New Model of Reactive Transport in Single-well Push-Pull Test with Aquitard Effect

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Supplementary Materials

S1. Derivation of the analytical solutions for the SWPP test

S2. Numerical solutions

S3. References for Table 4

Supplementary Materials

S1. Derivation of analytical solutions for the SWPP test

To reduce the complexity in analyzing the influence of input parameters on the output, the dimensionless parameters are introduced as follows: $C_{mD}=\frac{C_m}{C_0}$, $C_{imD}=\frac{C_{im}}{C_0}$, $C_{inj,mD}=\frac{C_{inj,m}}{C_0}$, $C_{inj,imD}=\frac{C_{inj,im}}{C_0}$, $C_{cha,mD}=\frac{C_{cha,m}}{C_0}$, $C_{cha,imD}=\frac{C_{cha,im}}{C_0}$, $C_{res,mD}=\frac{C_{res,m}}{C_0}$, $C_{res,imD}=\frac{C_{res,im}}{C_0}$, $C_{ext,mD}=\frac{C_{ext,m}}{C_0}$, $C_{ext,imD}=\frac{C_{ext,im}}{C_0}$, $C_{umD}=\frac{C_{um}}{C_0}$, $C_{uimD}=\frac{C_{uim}}{C_0}$, $C_{lmD}=\frac{C_{lm}}{C_0}$, $C_{limD}=\frac{C_{lim}}{C_0}$, $t_D=\frac{|A|}{\alpha_r^2 R_m}t$, $r_D=\frac{r}{\alpha_r}$, $r_{wD}=\frac{r_w}{\alpha_r}$, $z_D=\frac{z}{B}$, $\mu_{mD}=\frac{\alpha_r^2\mu_m}{A}$, $\mu_{imD}=\frac{\alpha_r^2 R_m\mu_{im}}{R_{im}A}$, $\mu_{umD}=\frac{\alpha_r^2\mu_{um}}{A}$, $\mu_{uimD}=\frac{\alpha_r^2 R_m\mu_{uim}}{R_{im}A}$, $\mu_{lmD}=\frac{\alpha_r^2\mu_{lm}}{A}$ and $\mu_{limD}=\frac{\alpha_r^2 R_m\mu_{lim}}{R_{im}A}$, where the subscript "*D*" represents the dimensionless parameter hereinafter, $A=\frac{Q}{4\pi B\theta_m}$. By substituting these dimensionless parameters into the governing equations, one could obtain the dimensionless model of the SWPP test:

$$\frac{\partial C_{mD}}{\partial t_D}=\frac{1}{r_D}\frac{\partial^2 C_{mD}}{\partial r_D^2}-\frac{1}{r_D}\frac{\partial C_{mD}}{\partial r_D}-\varepsilon_m(C_{mD}-C_{imD})-\mu_{mD}C_{mD}-\left(\frac{\theta_{um}\alpha_r^2 v_{um}}{2A\theta_m B}C_{umD}-\frac{\theta_{um}\alpha_r^2 D_u}{2A\theta_m B^2}\frac{\partial C_{umD}}{\partial z_D}\right)\Big|_{z_D=1}+\left(\frac{\theta_{lm}\alpha_r^2 v_{lm}}{2AB\theta_m}C_{lmD}-\frac{\theta_{lm}\alpha_r^2 D_l}{2AB^2\theta_m}\frac{\partial C_{lmD}}{\partial z_D}\right)\Big|_{z_D=-1}, r_D\geq r_{wD}, \quad \text{(S1a)}$$

$$\frac{\partial C_{imD}}{\partial t_D}=\varepsilon_{im}(C_{mD}-C_{imD})-\mu_{imD}C_{imD}, r_D\geq r_{wD}, \quad \text{(S1b)}$$

$$\frac{\partial C_{umD}}{\partial t_D}=\frac{R_m\alpha_r^2 D_u}{AB^2R_{um}}\frac{\partial^2 C_{umD}}{\partial z_D^2}-\frac{R_m v_{um}\alpha_r^2}{ABR_{um}}\frac{\partial C_{umD}}{\partial z_D}-\varepsilon_{um}(C_{umD}-C_{uimD})-\mu_{umD}C_{umD},$$

$$z_D\geq 1, \quad \text{(S2a)}$$

$$\frac{\partial C_{uimD}}{\partial t_D}=\varepsilon_{uim}(C_{umD}-C_{uimD})-\mu_{uimD}C_{uimD}, z_D\geq 1, \quad \text{(S2b)}$$

$$\frac{\partial C_{lmD}}{\partial t_D}=\frac{R_m\alpha_r^2 D_l}{AB^2R_{lm}}\frac{\partial^2 C_{lmD}}{\partial z_D^2}+\frac{R_m v_{lm}\alpha_r^2}{ABR_{lm}}\frac{\partial C_{lmD}}{\partial z_D}-\varepsilon_{lm}(C_{lmD}-C_{limD})-\mu_{lmD}C_{lmD},$$

$$z_D\leq -1, \quad \text{(S3a)}$$

$$\frac{\partial C_{limD}}{\partial t_D} = \varepsilon_{lim}(C_{lmD} - C_{limD}) - \mu_{limD} C_{limD}, z_D \leq -1, \quad \text{(S3b)}$$

where $\varepsilon_m = \frac{\omega_a \alpha_r^2}{A\theta_m}$, $\varepsilon_{im} = \frac{\omega_a \alpha_r^2 R_m}{A\theta_m R_{im}}$, $\varepsilon_{um} = \frac{\omega_u \alpha_r^2 R_m}{A\theta_{um} R_{um}}$, $\varepsilon_{uim} = \frac{\omega_u \alpha_r^2 R_m}{A\theta_{um} R_{uim}}$, $\varepsilon_{lm} = \frac{\omega_l \alpha_r^2 R_m}{A\theta_{lm} R_{lm}}$, $\varepsilon_{lim} = \frac{\omega_l \alpha_r^2 R_m}{A\theta_{lm} R_{lim}}$.

The analytical solution will be derived using the Laplace transform method and the Green's functions method, and the detailed information could be seen in the following sections.

S1.1 Solutions in the injection phase: Eqs. (25a) and (25f)

Substituting the dimensionless parameters into Eqs. (5) - (6), one could obtain the dimensionless boundary conditions and dimensionless initial conditions for the injection phase:

$$C_{mD}(r_D, t_D)|_{t_D=0} = C_{imD}(r_D, t_D)|_{t_D=0} = C_{umD}(r_D, z_D, t_D)|_{t_D=0} = C_{uimD}(r_D, z_D, t_D)|_{t_D=0} = C_{lmD}(r_D, z_D, t_D)|_{t_D=0} = C_{limD}(r_D, z_D, t_D)|_{t_D=0} = 0, \quad \text{(S4)}$$

$$C_{mD}(r_D, t_D)|_{r_D\to\infty} = C_{imD}(r_D, t_D)|_{r_D\to\infty} = C_{umD}(r_D, z_D, t_D)|_{z_D\to\infty} = C_{uimD}(r_D, z_D, t_D)|_{z_D\to\infty} = C_{lmD}(r_D, z_D, t)|_{z_D\to-\infty} = C_{limD}(r_D, z_D, t_D)|_{z_D\to-\infty} = 0, \quad \text{(S5)}$$

$$C_{mD}(r_D, t_D) = C_{umD}(r_D, z_D = 1, t_D), \quad \text{(S6a)}$$

$$C_{mD}(r_D, t_D) = C_{lmD}(r_D, z_D = -1, t_D). \quad \text{(S6b)}$$

Conducting Laplace transform to Eqs. (S2a) - (S2b), one has:

$$s\bar{C}_{umD} = \frac{R_m \alpha_r^2 D_u}{AB^2 R_{um}} \frac{\partial^2 \bar{C}_{umD}}{\partial z_D^2} - \frac{R_m v_{um} \alpha_r^2}{ABR_{um}} \frac{\partial \bar{C}_{umD}}{\partial z_D} - (\varepsilon_{um} + \mu_{umD})\bar{C}_{umD} + \varepsilon_{um}\bar{C}_{uimD},$$

$$z_D \geq 1, \quad \text{(S7a)}$$

$$s\bar{C}_{uimD} = \varepsilon_{uim}(\bar{C}_{umD} - \bar{C}_{uimD}) - \mu_{uimD}\bar{C}_{uimD}, z_D \geq 1, \quad \text{(S7b)}$$

Substituting Eq. (S7b) into Eq. (S7a) will lead to:

$$s\bar{C}_{umD} = \frac{R_m \alpha_r^2 D_u}{AB^2 R_{um}} \frac{\partial^2 \bar{C}_{umD}}{\partial z_D^2} - \frac{R_m v_{um} \alpha_r^2}{ABR_{um}} \frac{\partial \bar{C}_{umD}}{\partial z_D} - \left(\varepsilon_{um} + \mu_{umD} - \frac{\varepsilon_{um}\varepsilon_{uim}}{s + \mu_{uimD} + \varepsilon_{uim}}\right)\bar{C}_{umD},$$

$$z_D \geq 1, \tag{S8}$$

Similarly, Eqs. (S3a) - (S3b) become:

$$s\bar{C}_{lmD} = \frac{R_m \alpha_r^2 D_l}{AB^2 R_{lm}} \frac{\partial^2 \bar{C}_{lmD}}{\partial z_D^2} + \frac{R_m v_{lm} \alpha_r^2}{ABR_{lm}} \frac{\partial \bar{C}_{lmD}}{\partial z_D} - (\varepsilon_{lm} + \mu_{lmD})\bar{C}_{lmD} + \varepsilon_{lm}\bar{C}_{limD},$$

$$z_D \leq -1, \tag{S9a}$$

$$s\bar{C}_{limD} = \varepsilon_{lim}(\bar{C}_{lmD} - \bar{C}_{limD}) - \mu_{limD}\bar{C}_{limD}, z_D \leq -1, \tag{S9b}$$

Substituting Eq. (S9b) into Eq.(S9a) results in:

$$s\bar{C}_{lmD} = \frac{R_m \alpha_r^2 D_l}{AB^2 R_{lm}} \frac{\partial^2 \bar{C}_{lmD}}{\partial z_D^2} + \frac{R_m v_{lm} \alpha_r^2}{ABR_{lm}} \frac{\partial \bar{C}_{lmD}}{\partial z_D} - \left(\varepsilon_{lm} + \mu_{lmD} - \frac{\varepsilon_{lm}\varepsilon_{lim}}{s+\mu_{limD}+\varepsilon_{lim}}\right)\bar{C}_{lmD},$$

$$z_D \leq -1, \tag{S10}$$

where overbar represents the variables in Laplace domain hereinafter; *s* is the Laplace transform parameter in respect to dimensionless time.

