2\pi}{365} (t - 37) \right]$$

Where t is the time in days and T is in Celsius. The temperature gradient is zero at large depth (assume 20 m is “large”),

$$\frac{\partial T}{\partial x} = 0 \quad \text{at } x = 20 \text{ m}$$

The thermal diffusivity of soil $\alpha = 0.081 \text{ m}^2/\text{day}$.

- Solve this problem using the method of lines. Use a node spacing of $\Delta x = 2 \text{ m}$, model the soil temperature to a depth of 20 m over a 4-year (1460 day) period. Assume that the soil is initially at 10°C .
- Make suitable plot(s) to illustrate your results.
- Why was it necessary to solve over more than one year? [write a brief comment in the file]

Hint: in developing your solution, you may find it convenient to first obtain a solution for a constant surface temperature $T(t,0)$ of, say, 20°C (note: do not choose 10°C , since this will just give $T(t,x) = \text{constant!}$) before substituting the actual boundary condition above.

Solution

Please see code file.