

## Supplementary S1. Derivation of the solution for the steady-state problem.

The governing equations for the steady-state problem are as follows

$$\frac{D_i}{R_{d,i}} \frac{d^2 \eta_i(x)}{dx^2} - \frac{v_i}{R_{d,i}} \frac{d \eta_i(x)}{dx} = 0, \quad (i = 1, 2, 3, 4) \quad (1.1)$$

The steady-state problem's boundary conditions can be obtained using the earlier presumptions. For the steady-state problem, the inlet boundary condition is as follows:

$$\eta_1(0) = C_0 \quad (1.2)$$

For the steady-state problem, the outlet boundary condition is as follows:

$$\frac{\partial \eta_4(L)}{\partial x} = 0 \quad (1.3)$$

Where  $L$  [M] represents the thickness of the entire SB/GCL/SB-aquifer system

In this problem, the following normalization can be applied to each interface's concentration and mass flux continuity conditions:

$$\eta_i(L_i) = \eta_{i+1}(L_i) \quad (1.4)$$

$$n_i D_i \frac{\partial \eta_i(L_i)}{\partial x} = n_{i+1} D_{i+1} \frac{\partial \eta_{i+1}(L_i)}{\partial x} \quad (1.5)$$

The solution satisfying all the relevant conditions of sub-problem 1 is as follows

$$\eta_i(x) = j_{i,1} e^{r_{i,1} x} + j_{i,2} e^{r_{i,2} x} \quad (1.6)$$

$r_{i,1}$  and  $r_{i,2}$  can be expressed as follows

$$r_{i,1} = 0, \quad r_{i,2} = \frac{v_i}{D_i} \quad (1.7)$$

The coefficients  $j_{i,1}$  and  $j_{i,2}$  are determined in a similar manner to the coefficient determination in the transient-state problem. The boundary conditions (Eqs. (1.2) and (1.3)) and the continuity conditions (Eqs. (1.4) and (1.5)) for the steady-state problem are substituted

into Eqs. (1.1) and (1.6) to obtain the desired results.

### Supplementary S2. Derivation of the solution for the transient problem.

The governing equations for the transient -state problem are as follows

$$R_{d,i} \frac{\partial \delta_i(x,t)}{\partial t} = D_i \frac{\partial^2 \delta_i(x,t)}{\partial x^2} - v_i \frac{\partial \delta_i(x,t)}{\partial x}, \quad (i=1,2,3,4) \quad (2.1)$$

The following initial conditions apply to the transient-state problem since there was no initial contamination:

$$\delta_i(x, 0) = 0, \quad (i=1,2,3,4) \quad (2.2)$$

The boundary conditions for the transient-state problem can be derived as follows, based on the presumptions mentioned earlier.

The transient-state problem's inlet boundary condition is as follows:

$$\delta_i(0,t) = 0 \quad (2.3)$$

For the transient-state problem, the outlet boundary condition is as follows:

$$\frac{\partial \delta_4(L,t)}{\partial x} = 0 \quad (2.4)$$

For every interface in the transient-state problem, the concentration continuity conditions and mass flux continuity conditions can be normalized in the following ways:

$$\delta_i(L_i, t) = \delta_{i+1}(L_i, t) \quad (2.5)$$

$$n_i D_i \frac{\partial \delta_i(L_i, t)}{\partial x} = n_{i+1} D_i \frac{\partial \delta_{i+1}(L_i, t)}{\partial x} \quad (2.6)$$

The general solution that satisfies the transient-state problem can be defined as follows using the variable separation method:

$$\delta_i(x,t) = \sum_{m=1}^{\infty} Q_m g_{m,i}(x) e^{\alpha_i x - \beta_m t}, \quad (i=1,2,3,4) \quad (2.7)$$

Where  $Q_m$ ,  $\alpha_i$  are coefficients,  $\beta_m$  is an eigenvalue, and  $g_{m,i}$  is a characteristic function with respect to  $x$ , and can be described as

$$g_{m,i}(x) = \begin{cases} A_{m,i} \sin\left(\mu_i \varepsilon_{m,i} \frac{x}{L}\right) + B_{m,i} \cos\left(\mu_i \varepsilon_{m,i} \frac{x}{L}\right) & (\sigma \geq 0) \\ A_{m,i} \sinh\left(\mu_i \varepsilon_{m,i} \frac{x}{L}\right) + B_{m,i} \cos\left(\mu_i \varepsilon_{m,i} \frac{x}{L}\right) & (\sigma < 0) \end{cases} \quad (i=1,2,3,4) \quad (2.8)$$