Eqs. (S5), (S6a)-(S6b) and (S8) compose a model of the second-order ordinary differential equation (ODE) with boundary conditions, the general solution of Eq. (S8) is:

$$\bar{C}_{umD} = A_1 e^{a_1 z_D} + B_1 e^{a_2 z_D}. \tag{S11a}$$

Similarly, the general solution of Eq. (S10) is:

$$\bar{C}_{lmD} = A_2 e^{b_1 z_D} + B_2 e^{b_2 z_D}. \tag{S11b}$$

where $a_1 = \dfrac{\frac{R_m v_{um}\alpha_r^2}{ABR_{um}} + \sqrt{\left(\frac{R_m v_{um}\alpha_r^2}{ABR_{um}}\right)^2 + 4\frac{R_m\alpha_r^2 D_u}{AB^2 R_{um}}\left(s+\varepsilon_{um}+\mu_{umD}-\frac{\varepsilon_{um}\varepsilon_{uim}}{s+\mu_{uimD}+\varepsilon_{uim}}\right)}}{2\frac{R_m\alpha_r^2 D_u}{AB^2 R_{um}}}$,

$$a_2 = \frac{\frac{R_m v_{um}\alpha_r^2}{ABR_{um}} - \sqrt{\left(\frac{R_m v_{um}\alpha_r^2}{ABR_{um}}\right)^2 + 4\frac{R_m\alpha_r^2 D_u}{AB^2 R_{um}}\left(s+\varepsilon_{um}+\mu_{umD}-\frac{\varepsilon_{um}\varepsilon_{uim}}{s+\mu_{uimD}+\varepsilon_{uim}}\right)}}{2\frac{R_m\alpha_r^2 D_u}{AB^2 R_{um}}},$$

$$b_1 = \frac{-\frac{R_m v_{lm}\alpha_r^2}{ABR_{lm}} + \sqrt{\left(\frac{R_m v_{lm}\alpha_r^2}{ABR_{lm}}\right)^2 + 4\frac{R_m\alpha_r^2 D_l}{AB^2 R_{lm}}\left(s+\varepsilon_{lm}+\mu_{lmD}-\frac{\varepsilon_{lm}\varepsilon_{lim}}{s+\mu_{limD}+\varepsilon_{lim}}\right)}}{2\frac{R_m\alpha_r^2 D_l}{AB^2 R_{lm}}} \text{ and}$$

$$b_2 = \frac{-\frac{R_m v_{lm} \alpha_r^2}{ABR_{lm}} - \sqrt{\left(\frac{R_m v_{lm} \alpha_r^2}{ABR_{lm}}\right)^2 + 4\frac{R_m \alpha_r^2 D_l}{AB^2 R_{lm}}\left(s + \varepsilon_{lm} + \mu_{lmD} - \frac{\varepsilon_{lm}\varepsilon_{lim}}{s + \mu_{limD} + \varepsilon_{lim}}\right)}}{2\frac{R_m \alpha_r^2 D_l}{AB^2 R_{lm}}}.$$

Substituting Eqs. (S11a) - (S11b) into Eqs. (S5)-(S6b) leads to:

$$\bar{C}_{umD} = B_1 e^{a_2 z_D}. \quad \text{(S12a)}$$

$$\bar{C}_{lmD} = A_2 e^{b_1 z_D}. \quad \text{(S12b)}$$

where $B_1 = \bar{C}_{mD} exp(-a_2)$, $B_2 = 0$, $A_1 = 0$ and $A_2 = \bar{C}_{mD} exp(b_1)$.

Thus, we could obtain the solutions for the aquitards as:

$$\bar{C}_{umD} = \bar{C}_{mD} exp(a_2 z_D - a_2). \quad \text{(S13a)}$$

$$\bar{C}_{uimD} = \frac{\varepsilon_{uim}}{s + \varepsilon_{uim} + \mu_{uimD}} \bar{C}_{umD}, \quad \text{(S13b)}$$

$$\bar{C}_{lmD} = \bar{C}_{mD} exp(b_1 z_D + b_1). \quad \text{(S14a)}$$

$$\bar{C}_{limD} = \frac{\varepsilon_{lim}}{s + \varepsilon_{lim} + \mu_{limD}} \bar{C}_{lmD}, \quad \text{(S14b)}$$

In the injection phase, the dimensional boundary conditions Eq. (8) and Eqs. (12a)-(12b) are transformed into their dimensionless forms:

$$\left[C_{mD} - \frac{\partial C_{mD}(r_D, t_D)}{\partial r_D}\right]\bigg|_{r=r_{wD}} = C_{inj,mD}(t_D), 0 < t_D \le t_{inj,D} \quad \text{(S15)}$$

$$\beta_{inj} \frac{dC_{inj,mD}(t_D)}{dt_D} = 1 - C_{inj,mD}(t_D), 0 < t_D \le t_{inj,D}, \quad \text{(S16a)}$$

$$C_{inj,mD}(t_D = 0) = 0, \quad \text{(S16b)}$$

where $\beta_{inj} = \frac{V_{w,inj} r_{wD}}{\xi R_m \alpha_r}$.

Conducting Laplace transform to Eqs. (S1a) - (S1b), one has:

$$s\bar{C}_{mD} = \frac{1}{r_D}\frac{\partial^2 \bar{C}_{mD}}{\partial r_D^2} - \frac{1}{r_D}\frac{\partial \bar{C}_{mD}}{\partial r_D} - (\varepsilon_m + \mu_{mD})\bar{C}_{mD} + \varepsilon_m \bar{C}_{imD} -$$

$$\left(\frac{\theta_{um}\alpha_r^2 v_{um}}{2A\theta_m B}\bar{C}_{umD} - \frac{\theta_{um}\alpha_r^2 D_u}{2A\theta_m B^2}\frac{\partial \bar{C}_{umD}}{\partial z_D}\right)\bigg|_{z_D=1} + \left(\frac{\theta_{lm}\alpha_r^2 v_{lm}}{2A\theta_m B}\bar{C}_{lmD} - \frac{\theta_{lm}\alpha_r^2 D_l}{2AB^2\theta_m}\frac{\partial \bar{C}_{lmD}}{\partial z_D}\right)\bigg|_{z_D=-1},$$

$$r_D \geq r_{wD}. \tag{S17a}$$

$$\bar{C}_{imD} = \frac{\varepsilon_{im}}{(s+\mu_{imD}+\varepsilon_{im})}\bar{C}_{mD}, r_D \geq r_{wD}, \tag{S17b}$$

Substituting Eqs. (S13a), (S14a) and (S17b) into Eq. (S17a),one has:

$$\frac{1}{r_D}\frac{\partial^2 \bar{C}_{mD}}{\partial r_D^2} - \frac{1}{r_D}\frac{\partial \bar{C}_{mD}}{\partial r_D} - E\bar{C}_{mD} = 0. \tag{S18}$$

where

$$E = s + \varepsilon_m + \mu_{mD} - \frac{\varepsilon_m \varepsilon_{im}}{s+\mu_{imD}+\varepsilon_{im}} + \frac{\theta_{um}\alpha_r^2 v_{um}}{2A\theta_m B} - \frac{\theta_{lm}\alpha_r^2 v_{lm}}{2AB\theta_m} - \frac{a_2\theta_{um}\alpha_r^2 D_u}{2A\theta_m B^2} + \frac{b_1\theta_{lm}\alpha_r^2 D_l}{2AB^2\theta_m}.$$

The boundary conditions of the wellbore and infinity in the Laplace domain are:

$$\left[\bar{C}_{mD} - \frac{\partial \bar{C}_{mD}(r_D,s)}{\partial r_D}\right]\Big|_{r=r_{wD}} = \bar{C}_{inj,mD}(s), \tag{S19a}$$

$$\bar{C}_{mD}(r_D,s)|_{r_D\to\infty} = 0. \tag{S19b}$$

Conducting Laplace transform on Eqs. (S16a)- (S16b), one has:

$$\bar{C}_{inj,mD}(r_w,s) = \frac{1}{s(s\beta_{inj}+1)}, \tag{S20}$$

Eqs. (S18), (S19a)-(S19b), and (S20) compose a model of the second-order ordinary differential equation (ODE) with boundary conditions. The general solution of Eq. (S18) is:

$$\bar{C}_{mD}(r_D,s) = \phi_1\, exp\left(\frac{y_{inj}}{2}\right)A_i\left(E^{1/3}y_{inj}\right) + \phi_2 \exp\left(\frac{y_{inj}}{2}\right)B_i\left(E^{1/3}y_{inj}\right). \tag{S21}$$

where $y_{inj} = r_D + \frac{1}{4E}$, $y_{inj,w} = r_{wD} + \frac{1}{4E}$; ϕ_1 and ϕ_2 are constants which could be determined by the boundary conditions; $A_i(\cdot)$ and $B_i(\cdot)$ are the Airy functions of the first kind and second kind, respectively. As $B_i(r_D)$ diverges when $r_D \to \infty$, ϕ_2 has to be zero.

