Analysis of Bromide Tracer Transport in a Soil Column Leaching Test

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1 Experimental Setup

The soil column used in this study had a radius of 0.0075 m and a length of 0.1 m. The porosity of the soil was estimated to be 0.56. A bromide tracer solution was injected into the column at a flow rate of 1 mL/min. The effluent concentration of bromide was monitored over time, and the injection was stopped after 10 pore volumes (PV) had passed through the column.

2 Analytical Solution and Parameter Estimation

2.1 Basic Parameter Calculation

The volume of the soil column (V_{column}) was calculated as:

$$V_{column} = \pi \times (0.0075)^2 \times 0.1 = 1.767 \times 10^{-5}\,\mathrm{m}^3 = 17.67\,\mathrm{mL}$$

The pore volume (PV) was estimated using the porosity ($\theta = 0.56$):

$$PV = V_{column} \times \theta = 17.67 \times 0.56 \approx 10\,\mathrm{mL}$$

The time corresponding to one pore volume at a flow rate of $Q = 1\,\mathrm{mL/min}$ is:

$$t_{PV} = \frac{PV}{Q} = \frac{10\,\mathrm{mL}}{1\,\mathrm{mL/min}} = 10\,\mathrm{min}$$

2.2 Pore Water Velocity (v)

The breakthrough time t_{50} (time at which the normalized concentration C/C = 0.5) was estimated from the experimental data using linear interpolation. Based on the data points around C/C = 0.5, t_{50} was found to be approximately 20.34 minutes (using the original report's method of treating PV directly as time for interpolation, although a 5-minute interval per PV was noted). The pore water velocity was then calculated as:

$$v = \frac{L}{t_{50}} = \frac{0.1\,\mathrm{m}}{20.34 \times 60\,\mathrm{s}} = \frac{0.1\,\mathrm{m}}{1220.4\,\mathrm{s}} \approx 8.2 \times 10^{-5}\,\mathrm{m/s}$$

2.3 Hydraulic Conductivity (K)

The hydraulic conductivity was estimated using Darcy's Law:

$$K = \frac{Q \cdot L}{A \cdot \Delta H}$$

Where $Q = \frac{1\,\mathrm{mL/min}}{60\,\mathrm{s/min} \times 10^6\,\mathrm{mL/m^3}} = 1.67 \times 10^{-8}\,\mathrm{m^3/s}$, $L = 0.1\,\mathrm{m}$, $A = \pi \times (0.0075)^2\,\mathrm{m}^2 = 1.767 \times 10^{-4}\,\mathrm{m}^2$, and assuming $\Delta H = 0.1\,\mathrm{m}$, we get:

$$K = \frac{(1.67 \times 10^{-8}\,\mathrm{m^3/s}) \cdot (0.1\,\mathrm{m})}{(1.767 \times 10^{-4}\,\mathrm{m}^2) \cdot (0.1\,\mathrm{m})} \approx 9.45 \times 10^{-5}\,\mathrm{m/s}$$

2.4 Dispersion Coefficient (D) and Dispersivity (α)

The convection-dispersion equation was used to estimate the dispersion coefficient. Using a single data point (PV = 1.5, t = 15 min = 900 s, C/C = 0.176) and the analytical solution:

$$\frac{C}{C_0} = \frac{1}{2}\text{erfc}\left(\frac{L - vt}{2\sqrt{Dt}}\right)$$

The dispersion coefficient D was estimated to be approximately $3.6 \times 10^{-7}\,\text{m}^2/\text{s}$. The dispersivity ($\alpha$) was then calculated as:

$$\alpha = \frac{D}{v} = \frac{3.6 \times 10^{-7}\,\text{m}^2/\text{s}}{8.2 \times 10^{-5}\,\text{m/s}} \approx 0.0044\,\text{m} = 4.4\,\text{mm}$$

2.5 Mass Balance Verification

The mass balance was checked by comparing the total injected tracer mass with the recovered mass from the effluent. The recovery rate was estimated to be 97.6%.

3 Numerical Model

A one-dimensional numerical model based on the convection-dispersion equation was developed to simulate the transport of the bromide tracer through the soil column. The column was discretized into $N = 300$ cells, and the transport was simulated over time using an explicit finite difference scheme. The governing equation was approximated as:

$$C_i^{j+1} = C_i^j + \Delta t \left[D\frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{(\Delta x)^2} - v\frac{C_i^j - C_{i-1}^j}{\Delta x} \right]$$

The inlet boundary condition was set to the initial tracer concentration for the first 10 pore volumes and then switched to zero. An advective outflow boundary condition was applied at the outlet. The initial condition assumed a tracer-free soil column. The simulation was run with a Courant number of 0.05 to ensure numerical stability.

