Leachate diffusion from two-layer soil

Problem Statement

Compacted clay liner (CCL) at the top, natural stratum at the bottom. Leachate seeps from the top to bottom. This benchmark problem is taken from Li and Cleall (2010). The analytical solution in terms of a Fourier series are coded as a Visual Basic function.

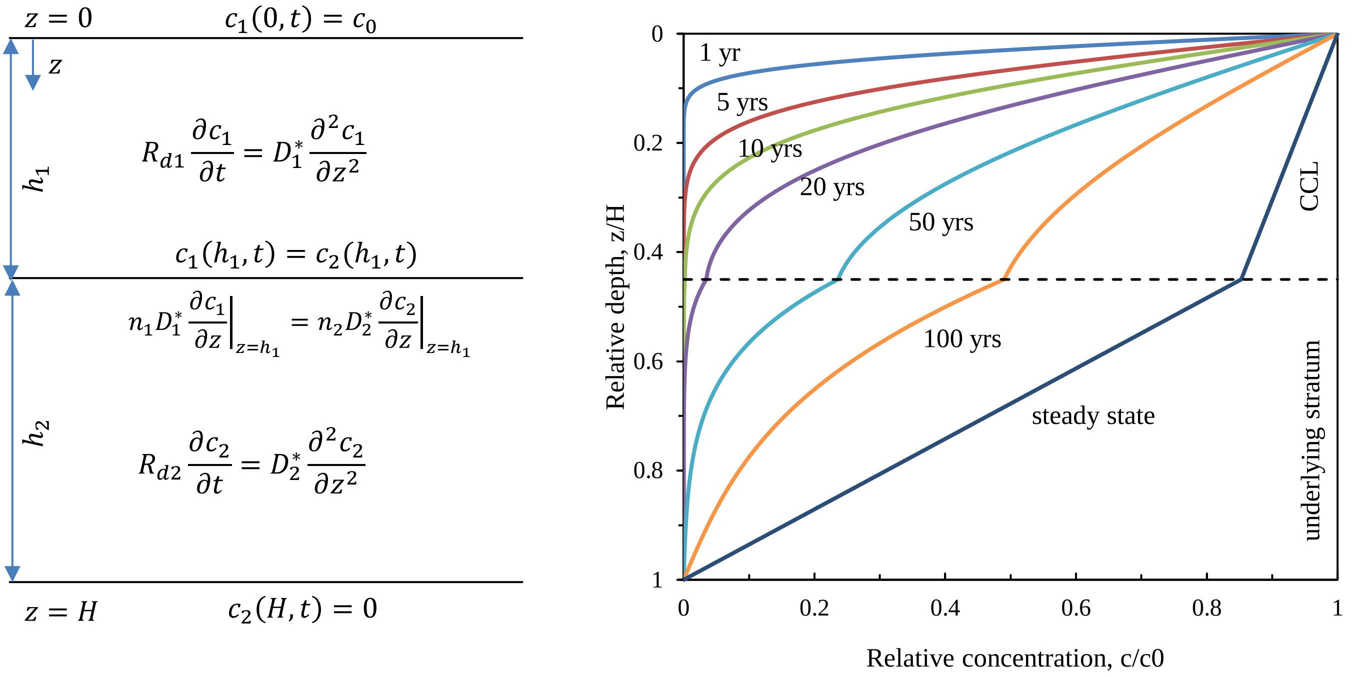


Figure 1. Left: Problem statement; Right: analytical solution using Fourier series

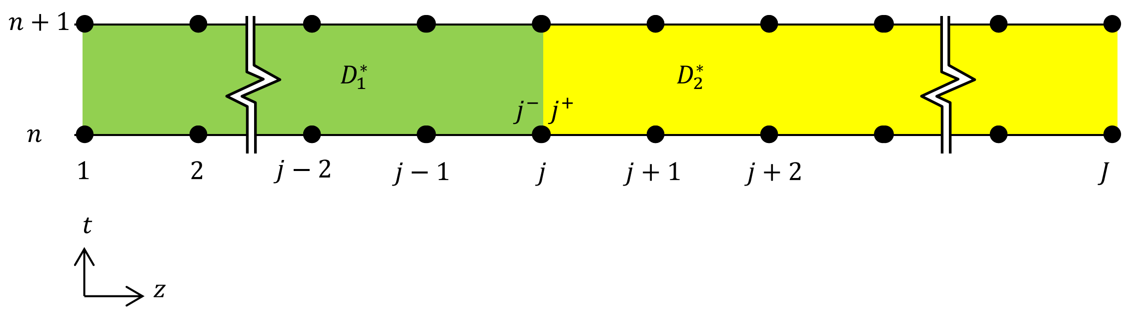
Diffusion coefficient: $D_1^* = 4 \times 10^{-10}\ \mathrm{m^2/s}$, $D_2^* = 1 \times 10^{-10}\ \mathrm{m^2/s}$,
Retardation factor: $R_{d1} = 3.3, R_{d2} = 1.0$, Porosity: $n_1 = 0.444, n_2 = 0.375$,
Layer thicknesses: $h_1 = 0.9$ m, $h_2 = 1.1$ m, $H = h_1 + h_2$

Initial condition: $c_1(z,0) = 0$ for $0 \le z \le h_1$, $c_2(z,0) = 0$ for $h_1 \le z \le H$.
The boundary conditions are of Dirichlet type at top & bottom. At the interface, the BC is continuity of C and mass flux of C.