Substituting Eqs. (S21), (S20) and $\phi_2 = 0$ into Eq. (S19a), the value of ϕ_1 is:

$$\phi_1 = \frac{1}{s(s\beta_{inj}+1)}\frac{1}{exp\left(\frac{y_{inj,w}}{2}\right)\left[\frac{A_i\left(E^{1/3}y_{inj,w}\right)}{2} - E^{1/3}A_i'\left(E^{1/3}y_{inj}\right)\right]}. \tag{S22}$$

where $A_i'(\cdot)$ is the derivative of the Airy function.

Substituting Eq. (S22) and $\phi_2 = 0$ into Eqs. (S21) and (S17b), one could obtain the Laplace-domain analytical solution of solute transport in the injection phase of the SWPP test.

S1.2 Solutions in the chaser phase: Eqs. (26a) - (26g)

For the chaser phase, conducting Laplace transform on Eqs. (S2a)-(S2b), one has:

$$\frac{R_m \alpha_r^2 D_u}{AB^2 R_{um}} \frac{\partial^2 \bar{C}_{umD}}{\partial z_D^2} - \frac{R_m v_{um} \alpha_r^2}{ABR_{um}} \frac{\partial \bar{C}_{umD}}{\partial z_D} - (s + \varepsilon_{um} + \mu_{umD})\bar{C}_{umD} + \varepsilon_{um}\bar{C}_{uimD} + C_{umD}(r_D, z_D, t_{inj,D}) = 0, \quad z_D \geq 1, \tag{S23a}$$

$$s\bar{C}_{uimD} - C_{uimD}(r_D, z_D, t_{inj,D}) = \varepsilon_{uim}(\bar{C}_{umD} - \bar{C}_{uimD}) - \mu_{uimD}\bar{C}_{uimD}\ , \tag{S23b}$$

Eq. (S23b) could be rewritten as :

$$\bar{C}_{uimD} = \frac{\varepsilon_{uim}}{s+\varepsilon_{uim}+\mu_{uimD}} \bar{C}_{umD} + \frac{C_{uimD}(r_D, z_D, t_{inj,D})}{s+\varepsilon_{uim}+\mu_{uimD}}, \tag{S23c}$$

Substituting Eq. (S23c) into Eq. (S23a), one has:

$$\frac{R_m \alpha_r^2 D_u}{AB^2 R_{um}} \frac{\partial^2 \bar{C}_{umD}}{\partial z_D^2} - \frac{R_m v_{um} \alpha_r^2}{ABR_{um}} \frac{\partial \bar{C}_{umD}}{\partial z_D} - \left(s + \varepsilon_{um} + \mu_{umD} - \frac{\varepsilon_{um}\varepsilon_{uim}}{s+\varepsilon_{uim}+\mu_{uimD}}\right)\bar{C}_{umD} + C_{umD}(r_D, z_D, t_{inj,D}) + \frac{\varepsilon_{um} C_{uimD}(r_D, z_D, t_{inj,D})}{s+\varepsilon_{uim}+\mu_{uimD}} = 0.\ z_D \geq 1, \tag{S24}$$

Similarly, Eqs. (S3a) - (S3b) become:

$$\frac{R_m \alpha_r^2 D_l}{AB^2 R_{lm}} \frac{\partial^2 \bar{C}_{lmD}}{\partial z_D^2} + \frac{R_m v_{lm} \alpha_r^2}{ABR_{lm}} \frac{\partial \bar{C}_{lmD}}{\partial z_D} - (s + \varepsilon_{lm} + \mu_{lmD})\bar{C}_{lmD} + \varepsilon_{lm}\bar{C}_{limD} + C_{lmD}(r_D, z_D, t_{inj,D}) = 0, \quad z_D \leq -1, \tag{S25a}$$

$$s\bar{C}_{limD} - C_{limD}(r_D, z_D, t_{inj,D}) = \varepsilon_{lim}(\bar{C}_{lmD} - \bar{C}_{limD}) - \mu_{limD}C_{limD}\ , \tag{S25b}$$

Eq. (S23b) could be rewritten as :

$$\bar{C}_{limD} = \frac{\varepsilon_{lim}}{s+\varepsilon_{lim}+\mu_{limD}} \bar{C}_{lmD} + \frac{C_{limD}(r_D, z_D, t_{inj,D})}{s+\varepsilon_{lim}+\mu_{limD}}, \tag{S25c}$$

Substituting Eq. (S25c) into Eq. (S25a), one has:

$$\frac{R_m \alpha_r^2 D_l}{AB^2 R_{lm}} \frac{\partial^2 \bar{C}_{lmD}}{\partial z_D^2} + \frac{R_m v_{lm} \alpha_r^2}{ABR_{lm}} \frac{\partial \bar{C}_{lmD}}{\partial z_D} - \left(s + \varepsilon_{lm} + \mu_{lmD} - \frac{\varepsilon_{lm}\varepsilon_{lim}}{s+\varepsilon_{lim}+\mu_{limD}}\right) \bar{C}_{lmD} +$$

$$C_{lmD}\left(r_D, z_D, t_{inj,D}\right) + \frac{\varepsilon_{lm} C_{limD}\left(r_D, z_D, t_{inj,D}\right)}{s+\varepsilon_{lim}+\mu_{limD}} = 0.\ z_D \leq -1, \tag{S26}$$

where $C_{umD}\left(r_D, z_D, t_{inj,D}\right)$ and $C_{uimD}\left(r_D, z_D, t_{inj,D}\right)$ are respectively the mobile and immobile concentrations [ML^{-3}] of the upper aquitard at the end of the injection phase, $C_{lmD}\left(r_D, z_D, t_{inj,D}\right)$ and $C_{limD}\left(r_D, z_D, t_{inj,D}\right)$ are respectively the mobile and immobile concentrations [ML^{-3}] of the lower aquitard at the end of the injection phase. In this study, we use the Green's function method to derive the analytical solution of Eqs. (S24) and (S26).

Notice that the boundary condition of Eq. (S6a) is inhomogeneous, thus we need to homogenize it first. Letting $\bar{C}_{umD} = \mathscr{k}(z_D) + \mathscr{s}_1 + \mathscr{s}_2 z_D$, and substituting them into Eqs. (S5) and (S6a) yields:

$$[\mathscr{k}(z_D)]|_{z_D \to \infty} = 0, \tag{S27a}$$

$$[\mathscr{k}(z_D)]|_{z_D = 1} = 0, \tag{S27b}$$

where $\mathscr{s}_1 = -\mathscr{s}_2 z_{eD}$ and $\mathscr{s}_2 = \frac{\bar{C}_{mD}(r_D, s)}{1 - z_{eD}}$.

Defining the spatial operator: $L_u = -\left[\frac{R_m \alpha_r^2 D_u}{AB^2 R_{um}} \frac{d^2}{dz_D^2} - \frac{R_m v_{um} \alpha_r^2}{ABR_{um}} \frac{d}{dz_D} - E_u\right]$, one has:

$$L_u \bar{C}_{umD} = L_u[\mathscr{k}(z_D) + \mathscr{s}_1] = F_u(z_D), \tag{S28}$$

Let $f_u(z_D) = F_u(z_D) - L_u[\mathscr{s}_1 + \mathscr{s}_2 z_D]$, one has:

$$\frac{R_m \alpha_r^2 D_u}{AB^2 R_{um}} \frac{d^2 \mathscr{k}}{dz_D^2} - \frac{R_m v_{um} \alpha_r^2}{ABR_{um}} \frac{d\mathscr{k}}{dz_D} - E_u \mathscr{k} = -f_u(z_D)\ , \tag{S29}$$

where $E_u = s + \varepsilon_{um} + \mu_{umD} - \frac{\varepsilon_{um}\varepsilon_{uim}}{s+\varepsilon_{uim}+\mu_{uimD}}$,

$F_u(z_D) = C_{umD}\left(r_D, z_D, t_{inj,D}\right) + \frac{\varepsilon_{um} C_{uimD}\left(r_D, z_D, t_{inj,D}\right)}{s+\varepsilon_{uim}+\mu_{uimD}}$ and $f_u(z_D) = C_{umD}\left(r_D, z_D, t_{inj,D}\right) + \frac{\varepsilon_{um} C_{uimD}\left(r_D, z_D, t_{inj,D}\right)}{s+\varepsilon_{uim}+\mu_{uimD}} - \frac{R_m v_{um} \alpha_r^2}{ABR_{um}} \mathscr{s}_2 - E_u(\mathscr{s}_1 + \mathscr{s}_2 z_D)$.

