Seminar 1: Diffusion and Convection

Transport of contaminants in porous media
Applied Hydropedology

1 Background

Baetslé formulated a simple analytical model for the spread of contaminants dependent on diffusion coefficient, D, and convection, $\vec{q} = q_x$:

$$c(x,t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x-q_x t)^2}{4Dt}}. \tag{1}$$

This equation resembles Gaussian normal distribution with the mean, $\mu = q_x t$, and the standard deviation, $\sigma = \sqrt{2Dt}$, for conservative transport (no reactions present). If we include zero-order reactions the model (1) is updated as follows

$$c(x,t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x-q_x t)^2}{4Dt}} + \lambda_0 t, \tag{2}$$

and for the first order reactions, such as the radioactive decay, the model is assembled as follows

$$c(x,t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x-q_x t)^2}{4Dt} + \lambda_1 t}, \tag{3}$$

where λ_1 is the first order reaction kinetics, which is related to particle half-live $T_{1/2}$ as follows

$$T_{1/2} = \frac{\ln 2}{\lambda_1}. \tag{4}$$

2 Tasks

Answer following questions:

1. Set $q_x = 0$. Look at $x = 50$ at time unit t=1. Why is the concentration of the contaminant at this location higher with $D = 200$ compared to $D = 100$?
2. Repeat task 1 for $x = 5$. Why is the concentration of the contaminant at this location lower with $D = 200$ compared to $D = 100$?
3. Set q_x so that the center of the pollution is at location 350 after 5 time units. What is the value of q_x?
4. Set q_x so that the center of the pollution is at location -150 after 2 time units. What is the value of q_x?
5. Why is the location in task (3) to the right of the starting point and why is the location in task ((4) to the left of the starting position?
6. Set the zero order reaction term to a negative number. Why is the concentration negative? Does it make sense?

7. Set the zero order reaction term to zero and the first order reaction term to a negative number. Why does the concentration never reach zero?

8. Compute numerically with the trapezoid method the total amount of the dissolved contaminant for different values of t. The integral is given by

$$M(t) = \int_{-\infty}^{+\infty} c(t)\mathrm{d}x.$$

The approximation using the trapezoid method is

$$M(t) \approx \sum_{i=1}^{n-1} \frac{c_i(t) + c_{i+1}(t)}{2} \mathrm{dx}.$$

where dx is the discretization step.

(a) Set q_x and the reaction terms to zero. Calculate the total amount of the dissolved contaminant for $D = 100$ and $D = 10$ for time unit $t = 1$ for $\mathrm{dx} = 20$, 5 and 1. Compare the results to the analytical solution. If you cannot calculate the analytical solution of the integral, use Wolfram alpha. Why can you use a larger discretization step for a higher diffusion coefficient?

(b) Repeat 8a for $t = 3$. What does mass conservative mean?

(c) Repeat 8a with a positive and a negative reaction term.