4 Optimization of Dispersion Coefficient

To improve the fit between the simulated and experimental breakthrough curves, the dispersion coefficient (D) was optimized using the 'minimize' function from the 'scipy.optimize' library with the 'Nelder-Mead' method. The objective function to be minimized was the sum of squared errors (SSE) between the simulated and experimental normalized effluent concentrations at the experimental time points. The optimization was performed with bounds set for the dispersion coefficient (10^{-8} to 10^{-5}).

The optimized value for the dispersion coefficient was found to be approximately $7.99 \times 10^{-7}\,\text{m}^2/\text{s}$.

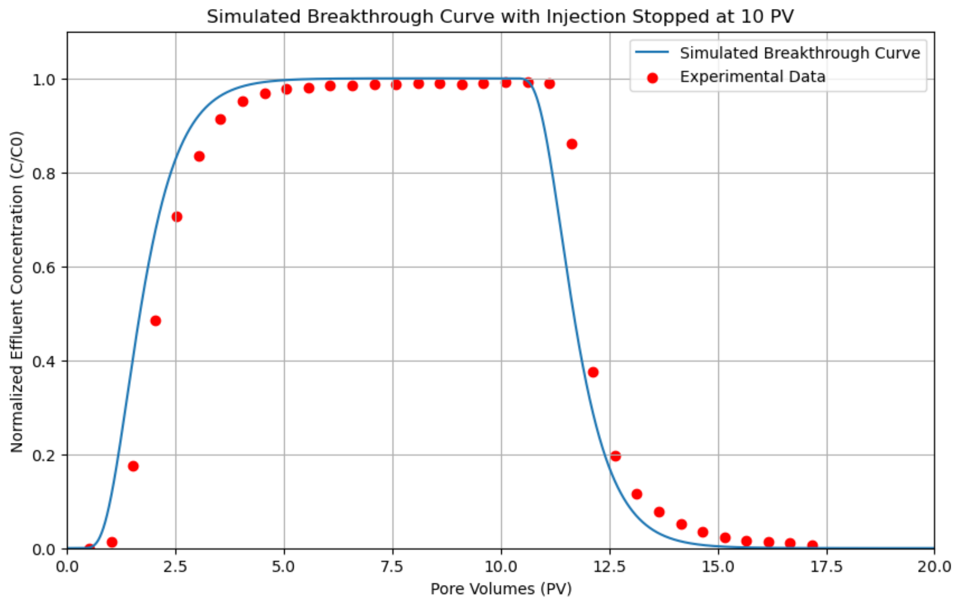

Figure 1: Simulated and Experimental Breakthrough Curve with Optimized Dispersion Coefficient ($D = 7.99 \times 10^{-7}\,\mathrm{m}^2/\mathrm{s}$)

Figure 1 shows the experimental data along with the simulated breakthrough curve using the optimized dispersion coefficient. The plot indicates a reasonable agreement between the model and the experimental results, particularly in capturing the initial breakthrough and the subsequent washout after the tracer injection was stopped.

5 Discussion

The initial analytical estimate of the dispersion coefficient ($3.6 \times 10^{-7}\,\mathrm{m}^2/\mathrm{s}$) showed some discrepancy with the experimental data. The numerical optimization process yielded a value of $7.99 \times 10^{-7}\,\mathrm{m}^2/\mathrm{s}$, which resulted in a better fit to the experimental breakthrough curve. The difference between the initial estimate and the optimized value could be attributed to the simplified assumptions made in the analytical solution based on a single data point. The numerical model, by simulating the entire breakthrough curve, allowed for a more comprehensive optimization.

The remaining discrepancies between the simulated and experimental data might be due to several factors, including the inherent simplifications in the 1D model (which assumes homogeneity and neglects potential radial variations in flow and concentration), experimental errors, or the limitations of the chosen numerical scheme.

6 Conclusion

The soil column leaching test was analyzed using both analytical and numerical methods. The hydraulic conductivity was estimated using Darcy's Law, and an initial estimate of the dispersion coefficient was obtained from the analytical solution of the convection-dispersion equation. A numerical model was developed and used to optimize the dispersion coefficient using the Nelder-Mead method, resulting in an improved fit to the experimental breakthrough curve. The optimized dispersion coefficient of $7.99 \times 10^{-7}\,\mathrm{m}^2/\mathrm{s}$ provides a more accurate representation of the solute transport behavior in the soil column under the given experimental conditions.