The general solution of Eq. (S24) is:

$$\bar{C}_{umD} = \int_1^{\infty} g_u(z_D, E_u; \eta_u)\, f_u(\eta_u) d\eta_u + \frac{z_D - z_{eD}}{1 - z_{eD}} \bar{C}_{mD}(r_D, s),\ z_D \geq 1. \qquad \text{(S30)}$$

where $f_u(\eta_u) = C_{umD}\left(r_D, \eta_u, t_{inj,D}\right) + \frac{\varepsilon_{um} C_{uimD}\left(r_D, \eta_u, t_{inj,D}\right)}{s + \varepsilon_{uim} + \mu_{uimD}} - \frac{R_m v_{um} \alpha_r^2}{ABR_{um}} \mathscr{s}_2 - E_u(\mathscr{s}_1 + \mathscr{s}_2 \eta_u)$, η_u is a positive value varying between 1 and ∞ (e.g. $1 \leq \eta_u \leq \infty$); $g_u(z_D, E_u; \eta_u)$ is the Green's function, and could be expressed as :

$$g_u(z_D, E_u; \eta_u) = \begin{cases} g_{u1}(z_D, E_u; \eta_u) = N_1 exp(a_1 z_D) + N_2 exp(a_2 z_D) & 1 \leq z_D < \eta_u \\ g_{u2}(z_D, E_u; \eta_u) = N_3 exp(a_1 z_D) + N_4 exp(a_2 z_D) & \eta_u \leq z_D < \infty \end{cases}, \qquad \text{(S31)}$$

where N_1, N_2, N_3 and N_4 are coefficients to be detrmined using the following conditions [*Chen and Woodside* ,1988]:

a) $g_u(z_D, E_u; \eta_u)$ satisfying the model of Eqs. (S29) and (S27a)-(S27b);

b) $g_{u1}(z_D, E_u; \eta_u) = g_{u2}(z_D, E_u; \eta_u)$;

c) $\left.\frac{dg_{u2}}{dz_D}\right|_{z_D = \eta_u^{+}} - \left.\frac{dg_{u1}}{dz_D}\right|_{z_D = \eta_u^{-}} = -\frac{AB^2 R_{um}}{R_m \alpha_r^2 D_u}$;

Substituting Eq. (S31) into Eq. (S27a), one has:

$$N_3 = 0, \qquad \text{(S32)}$$

Substituting Eq. (S31) into Eq. (S27b), one has:

$$N_1 exp(a_1) + N_2 exp(a_2) = 0, \qquad \text{(S33a)}$$

According to Eq. (S33a), one has:

$$N_1 = -N_2 exp(a_2 - a_1), \qquad \text{(S33b)}$$

According to above condition of b), one has:

$$N_1 exp(a_1 \eta_u) + N_2 exp(a_2 \eta_u) = N_4 exp(a_2 \eta_u), \qquad \text{(S34)}$$

According to above condition of c), one has:

$$N_4 a_2 exp(a_2 \eta_u) - [N_1 a_1 exp(a_1 \eta_u) + N_2 a_2 exp(a_2 \eta_u)] = -\frac{AB^2 R_{um}}{R_m \alpha_r^2 D_u}. \qquad \text{(S35)}$$

In the chaser phase, the values of N_1, N_2 , $N_3$and N_4 could be determined by Eqs. (S33a) - (S35), namely:

$$N_1 = -N_2 exp(a_2 - a_1), N_2 = \frac{-AB^2 R_{um}}{R_m \alpha_r^2 D_u[(a_1 - a_2)exp(a_2 - a_1)exp(a_1 \eta_u)]}, N_3 = 0 \text{ and}$$

$$N_4 = N_2 - N_2 exp(a_2 - a_1) exp(a_1 \eta_u - a_2 \eta_u).$$

As for the analytical solution of the lower aquitard, one could use a similar approach as that used for deriving the analytical solution of the upper aquitard to obtain, and the general solution of Eq. (S26) could be described as:

$$\bar{C}_{lmD} = \int_{-1}^{-\infty} g_l(z_D, E_l; \eta_l)\, f_l(\eta_l) d\eta_l + \frac{z_{eD} + z_D}{z_{eD} - 1} \bar{C}_{mD}(r_D, z_D, s), z_D \leq -1. \qquad \text{(S36a)}$$

$$g_l(z_D, E_l; \eta_l) = \begin{cases} g_{l1}(z_D, E_l; \eta_l) = M_1 exp(b_1 z_D) + M_2 exp(b_2 z_D) & -1 \leq z_D < \eta_l \\ g_{l2}(z_D, E_l; \eta_l) = M_3 exp(b_1 z_D) + M_4 exp(b_2 z_D) & \eta_l \leq z_D < -\infty \end{cases}, \qquad \text{(S36b)}$$

$$f_l(\eta_l) = C_{lmD}(r_D, \eta_l, t_{inj,D}) + \frac{\varepsilon_{lm} C_{limD}(r_D, \eta_l, t_{inj,D})}{s + \varepsilon_{lim} + \mu_{limD}} + \frac{R_m v_{lm} \alpha_r^2}{ABR_{lm}} \frac{\bar{C}_{mD}}{z_{eD} - 1} - \bar{C}_{mD} E_l \frac{z_{eD} + \eta_l}{z_{eD} - 1}, \qquad \text{(S36c)}$$

where η_l is a negative value varying between -1 and $-\infty$ (e.g.$-1 \leq \eta_l \leq -\infty$); $g_l(z_D, E_l; \eta_l)$ is the Green's function, $E_l = s + \varepsilon_{lm} + \mu_{lmD} - \frac{\varepsilon_{lm} \varepsilon_{lim}}{s + \varepsilon_{lim} + \mu_{limD}}$, and the values of M_1, M_2 , $M_3$and M_4 could be described as: $M_1 = -M_2 exp(b_1 - b_2)$, $M_2 = \frac{-AB^2 R_{lm}}{R_m \alpha_r^2 D_l[exp(b_2 \eta_l - b_1 \eta_l) - b_2 exp(b_2 \eta_l)]}$, $M_3 = M_2 exp(b_2 \eta_l - b_1 \eta_l) - M_2 exp(b_1 - b_2)$, $M_4 = 0$, and the values of a_1, a_2 , b_1 and b_2 are the same as used in the injection phase.

In the chaser phase, the dimensional boundary conditions Eqs. (15a)-(15b) are transformed into dimensionless forms as:

$$\beta_{cha,D} \frac{\partial C_{mD}(r_D, t_D)}{\partial t_D}\bigg|_{r_D = r_{wD}} = C_{mD}(r_D, t_D), t_{inj,D} < t_D \leq t_{cha,D}, \qquad \text{(S37a)}$$

$$C_{cha,mD}(r_D, t_D)\big|_{t_D = t_{inj,D}} = C_{inj,mD}(r_D, t_D)\big|_{t_D = t_{inj,D}}, t_{inj,D} < t_D \leq t_{cha,D}. \qquad \text{(S37b)}$$

where $\beta_{cha,D} = -\frac{V_{w,cha} r_{wD}}{\xi R_m \alpha_r}$.

Conducting Laplace transform on Eqs. (S1a)-(S1b) in the chaser phase, one has:

$$s\bar{C}_{mD} - C_{mD}\left(r_D, t_{inj,D}\right) = \frac{1}{r_D}\frac{\partial^2 \bar{C}_{mD}}{\partial r_D^2} - \frac{1}{r_D}\frac{\partial \bar{C}_{mD}}{\partial r_D} - (\varepsilon_m + \mu_{mD})\bar{C}_{mD} + \varepsilon_m \bar{C}_{imD} -$$

$$\left(\frac{\theta_{um}\alpha_r^2 v_{um}}{2A\theta_m B}\bar{C}_{umD} - \frac{\theta_{um}\alpha_r^2 D_u}{2A\theta_m B^2}\frac{\partial \bar{C}_{umD}}{\partial z_D}\right)\Big|_{z_D=1} + \left(\frac{\theta_{lm}\alpha_r^2 v_{lm}}{2A\theta_m B}\bar{C}_{lmD} - \frac{\theta_{lm}\alpha_r^2 D_l}{2AB^2\theta_m}\frac{\partial \bar{C}_{lmD}}{\partial z_D}\right)\Big|_{z_D=-1},$$

$$r_D \geq r_{wD}. \quad \text{(S38a)}$$

$$\bar{C}_{imD} = \frac{\varepsilon_{im}}{(s+\mu_{imD}+\varepsilon_{im})}\bar{C}_{mD} + \frac{C_{imD}\left(r_D, t_{inj,D}\right)}{(s+\mu_{imD}+\varepsilon_{im})}, r_D \geq r_{wD}, \quad \text{(S38b)}$$

where $C_{mD}\left(r_D, t_{inj,D}\right)$ and $C_{imD}\left(r_D, t_{inj,D}\right)$ are respectively the mobile and immobile concentrations [ML^{-3}] of the aquifer at the end of the injection phase, which could be calculated by Eqs. (S21) and (S17b).

After substituting Eqs. (S30), (S36a)-(S36c) and (S38b) into Eq. (S38a), one has:

$$\frac{1}{r_D}\frac{\partial^2 \bar{C}_{mD}}{\partial r_D^2} - \frac{1}{r_D}\frac{\partial \bar{C}_{mD}}{\partial r_D} - E_a \bar{C}_{mD} + F = 0, r_D \geq r_{wD}, \quad \text{(S39)}$$

where $E_a = s + \varepsilon_m + \mu_{mD} - \frac{\varepsilon_m \varepsilon_{im}}{s+\mu_{imD}+\varepsilon_{im}} + \frac{\theta_{um}\alpha_r^2 v_{um}}{2A\theta_m B} - \frac{\theta_{lm}\alpha_r^2 v_{lm}}{2AB^2\theta_m} - \frac{1}{1-z_{eD}}\frac{\theta_{um}\alpha_r^2 D_u}{2A\theta_m B^2} + \frac{1}{z_{eD}-1}\frac{\theta_{lm}\alpha_r^2 D_l}{2AB^2\theta_m}$

and $F = C_{mD}\left(r_D, t_{inj,D}\right) + \frac{\varepsilon_m C_{imD}\left(r_D, t_{inj}\right)}{s+\mu_{imD}+\varepsilon_{im}}$.