Find $c_1(z,t)/c_0$ and $c_2(z,t)/c_0$ for t = 1, 5, 10, 20, 50, 100 and 1000 years. The time has units of seconds (s), as a result, multiply years by (365 day/year)×(86400 s/day).

Finite difference implementation

This part is based on Hickson et al. (2010).



In points for domain 1 (green), we have $\frac{\partial c}{\partial t} = D_1 \frac{\partial^2 c}{\partial x^2}$. The term $\frac{\partial^2 c}{\partial x^2}$ is calculated with the central difference formula.

$$\frac{\partial^2 c_{j-1}^n}{\partial x^2} = \frac{c_{j-2}^n - 2c_{j-1}^n + c_{j-1}^n}{\Delta x^2}.$$

The time marching algorithm is:

$$\frac{dc_{j-1}}{dt} = \frac{D_1^*}{R_{d1}} \frac{c_{j-2} - 2c_{j-1} + c_j}{\Delta x^2}$$

This formula can be solved with the desired time marching algorithm. Similar equation can be written for other interior nodes within domain 1 (nodes 2 until $j-1$). For nodes $j+1$ we have:

$$\frac{dc_{j+1}}{dt} = \frac{D_2^*}{R_{d2}} \frac{c_j - 2c_{j+1} + c_{j+2}}{\Delta x^2}$$

Similar formulas can be written for nodes $j+1$ until $J-1$. For node j itself, we write the governing equation as:

$$\frac{dc_j}{dt} = \frac{1}{2}\left(\frac{D_1^*}{R_{d1}} \frac{\partial^2 c_{j^-}}{\partial z^2} + \frac{D_2^*}{R_{d2}} \frac{\partial^2 c_{j^+}}{\partial z^2} \right) \quad (1)$$

The boundary conditions are:

$$c_{j^-} = c_{j^+} \quad (2)$$

$$n_1 D_1^* \frac{\partial c_{j^-}}{\partial z} = n_2 D_2^* \frac{\partial c_{j^+}}{\partial z} \quad (3)$$

The Taylor series for c_{j-2} and c_{j-1} with respect to c_{j^-} are:

$$c_{j-1} = c_{j^-} - \Delta z \frac{\partial c_{j^-}}{\partial z} + \frac{\Delta z^2}{2} \frac{\partial^2 c_{j^-}}{\partial z^2} \quad (4)$$

$$c_{j-2} = c_{j^-} - 2\Delta z \frac{\partial c_{j^-}}{\partial z} + 2\Delta z^2 \frac{\partial^2 c_{j^-}}{\partial z^2} \quad (5)$$

Similarly:

$$c_{j+1} = c_{j^+} + \Delta z \frac{\partial c_{j^+}}{\partial z} + \frac{\Delta z^2}{2} \frac{\partial^2 c_{j^+}}{\partial z^2} \quad (6)$$

$$c_{j+2} = c_{j^+} + 2\Delta z \frac{\partial c_{j^+}}{\partial z} + 2\Delta z^2 \frac{\partial^2 c_{j^+}}{\partial z^2} \quad (7)$$

Equations. (2-7) are 6 equations with 6 unknowns: $c_{j^-}, c_{j^+}, \frac{\partial c_{j^-}}{\partial z}, \frac{\partial c_{j^+}}{\partial z}, \frac{\partial^2 c_{j^-}}{\partial z^2}$ and $\frac{\partial^2 c_{j^+}}{\partial z^2}$. After solving them and substituting in the right hand side of Equation (1), we have:

$$\frac{dc_j}{dt} = a_1 c_{j-2} + a_2 c_{j-1} + a_3 c_{j+1} + a_4 c_{j+2}$$

Notice that c_j itself does not appear on the right side. The coefficients are:

a1 = (((2 * Ds1 ^ 2 * Rd2 - Ds1 * Ds2 * Rd1) * n1 + 3 * Ds2 * n2 * Ds1 * Rd2) / Rd1 / dz ^ 2 / (Ds1 * n1 + Ds2 * n2) / Rd2) / 0.6e1;
a2 = -(((Ds1 * Rd2 - 2 * Ds2 * Rd1) * n1 + 3 * Ds2 * Rd2 * n2) * Ds1 / Rd1 / dz ^ 2 / (Ds1 * n1 + Ds2 * n2) / Rd2) / 0.3e1;
a3 = (((2 * Ds1 * Ds2 * Rd2 - Ds2 ^ 2 * Rd1) * n2 - 3 * Ds2 * Ds1 * n1 * Rd1) / Rd1 / dz ^ 2 / (Ds1 * n1 + Ds2 * n2) / Rd2) / 0.3e1;
a4 = (((-Ds1 * Ds2 * Rd2 + 2 * Ds2 ^ 2 * Rd1) * n2 + 3 * Ds2 * Ds1 * n1 * Rd1) / Rd1 / dz ^ 2 / (Ds1 * n1 + Ds2 * n2) / Rd2) / 0.6e1;

References

[1] Li, Y. C., & Cleall, P. J. (2010). Analytical solutions for contaminant diffusion in double-layered porous media. *Journal of Geotechnical and Geoenvironmental Engineering*, *136*(11), 1542-1554. https://ascelibrary.org/doi/abs/10.1061/(ASCE)GT.1943-5606.0000365

[2] Hickson, R. I., Barry, S. I., Mercer, G. N., & Sidhu, H. S. (2011). Finite difference schemes for multilayer diffusion. Mathematical and Computer Modelling, 54(1-2), 210-220. https://www.sciencedirect.com/science/article/pii/S0895717711000938