Where  $\sigma = \beta_m - v_i^2 / (4D_i R_{d,i})$ , by substituting Eq. (2.7) and Eq. (2.8) into Eq. (2.1) and setting  $t = 0$ , we obtain  $\alpha_i$

$$\alpha_i = \frac{v_i}{2D_i}, \quad (i=1,2,3,4) \quad (2.9)$$

Substituting the obtained  $\alpha_i$  into Eqs. (2.1), (2.7), and (2.8), we can solve for  $\varepsilon_{m,i}$

$$\varepsilon_{m,i} = \sqrt{\left| \beta_m - \frac{v_i^2}{4D_i R_{d,i}} \right|}, \quad (i=1,2,3,4) \quad (2.10)$$

Substituting Eq (2.9) and Eq (2.10) back into Eq (2.8), obtained

$$\mu_i = L \sqrt{\frac{R_{d,i}}{D_i}}, \quad (i=1,2,3,4) \quad (2.11)$$

To obtain  $\beta_m$ , it is necessary to derive the transfer Eqs for the coefficients  $A_{m,i}$  and  $B_{m,i}$  by substituting Eqs. (2.7) and (2.8) into the continuity conditions given by Eqs. (2.5) and (2.6).

$$\begin{bmatrix} A_{m,i} \\ B_{m,i} \end{bmatrix} = P_{i-1} \begin{bmatrix} A_{m,i-1} \\ B_{m,i-1} \end{bmatrix}, \quad (i=2,3,4) \quad (2.12)$$

where

$$P_i = \frac{e^{(\alpha_i - \alpha_{i+1})x_i}}{n_{i+1} D_{i+1} \mu_{i+1} \theta_{m,i+1}} \begin{bmatrix} A_i^\# H_i^\# + D_i^\# E_i^\# & C_i^\# H_i^\# - D_i^\# G_i^\# \\ A_i^\# F_i^\# - B_i^\# E_i^\# & B_i^\# G_i^\# + C_i^\# F_i^\# \end{bmatrix}, \quad (i=1,2,3) \quad (2.13)$$

where

$$A_i^\# = \begin{cases} \sin(\mu_i \varepsilon_{m,i} x) & \sigma_i \geq 0 \\ \sinh(\mu_i \varepsilon_{m,i} x) & \sigma_i < 0 \end{cases} \quad (2.14)$$

$$B_i^\# = \begin{cases} \sin(\mu_{i+1} \varepsilon_{m,i+1} x) & \sigma_{i+1} \geq 0 \\ \sinh(\mu_{i+1} \varepsilon_{m,i+1} x) & \sigma_{i+1} < 0 \end{cases} \quad (2.15)$$

$$C_i^\# = \begin{cases} \cos(\mu_i \varepsilon_{m,i} x) & \sigma_i \geq 0 \\ \cosh(\mu_i \varepsilon_{m,i} x) & \sigma_i < 0 \end{cases} \quad (2.16)$$

$$D_i^\# = \begin{cases} \cos(\mu_{i+1} \varepsilon_{m,i+1} x) & \sigma_{i+1} \geq 0 \\ \cosh(\mu_{i+1} \varepsilon_{m,i+1} x) & \sigma_{i+1} < 0 \end{cases} \quad (2.17)$$

$$E_i^\# = \begin{cases} n_i D_i \mu_i \varepsilon_{m,i} \cos(\mu_i \varepsilon_{m,i} x) - n_i D_i \alpha_i \sin(\mu_i \varepsilon_{m,i} x) & \sigma_i \geq 0 \\ n_i D_i \mu_i \varepsilon_{m,i} \cosh(\mu_i \varepsilon_{m,i} x) - n_i D_i \alpha_i \sinh(\mu_i \varepsilon_{m,i} x) & \sigma_i < 0 \end{cases} \quad (2.18)$$