The boundary conditions of Eqs. (S37a)-(S37b) in Laplace domain becomes:

$$\bar{C}_{cha,mD}(r_{wD}, s) = \frac{\beta_{cha,D}}{s\beta_{cha,D}+1} C_{inj,mD}(r_D, t_D)\big|_{t_D = t_{inj,D}}. \quad \text{(S40)}$$

The boundary conditions of the wellbore and infinity in Laplace domain are:

$$\left[\bar{C}_{mD} - \frac{\partial \bar{C}_{mD}(r_D, s)}{\partial r_D}\right]\Big|_{r=r_{wD}} = \frac{\beta_{cha,D}}{s\beta_{cha,D}+1} C_{inj,mD}(r_D, t_D)\big|_{t_D = t_{inj,D}}, \quad \text{(S41a)}$$

$$\bar{C}_{cha,mD}(r_{wD}, s)\big|_{r_D \to \infty} = 0, \quad \text{(S41b)}$$

Similar to the model of the SWPP test in the injection phase, Eqs. (S39) and (S40)-(S41b) compose a model of the second-order ordinary differential equation (ODE) with boundary conditions, however, the governing equation is an inhomogeneous differential equation. In this study, we use the Green's function method to derive the analytical solution of Eq. (S39).

Notice that the boundary condition of Eq. (S41a) is inhomogeneous, and we need to homogenize it first. Assigning $\bar{C}_{mD} = \Psi(r_D) + \delta_1 + \delta_2 r_D$, and substituting it into Eqs. (S41a) and (S41b) yields:

$$\left[\Psi(r_D, s) - \frac{\partial \Psi(r_D,s)}{\partial r_D}\right]\Bigg|_{r=r_{wD}} = 0, \tag{S42a}$$

$$\Psi(r_D, s)|_{r_D\to\infty} = 0, \tag{S42b}$$

where $\delta_1 = -\frac{\beta_{cha,D}}{s\beta_{cha,D}+1}\frac{r_D|_{r_D\to\infty}}{(r_{wD}-r_D|_{r_D\to\infty}-1)}C_{inj,mD}(r_D,t_D)\Big|_{t_D=t_{inj,D}}$ and

$$\delta_2 = \frac{\beta_{cha,D}}{s\beta_{cha,D}+1}\frac{1}{(r_{wD}-r_D|_{r_D\to\infty}-1)}C_{inj,mD}(r_D,t_D)\Big|_{t_D=t_{inj,D}}.$$

Defining a spatial operator: $L = -\left[\frac{d^2}{dr_D^2} - \frac{d}{dr_D} - r_D E_a\right]$, one has:

$$L\bar{C}_{mD} = L[\Psi(r_D) + \delta_1 + \delta_2 r_D] = F r_D, \tag{S43}$$

Let $\varphi(r_D) = F r_D - L(\delta_1 + \delta_2 r_D)$, one has:

$$\frac{\partial^2 \Psi}{\partial r_D^2} - \frac{\partial \Psi}{\partial r_D} - r_D E_a \Psi = -\varphi(r_D). \tag{S44}$$

where $\varphi(r_D) = F r_D - [\delta_2 + r_D E_a(\delta_1 + \delta_2 r_D)]$.

The general solution of Eqs. (S42a) - (S44) is:

$$\Psi(r_D, E_a; \eta) = \int_{r_{wD}}^{\infty} g(r_D, E_a; \eta)\, \varphi(\eta) d\eta. \tag{S45}$$

where η is a positive value varying between r_{wD} and ∞ (e.g. $r_{wD} \le \eta \le \infty$); $g(r_D, E_a; \eta)$ is the Green's function, and could be expressed as :

$$g(r_D, E_a; \eta) = \begin{cases} g_1(r_D, E_a; \eta) = \mathcal{T}_1 exp(\frac{y_{cha}}{2}) A_i\left(E_a^{\frac{1}{3}} y_{cha}\right) + \mathcal{T}_2\, exp\left(\frac{y_{cha}}{2}\right) B_i\left(E_a^{\frac{1}{3}} y_{cha}\right) r_{wD} \le y_{cha} \le \eta \\ g_2(r_D, E_a; \eta) = \mathcal{T}_3 exp(\frac{y_{cha}}{2}) A_i\left(E_a^{\frac{1}{3}} y_{cha}\right) + \mathcal{T}_4\, exp\left(\frac{y_{cha}}{2}\right) B_i\left(E_a^{\frac{1}{3}} y_{cha}\right)\ \eta \le y_{cha} \le \infty \end{cases}. \tag{S46}$$

where $\varphi(\eta) = F\eta - [\delta_2 + \eta E_a(\delta_1 + \delta_2\eta)]$, $y_{cha} = r_D + \frac{1}{4E_a}$. As $B_i(r_D)$ diverges when $r_D \to \infty$, $\mathcal{T}_4$ has to be zero. Substituting Eq. (S45) into Eq. (S42a), one has:

$$\left[g_1 - \frac{\partial g_1}{\partial r_D}\right]\Big|_{r_D=r_{wD}} = 0, \quad \text{(S47)}$$

According to Eq. (S47), one has:

$$\mathcal{T}_1 = -\mathcal{T}_2 X. \quad \text{(S48)}$$

where $X = \frac{\frac{1}{2}B_i({E_a}^{1/3}y_{cha,w}) - {E_a}^{1/3}B_i'({E_a}^{1/3}y_{cha,w})}{\frac{1}{2}A_i({E_a}^{1/3}y_{cha,w}) - {E_a}^{1/3}A_i'({E_a}^{1/3}y_{cha,w})}$ and $y_{cha,w} = r_{wD} + \frac{1}{4E_a}$.

According to above condition of b), one has:

$$\mathcal{T}_1 A_i\left({E_a}^{\frac{1}{3}} y_{cha}|_{r_D=\eta^+}\right) + \mathcal{T}_2 B_i\left({E_a}^{\frac{1}{3}} y_{cha}|_{r_D=\eta^+}\right) = \mathcal{T}_3 A_i\left({E_a}^{1/3} y_{cha}|_{r_D=\eta^-}\right). \quad \text{(S49)}$$

According to above condition of c), one has:

$$\left[\frac{1}{2}\mathcal{T}_3\, exp\left(\frac{y_{cha}}{2}\right) A_i\left({E_a}^{\frac{1}{3}} y_{cha}\right) + {E_a}^{\frac{1}{3}}\mathcal{T}_3\, exp\left(\frac{y_{cha}}{2}\right) A_i'\left({E_a}^{\frac{1}{3}} y_{cha}\right)\right]\Big|_{r_D=\eta^-} -$$
$$\left[0.5\mathcal{T}_1\, exp\left(\frac{y_{cha}}{2}\right) A_i\left({E_a}^{\frac{1}{3}} y_{cha}\right) + {E_a}^{\frac{1}{3}}\mathcal{T}_1\, exp\left(\frac{y_{cha}}{2}\right) A_i'\left({E_a}^{\frac{1}{3}} y_{cha}\right)\right]\Big|_{r_D=\eta^+} -$$
$$\left[\frac{1}{2}\mathcal{T}_2\, exp\left(\frac{y_{cha}}{2}\right) B_i\left({E_a}^{\frac{1}{3}} y_{cha}\right) + {E_a}^{\frac{1}{3}}\mathcal{T}_2\, exp\left(\frac{y_{cha}}{2}\right) B_i'\left({E_a}^{\frac{1}{3}} y_{cha}\right)\right]\Big|_{r_D=\eta^+} = -1. \quad \text{(S50)}$$

For solution in the chaser phase, the values of $\mathcal{T}_1$, $\mathcal{T}_2$, $\mathcal{T}_3$ and $\mathcal{T}_4$ could be determined by Eqs. (S48) - (S50), namely:

$\mathcal{T}_1 = -\frac{\pi A_i\left(y_{ext}|_{r_D=\eta^+}\right)}{{E_a}^{1/3}} X$, $\mathcal{T}_2 = \frac{\pi A_i\left(y_{ext}|_{r_D=\eta^+}\right)}{{E_a}^{1/3}}$, $\mathcal{T}_3 = \frac{\pi A_i\left(y_{ext}|_{r_D=\eta^+}\right)}{{E_a}^{1/3}}\left[\frac{B_i\left(y_{ext}|_{r_D=\eta^+}\right)}{A_i\left(y_{ext}|_{r_D=\eta^+}\right)} - X\right]$ and $\mathcal{T}_4 = 0$.

S1.3 Solutions in the rest phase: Eqs. (27a) - (27f)

In the rest phase, the flow velocity become zero, and the advection and dispersion terms drop out of the governing equations. After conducting Laplace transform on Eqs. (S2a)-(S2b), the following equations would be obtained:

$$(s+\varepsilon_{um}+\mu_{umD})\bar{C}_{umD}-\varepsilon_{um}\bar{C}_{uimD}-C_{umD}(r_D,z_D,t_{cha,D})=0.\ z_D\geq 1. \quad \text{(S51a)}$$

$$\bar{C}_{uimD}=\frac{\varepsilon_{uim}}{s+\varepsilon_{uim}+\mu_{umD}}\bar{C}_{umD}+\frac{C_{uimD}(r_D,z_D,t_{cha,D})}{s+\varepsilon_{uim}+\mu_{umD}},\ z_D\geq 1, \quad \text{(S51b)}$$

Substituting Eq. (S51b) into Eq. (S51a), one has:

$$\left(s+\varepsilon_{um}+\mu_{umD}-\frac{\varepsilon_{um}\varepsilon_{uim}}{s+\varepsilon_{uim}+\mu_{uimD}}\right)\bar{C}_{umD}-C_{umD}(r_D,z_D,t_{cha,D})-\frac{\varepsilon_{um}C_{uimD}(r_D,z_D,t_{cha,D})}{s+\varepsilon_{uim}+\mu_{uimD}}=$$
$$0.\ z_D\geq 1. \quad \text{(S52)}$$