$$F_i^\# = \begin{cases} n_{i+1} D_{i+1} \mu_{i+1} \varepsilon_{m,i+1} \cos(\mu_{i+1} \varepsilon_{m,i+1} x) - n_{i+1} D_{i+1} \alpha_{i+1} \sin(\mu_{i+1} \varepsilon_{m,i+1} x) & \sigma_{i+1} \geq 0 \\ n_{i+1} D_{i+1} \mu_{i+1} \varepsilon_{m,i+1} \cosh(\mu_{i+1} \varepsilon_{m,i+1} x) - n_{i+1} D_{i+1} \alpha_{i+1} \sinh(\mu_{i+1} \varepsilon_{m,i+1} x) & \sigma_{i+1} < 0 \end{cases} \quad (2.19)$$

$$G_i^\# = \begin{cases} n_i D_i \mu_i \varepsilon_{m,i} \cos(\mu_i \varepsilon_{m,i} x) + n_i D_i \alpha_i \sin(\mu_i \varepsilon_{m,i} x) & \sigma_i \geq 0 \\ n_i D_i \mu_i \varepsilon_{m,i} \cosh(\mu_i \varepsilon_{m,i} x) + n_i D_i \alpha_i \sinh(\mu_i \varepsilon_{m,i} x) & \sigma_i < 0 \end{cases} \quad (2.20)$$

$$H_i^\# = \begin{cases} n_{i+1} D_{i+1} \mu_{i+1} \varepsilon_{m,i+1} \cos(\mu_{i+1} \varepsilon_{m,i+1} x) + n_{i+1} D_{i+1} \alpha_{i+1} \sin(\mu_{i+1} \varepsilon_{m,i+1} x) & \sigma_{i+1} \geq 0 \\ n_{i+1} D_{i+1} \mu_{i+1} \varepsilon_{m,i+1} \cosh(\mu_{i+1} \varepsilon_{m,i+1} x) + n_{i+1} D_{i+1} \alpha_{i+1} \sinh(\mu_{i+1} \varepsilon_{m,i+1} x) & \sigma_{i+1} < 0 \end{cases} \quad (2.21)$$

Eqs. (2.14) into (2.21) for  $i = 1, 2, 3$

The characteristic values  $\beta_m$  are determined by the following equation

$$P_4 P_3 P_2 P_1 P_0 = 0 \quad (2.22)$$

The value  $P_0$  is determined by substituting Eqs (2.7) and (2.8) into the inlet boundary condition of the transient -state problem (Eq (2.3))

$$P_0 = \begin{bmatrix} A_{m,1} \\ B_{m,1} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad (2.23)$$

The value  $P_4$  is obtained by substituting Eqs. (2.7) and (2.8) into the outlet boundary condition of the transient -state problem (Eq. (2.4))

$$P_4 = \begin{cases} \begin{bmatrix} \alpha_4 \sin(\mu_4 \varepsilon_{m,4}) + \mu_4 \varepsilon_{m,4} \cos(\mu_4 \varepsilon_{m,4}) \\ \alpha_4 \cos(\mu_4 \varepsilon_{m,4}) - \mu_4 \varepsilon_{m,4} \sin(\mu_4 \varepsilon_{m,4}) \end{bmatrix}^T & \sigma \geq 0 \\ \begin{bmatrix} \alpha_4 \sinh(\mu_4 \varepsilon_{m,4}) + \mu_4 \varepsilon_{m,4} \cosh(\mu_4 \varepsilon_{m,4}) \\ \alpha_4 \cosh(\mu_4 \varepsilon_{m,4}) + \mu_4 \varepsilon_{m,4} \sinh(\mu_4 \varepsilon_{m,4}) \end{bmatrix}^T & \sigma < 0 \end{cases} \quad (2.24)$$

The coefficients  $Q_m$  are obtained from the following orthogonality relationship

$$Q_m = \frac{\sum_{i=1}^4 \int_{x_{i-1}}^{x_i} \delta_i(x) n_i R_{d,i} g_{m,i}(x) e^{-\alpha_i x}}{\sum_{i=1}^4 \int_{x_{i-1}}^{x_i} q_i n_i R_{d,i} g_{m,i}^2(x)} \quad (2.25)$$

where

$$\begin{cases} q_1 = 1 \\ q_2 = e^{2(a_2 - a_1)x_1} \\ q_3 = e^{2(a_2 - a_1)x_1 + 2(a_3 - a_2)x_2} \\ q_4 = e^{2(a_2 - a_1)x_1 + 2(a_3 - a_2)x_2 + 2(a_4 - a_3)x_3} \end{cases} \quad (2.26)$$