Similarly, Eqs. (S3a) - (S3b) become:

$$(s+\varepsilon_{lm}+\mu_{lmD})\bar{C}_{lmD}-\varepsilon_{lm}\bar{C}_{limD}-C_{lmD}(r_D,z_D,t_{cha,D})=0.\ z_D\leq -1. \quad \text{(S53a)}$$

$$\bar{C}_{limD}=\frac{\varepsilon_{lim}}{s+\varepsilon_{lim}+\mu_{lmD}}\bar{C}_{lmD}+\frac{C_{limD}(r_D,z_D,t_{cha,D})}{s+\varepsilon_{lim}+\mu_{lmD}},\quad z_D\leq -1, \quad \text{(S53b)}$$

Substituting Eq. (S45b) into Eq. (S45a), one has:

$$\left(s+\varepsilon_{lm}+\mu_{lmD}-\frac{\varepsilon_{lm}\varepsilon_{lim}}{s+\varepsilon_{lim}+\mu_{limD}}\right)\bar{C}_{lmD}-C_{lmD}(r_D,z_D,t_{cha,D})-\frac{\varepsilon_{lm}C_{limD}(r_D,z_D,t_{cha,D})}{s+\varepsilon_{lim}+\mu_{limD}}=$$
$$0.\ z_D\leq -1. \quad \text{(S54)}$$

According to Eqs. (S52) and (S54), one has:

$$\bar{C}_{umD}=\frac{C_{umD}(r_D,z_D,t_{cha,D})+\frac{\varepsilon_{um}C_{uimD}(r_D,z_D,t_{cha,D})}{s+\varepsilon_{uim}+\mu_{uimD}}}{\left(s+\varepsilon_{um}+\mu_{umD}-\frac{\varepsilon_{um}\varepsilon_{uim}}{s+\varepsilon_{uim}+\mu_{uimD}}\right)},\ z_D\geq 1, \quad \text{(S55a)}$$

$$\bar{C}_{lmD}=\frac{C_{lmD}(r_D,z_D,t_{cha,D})+\frac{\varepsilon_{lm}C_{limD}(r_D,z_D,t_{cha,D})}{s+\varepsilon_{lim}+\mu_{limD}}}{\left(s+\varepsilon_{lm}+\mu_{lmD}-\frac{\varepsilon_{lm}\varepsilon_{lim}}{s+\varepsilon_{lim}+\mu_{limD}}\right)},\ z_D\leq -1, \quad \text{(S55b)}$$

where $C_{umD}(r_D,z_D,t_{cha,D})$and $C_{uimD}(r_D,z_D,t_{cha,D})$ are respectively the mobile and immobile concentrations [ML^{-3}] of the upper aquitard at the end of the chaser phase, $C_{lmD}(r_D,z_D,t_{cha,D})$

and $C_{limD}(r_D, z_D, t_{cha,D})$ are respectively the mobile and immobile concentrations [ML^{-3}] of the lower aquitard at the end of the chaser phase.

Similarly, the dimensionless governing equation of the mobile zone during the rest phase is:

$$\frac{\partial C_{mD}}{\partial t_D} = -\varepsilon_m (C_{mD} - C_{imD}) - \mu_{mD} C_{mD}, r_D \geq r_{wD}. \tag{S56a}$$

$$\frac{\partial C_{imD}}{\partial t_D} = \varepsilon_{im} (C_{mD} - C_{imD}) - \mu_{imD} C_{imD}, r_D \geq r_{wD}, \tag{S56b}$$

Conducting Laplace transform to Eqs. (S56a) and (S56b) for the rest phase, one has:

$$s\bar{C}_{mD} - C_{mD}(r_D, t_{cha,D}) = -\varepsilon_m (\bar{C}_{mD} - \bar{C}_{imD}) - \mu_{mD} \bar{C}_{mD}, r_D \geq r_{wD}. \tag{S57a}$$

$$s\bar{C}_{imD} - C_{imD}(r_D, t_{cha,D}) = \varepsilon_{im} (\bar{C}_{mD} - \bar{C}_{imD}) - \mu_{imD} \bar{C}_{imD}, r_D \geq r_{wD}, \tag{S57b}$$

According to Eqs. (S57a)-(S57b) , one has:

$$\bar{C}_{mD} = \frac{C_{mD}(r_D, t_{cha,D}) + \frac{\varepsilon_m C_{imD}(r_D, t_{cha,D})}{(s + \mu_{imD} + \varepsilon_{im})}}{\left[s + \varepsilon_m + \mu_{mD} - \frac{\varepsilon_m \varepsilon_{im}}{(s + \mu_{imD} + \varepsilon_{im})}\right]}. \tag{S58a}$$

$$\bar{C}_{imD} = \frac{C_{imD}(r_D, t_{cha,D})}{(s + \mu_{imD} + \varepsilon_{im})} + \frac{\varepsilon_{im} \bar{C}_{mD}}{(s + \mu_{imD} + \varepsilon_{im})}. \tag{S58b}$$

S1.4 Solutions in the extraction phase: Eqs. (28a) - (28g)

Contrary to the injection and chaser phases, the direction of advective flux is reversed in the extraction stage, Eqs. (S2a) and (S3a) are modified as:

$$\frac{\partial C_{umD}}{\partial t_D} = \frac{R_m \alpha_r^2 D_u}{AB^2 R_{um}} \frac{\partial^2 C_{umD}}{\partial z_D^2} + \frac{R_m v_{um} \alpha_r^2}{ABR_{um}} \frac{\partial C_{umD}}{\partial z_D} - \varepsilon_{um} (C_{umD} - C_{uimD}) - \mu_{umD} C_{umD},$$

$$z_D \geq 1, \tag{S59a}$$

$$\frac{\partial C_{lmD}}{\partial t_D} = \frac{R_m \alpha_r^2 D_l}{AB^2 R_{lm}} \frac{\partial^2 C_{lmD}}{\partial z_D^2} - \frac{R_m v_{lm} \alpha_r^2}{ABR_{lm}} \frac{\partial C_{lmD}}{\partial z_D} - \varepsilon_{lm} (C_{lmD} - C_{limD}) - \mu_{lmD} C_{lmD},$$

$$z_D \leq -1, \tag{S59b}$$

Conducting Laplace transform on Eqs. (S2b) and (S59a), one has:

$$s\bar{C}_{umD} - C_{umD}\left(r_D, z_D, t_{res,D}\right) = \frac{R_m \alpha_r^2 D_u}{AB^2 R_{um}} \frac{\partial^2 \bar{C}_{umD}}{\partial z_D^2} + \frac{R_m v_{um} \alpha_r^2}{ABR_{um}} \frac{\partial \bar{C}_{umD}}{\partial z_D} - \varepsilon_{um}(\bar{C}_{umD} - \bar{C}_{uimD}) -$$

$$\mu_{umD}\bar{C}_{umD},\ z_D \geq 1, \quad \text{(S60a)}$$

$$\bar{C}_{uimD} = \frac{\varepsilon_{uim}\bar{C}_{umD}}{s+\varepsilon_{uim}+\mu_{uimD}} + \frac{C_{uimD}(r_D, z_D, t_{res,D})}{s+\varepsilon_{uim}+\mu_{uimD}},\ z_D \geq 1, \quad \text{(S60b)}$$

Substituting Eqs. (S60b) into Eq. (S60a) ,one can has:

$$\frac{R_m \alpha_r^2 D_u}{AB^2 R_{um}} \frac{\partial^2 \bar{C}_{umD}}{\partial z_D^2} + \frac{R_m v_{um} \alpha_r^2}{ABR_{um}} \frac{\partial \bar{C}_{umD}}{\partial z_D} - \left(s + \varepsilon_{um} + \mu_{umD} - \frac{\varepsilon_{um}\varepsilon_{uim}}{s+\varepsilon_{uim}+\mu_{uimD}}\right)\bar{C}_{umD} +$$

$$C_{umD}\left(r_D, z_D, t_{res,D}\right) + \frac{\varepsilon_{um} C_{uimD}(r_D, z_D, t_{res,D})}{s+\varepsilon_{uim}+\mu_{uimD}} = 0.\ z_D \geq 1, \quad \text{(S61)}$$

Similarly, conducting Laplace transform on Eqs. (S3b) and (S59b), one has:

$$s\bar{C}_{lmD} - C_{lmD}\left(r_D, z_D, t_{res,D}\right) = \frac{R_m \alpha_r^2 D_l}{AB^2 R_{lm}} \frac{\partial^2 \bar{C}_{lmD}}{\partial z_D^2} - \frac{R_m v_{lm} \alpha_r^2}{ABR_{lm}} \frac{\partial \bar{C}_{lmD}}{\partial z_D} - \varepsilon_{lm}(\bar{C}_{lmD} - \bar{C}_{limD}) -$$

$$\mu_{lmD}\bar{C}_{lmD},\ z_D \leq -1, \quad \text{(S62a)}$$

$$\bar{C}_{limD} = \frac{\varepsilon_{lim}\bar{C}_{lmD}}{s+\varepsilon_{lim}+\mu_{limD}} + \frac{C_{limD}(r_D, z_D, t_{res,D})}{s+\varepsilon_{lim}+\mu_{limD}},\ z_D \leq -1, \quad \text{(S62b)}$$

Substituting Eqs. (S62b) into Eq.(S62a), one has:

$$\frac{R_m \alpha_r^2 D_l}{AB^2 R_{lm}} \frac{\partial^2 \bar{C}_{lmD}}{\partial z_D^2} - \frac{R_m v_{lm} \alpha_r^2}{ABR_{lm}} \frac{\partial \bar{C}_{lmD}}{\partial z_D} - \left(s + \varepsilon_{lm} + \mu_{lmD} - \frac{\varepsilon_{lm}\varepsilon_{lim}}{s+\varepsilon_{lim}+\mu_{limD}}\right)\bar{C}_{lmD} +$$

$$C_{lmD}\left(r_D, z_D, t_{res,D}\right) + \frac{\varepsilon_{lm} C_{limD}(r_D, z_D, t_{res,D})}{s+\varepsilon_{lim}+\mu_{limD}} = 0.\ z_D \leq -1, \quad \text{(S63)}$$

where $C_{umD}\left(r_D, z_D, t_{res,D}\right)$and $C_{uimD}\left(r_D, z_D, t_{res,D}\right)$ are respectively the mobile and immobile concentrations [ML^{-3}] of the upper aquitard at the end of the rest phase, $C_{lmD}\left(r_D, z_D, t_{res,D}\right)$ and $C_{limD}\left(r_D, z_D, t_{res,D}\right)$ are respectively the mobile and immobile concentrations [ML^{-3}] of the lower aquitard at the end of the rest phase.

One could use a similar approach of obtaining the analytical solution of aquitards in the chaser phase to derive the solution of aquitards in the extraction phase. The general solution of (S61) is:

$$\bar{C}_{umD} = \int_{1}^{\infty} g_u(z_D, E_u; \mathscr{b}_u)\, f_u(\mathscr{b}_u) d\mathscr{b}_u + \frac{z_D - z_{eD}}{1 - z_{eD}} \bar{C}_{mD}(r_D, s), z_D \geq 1, \quad \text{(S64a)}$$

$$g_u(z_D, E_u; \mathscr{b}_u) = \begin{cases} g_{u1}(z_D, E_u; \mathscr{b}_u) = H_1 exp(m_1 z_D) + H_2 exp(m_2 z_D) & 1 \leq z_D < \mathscr{b}_u \\ g_{u2}(z_D, E_u; \mathscr{b}_u) = H_3 exp(m_1 z_D) + H_4 exp(m_2 z_D) & \mathscr{b}_u \leq z_D < \infty \end{cases}, \quad \text{(S64b)}$$

$$f_u(\mathscr{b}_u) =$$

$$C_{umD}\left(r_D, \mathscr{b}_u, t_{res,D}\right) + \frac{\varepsilon_{um} C_{uimD}\left(r_D, \mathscr{b}_u, t_{res,D}\right)}{s + \varepsilon_{uim} + \mu_{uimD}} + \frac{R_m v_{um} \alpha_r^2}{ABR_{um}} \frac{\bar{C}_{mD}(r_D, s)}{1 - z_{eD}} - \frac{\mathscr{b}_u - z_{eD}}{1 - z_{eD}} E_u \bar{C}_{mD}(r_D, s),$$

(S64c)

The general solution of Eq. (S63) could be described as:

$$\bar{C}_{lmD} = \int_{-1}^{-\infty} g_l(z_D, E_l; \mathscr{b}_l)\, f_l(\mathscr{b}_l) d\mathscr{b}_l + \frac{z_D + z_{eD}}{z_{eD} - 1} \bar{C}_{mD}(r_D, s), z_D \leq -1, \quad \text{(S65a)}$$

$$g_l(z_D, E_l; \mathscr{b}_l) = \begin{cases} g_{l1}(z_D, E_l; \mathscr{b}_l) = I_1 exp(n_1 z_D) + I_2 exp(n_2 z_D) & -1 \leq z_D < \mathscr{b}_l \\ g_{l2}(z_D, E_l; \mathscr{b}_l) = I_3 exp(n_1 z_D) + I_4 exp(n_2 z_D) & \mathscr{b}_l \leq z_D < -\infty \end{cases}, \quad \text{(S65b)}$$

$$f_l(\mathscr{b}_l) =$$

$$C_{mD}\left(r_D, \mathscr{b}_l, t_{res,D}\right) + \frac{\varepsilon_{lm} C_{limD}\left(r_D, \mathscr{b}_l, t_{res,D}\right)}{s + \varepsilon_{lim} + \mu_{limD}} - \frac{R_m v_{lm} \alpha_r^2}{ABR_{lm}} \frac{\bar{C}_{mD}(r_D, s)}{z_{eD} - 1} - \frac{\mathscr{b}_l + z_{eD}}{z_{eD} - 1} E_l \bar{C}_{mD}(r_D, s),$$

(S65c)

where $\mathscr{b}_u$ is a positive value varying between 1 and ∞; $\mathscr{b}_l$ is a negative value varying between -1 and $-\infty$; $g_u(z_D, E_u; \mathscr{b}_u)$ and $g_l(z_D, E_l; \mathscr{b}_l)$ are the Green's functions, $H_1 \sim H_4$ and $I_1 \sim I_4$ are contants which could be determined by the boundary conditions and conditions of a)~c), the values of $H_1 \sim H_4$ and $I_1 \sim I_4$ are as follows: $H_1 = -H_2 exp(m_2 - m_1)$,

$H_2 = \frac{-AR_{um}B^2}{R_m \alpha_r^2 D_u [(m_1 - m_2) exp(m_2 - m_1) exp(m_1 \mathscr{b}_u)]}$, $H_3 = 0$, $H_4 = H_2 - H_2 exp(m_2 - m_1) exp(m_1 \mathscr{b}_u - m_2 \mathscr{b}_u)$,

$I_1 = -I_2 exp(n_1 - n_2)$, $I_2 = \frac{-AB^2 R_{lm}}{R_m \alpha_r^2 D_l [exp(n_2 \mathscr{b}_l - n_1 \mathscr{b}_l) - n_2 exp(n_2 \mathscr{b}_l)]}$,

$I_3 = I_2 exp(n_2 \mathscr{b}_l - n_1 \mathscr{b}_l) - I_2 exp(n_1 - n_2)$, $I_4 = 0$,

$$m_1 = \frac{-\frac{R_m v_{um} \alpha_r^2}{ABR_{um}} + \sqrt{\left(\frac{R_m v_{um} \alpha_r^2}{ABR_{um}}\right)^2 + 4 \frac{R_m \alpha_r^2 D_u}{AB^2 R_{um}} \left(s + \varepsilon_{um} + \mu_{umD} - \frac{\varepsilon_{um} \varepsilon_{uim}}{s + \mu_{uimD} + \varepsilon_{uim}}\right)}}{2 \frac{R_m \alpha_r^2 D_u}{AB^2 R_{um}}},$$

$$m_2 = \frac{-\frac{R_m v_{um}\alpha_r^2}{ABR_{um}} - \sqrt{\left(\frac{R_m v_{um}\alpha_r^2}{ABR_{um}}\right)^2 + 4\frac{R_m\alpha_r^2 D_u}{AB^2 R_{um}}\left(s+\varepsilon_{um}+\mu_{umD}-\frac{\varepsilon_{um}\varepsilon_{uim}}{s+\mu_{uimD}+\varepsilon_{uim}}\right)}}{2\frac{R_m\alpha_r^2 D_u}{AB^2 R_{um}}},$$

$$n_1 = \frac{\frac{R_m v_{lm}\alpha_r^2}{ABR_{lm}} + \sqrt{\left(\frac{R_m v_{lm}\alpha_r^2}{ABR_{lm}}\right)^2 + 4\frac{R_m\alpha_r^2 D_l}{AB^2 R_{lm}}\left(s+\varepsilon_{lm}+\mu_{lmD}-\frac{\varepsilon_{lm}\varepsilon_{lim}}{s+\mu_{limD}+\varepsilon_{lim}}\right)}}{2\frac{R_m\alpha_r^2 D_l}{AB^2 R_{lm}}} \text{ and}$$

$$n_2 = \frac{\frac{R_m v_{lm}\alpha_r^2}{ABR_{lm}} - \sqrt{\left(\frac{R_m v_{lm}\alpha_r^2}{ABR_{lm}}\right)^2 + 4\frac{R_m\alpha_r^2 D_l}{AB^2 R_{lm}}\left(s+\varepsilon_{lm}+\mu_{lmD}-\frac{\varepsilon_{lm}\varepsilon_{lim}}{s+\mu_{limD}+\varepsilon_{lim}}\right)}}{2\frac{R_m\alpha_r^2 D_l}{AB^2 R_{lm}}}.$$

Similarly, contrary to the injection and chaser phases, the direction of advective flux is reversed in the extraction stage, and Eq. (S1a) is modified as:

$$\frac{\partial C_{mD}}{\partial t_D} = \frac{1}{r_D}\frac{\partial^2 C_{mD}}{\partial r_D^2} + \frac{1}{r_D}\frac{\partial C_{mD}}{\partial r_D} - \varepsilon_m(C_{mD} - C_{imD}) - \mu_{mD}C_{mD} - \left(-\frac{\theta_{um}\alpha_r^2 v_{um}}{2A\theta_m B}C_{umD} - \frac{\theta_{um}\alpha_r^2 D_u}{2A\theta_m B}\frac{\partial C_{umD}}{\partial z_D}\right)\bigg|_{z=1} + \left(-\frac{\theta_{lm}\alpha_r^2 v_{lm}}{2AB^2\theta_m}C_{lmD} - \frac{\theta_{lm}\alpha_r^2 D_l}{2AB^2\theta_m}\frac{\partial C_{lmD}}{\partial z_D}\right)\bigg|_{z=-1}, r_D \geq r_{wD}. \quad \text{(S66)}$$

In the extraction phase, the dimensional boundary conditions Eqs. (14a)-(14b) are transformed to the dimensionless format:

$$\beta_{ext,D}\frac{\partial C_{mD}(r_D,t_D)}{\partial t_D}\bigg|_{r_D=r_{wD}} = \frac{\partial C_{mD}(r_D,t_D)}{\partial r_D}\bigg|_{r_D=r_{wD}}, t_{res,D} < t_D \leq t_{ext,D} \quad \text{(S67a)}$$

$$C_{mD}(r_D,t_D)|_{t_D=t_{res,D}} = C_{res,mD}(r_D,t_D)\big|_{t_D=t_{res,D}}. \quad \text{(S67b)}$$

where $\beta_{ext,D} = -\frac{V_{w,ext}r_{wD}}{\xi R_m\alpha_r}$.

Conducting Laplace transform on Eqs. (S58) and (S1b) in the extraction phase, one has:

$$s\bar{C}_{mD} - C_{mD}(r_D,t_{res}) = \frac{1}{r_D}\frac{\partial^2\bar{C}_{mD}}{\partial r_D^2} + \frac{1}{r_D}\frac{\partial\bar{C}_{mD}}{\partial r_D} - (\varepsilon_m + \mu_{mD})\bar{C}_{mD} + \varepsilon_m\bar{C}_{imD} - \left(-\frac{\theta_{um}\alpha_r^2 v_{um}\bar{C}_{umD}}{2A\theta_m b} - \frac{\theta_{um}\alpha_r^2 D_u}{2A\theta_m b}\frac{\partial\bar{C}_{umD}}{\partial z_D}\right)\bigg|_{z_D=1} - \left(\frac{\theta_{lm}\alpha_r^2 v_{lm}\bar{C}_{lmD}}{2Ab^2\theta_m} + \frac{\theta_{lm}\alpha_r^2 D_l}{2Ab^2\theta_m}\frac{\partial\bar{C}_{lmD}}{\partial z_D}\right)\bigg|_{z_D=-1},$$

$$r_D \geq r_{wD}. \quad \text{(S68a)}$$

$$\bar{C}_{imD} = \frac{\varepsilon_{im}}{(s+\mu_{imD}+\varepsilon_{im})}\bar{C}_{mD} + \frac{C_{imD}(r_D,t_{res})}{s+\mu_{imD}+\varepsilon_{im}}, r_D \geq r_{wD}, \quad \text{(S68b)}$$

After substituting Eqs. (S64a)- (S65c) and Eq. (S68b) into Eq. (S68a), one has

$$\frac{\partial^2 \bar{C}_{mD}}{\partial r_D^2} + \frac{\partial \bar{C}_{mD}}{\partial r_D} - r_D \zeta \bar{C}_{mD} + r_D \Lambda = 0. \quad \text{(S69)}$$

where $\zeta = s + \varepsilon_m + \mu_{mD} - \frac{\varepsilon_{im}\varepsilon_m}{s+\mu_{imD}+\varepsilon_{im}} - \frac{\theta_{um}\alpha_r^2 v_{um}}{2A\theta_m B} + \frac{\theta_{lm}\alpha_r^2 v_{lm}}{2AB^2\theta_m} - \frac{1}{1-z_{eD}}\frac{\theta_{um}\alpha_r^2 D_u}{2A\theta_m b} + \frac{1}{z_{eD}-1}\frac{\theta_{lm}\alpha_r^2 D_l}{2Ab^2\theta_m}$,

$\Lambda = C_{mD}(r_D, t_{res}) + \frac{\varepsilon_m C_{imD}(r_D,t_{res})}{s+\mu_{imD}+\varepsilon_{im}}$; $C_{imD}(r_D, t_{res})$ and $C_{mD}(r_D, t_{res})$ represent the initial concentrations in the immobile and mobile domains of the SWPP test in the rest phase.

The boundary condition of Eqs. (S67a)-(S67b) in Laplace domain becomes:

$$s\beta_{ext,D}\bar{C}_{mD}(r_D, s)|_{r_D=r_{wD}} - \beta_{ext,D}C_{res,m}(r_D, t_D)\big|_{t_D=t_{res,D}} = \frac{\partial \bar{C}_{mD}(r_D,s)}{\partial r_D}\bigg|_{r_D=r_{wD}}. \quad \text{(S70)}$$

Similar to the model of the SWPP test in the injection phase, Eqs. (S5), (S61) and (S70) compose a model of the second-order ordinary differential equation (ODE) with boundary conditions. However, the governing equation is an inhomogeneous differential equation. In this study, we use the Green's function method to derive the analytical solution of Eq. (S69).

Similar to *Chen and Woodside* [1988], Eq. (S69) could be transferred into a self-adjoint form:

$$\frac{\partial^2 G}{\partial r_D^2} - \left(r_D \zeta + \frac{1}{4}\right) G = -\ell(r_D). \quad \text{(S71)}$$

where $G = exp(r_D/2)\bar{C}_{mD}$ and $\ell(r_D) = exp(r_D/2)r_D\Lambda$.

The boundary conditions of Eqs. (S5) and (S70) could be rewritten as：

$$G(r_D, s)|_{r_D=\infty} = 0, \quad \text{(S72a)}$$

$$\left[\left(s\beta_{ext,D} + \frac{1}{2}\right) G - \frac{\partial G}{\partial r_D}\right]\bigg|_{r_D=r_{wD}} = \beta_{ext,D} exp(r_{wD}/2) C_{mD}\left(r_{wD}, t_{res,D}\right), \quad \text{(S72b)}$$

One could find that the boundary condition of Eq. (S72b) is inhomogeneous, and we need to homogenize it first. Assigning $G = U(r_D) + V(r_D)$ and $V(r_D) = \sigma_1 + \sigma_2 r_D$, and substituting them into Eqs. (S72a) and (S72b) yields:

$$U(r_D, s)|_{r_D=\infty} = 0, \quad \text{(S73a)}$$

$$\left[\left(s\beta_{ext,D} + \frac{1}{2}\right)U - \frac{\partial U}{\partial r_D}\right]\Big|_{r_D=r_{wD}} = 0, \quad \text{(S73b)}$$

where $\sigma_1 = -\frac{\beta_{ext,D} exp(r_{wD}/2) C_{mD}(r_{wD}, t_{res,D})}{\left(s\beta_{ext,D}+\frac{1}{2}\right)r_{wD}-1-\left(s\beta_{ext,D}+\frac{1}{2}\right)r_D|_{r_D\to\infty}} r_D|_{r_D\to\infty}$,

$$\sigma_2 = \frac{\beta_{ext,D} exp(r_{wD}/2) C_{mD}(r_{wD}, t_{res,D})}{\left(s\beta_{ext,D}+\frac{1}{2}\right)r_{wD}-1-\left(s\beta_{ext,D}+\frac{1}{2}\right)r_D|_{r_D\to\infty}}.$$

After defining a spatial operator:$\mathrm{L} = -\frac{d^2}{dr_D^2} + \left(r_D\zeta + \frac{1}{4}\right)$, one has:

$$LG = LU(r_D) + LV(r_D) = \ell(r_D), \quad \text{(S74)}$$

and

$$LU(r_D) = \ell(r_D) - LV(r_D). \quad \text{(S75)}$$

Let $f(r_D) = \ell(r_D) - LV(r_D)$, one has:

$$\frac{\partial^2 U}{\partial r_D^2} - \left(r_D\zeta + \frac{1}{4}\right)U = -f(r_D). \quad \text{(S76)}$$

where $f(r_D) = exp(r_D/2) r_D \Lambda - \left(r_D\zeta + \frac{1}{4}\right)(\sigma_1 + \sigma_2 r_D)$.

Right now, the model with an inhomogeneous boundary condition becomes a regular Sturm-Louisville problem. The general solution of Eqs. (S73a) - (S73b) and (S76) is:

$$U(r_D, \zeta; \varepsilon) = \int_{r_{wD}}^{\infty} g(r_D, \zeta; \varepsilon) f(\varepsilon) d\varepsilon. \quad \text{(S77)}$$

where ε is a positive value varying between r_{wD} and ∞ (e.g. $r_{wD} \le \varepsilon \le \infty$); $g(r_D, \zeta; \varepsilon)$ is the Green's function, and could be expressed as :

$$g(r_D, \zeta; \varepsilon) = \begin{cases} g_1(r_D, \zeta; \varepsilon) = P_1 A_i(y_{ext}) + P_2 B_i(y_{ext}) & r_{wD} \le y_{ext} \le \varepsilon \\ g_2(r_D, \zeta; \varepsilon) = P_3 A_i(y_{ext}) + P_4 B_i(y_{ext}) & \varepsilon \le y_{ext} \le \infty \end{cases}, \quad \text{(S78)}$$

where $f(\varepsilon)=exp(\varepsilon/2)\varepsilon\Lambda-\left(\varepsilon\zeta+\frac{1}{4}\right)(\sigma_1+\sigma_2\varepsilon)$, $y_{ext}=\zeta^{1/3}\left(r_D+\frac{1}{4\zeta}\right)$, P_1, P_2, P_3 and P_4 are coefficients to be determined. As $B_i(r_D)$ diverges when $r_D\to\infty$, P_4 has to be zero.

Substituting Eq. (S78) into Eq. (S73b), one has:

$$\left[\left(s\beta_{ext,D}+\frac{1}{2}\right)g_1-\frac{\partial g_1}{\partial r_D}\right]\Big|_{r_D=r_{wD}}=0, \tag{S79}$$

which leads to

$$P_1=-P_2W. \tag{S80}$$

where $W=\frac{\left(s\beta_{ext,D}+\frac{1}{2}\right)B_i(y_{ext,w})-\zeta^{1/3}B_i'(y_{ext,w})}{\left(s\beta_{ext,D}+\frac{1}{2}\right)A_i(y_{ext,w})-\zeta^{1/3}A_i'(y_{ext,w})}$, $y_{ext,w}=\zeta^{1/3}\left(r_{wD}+\frac{1}{4\zeta}\right)$.

According to the properties of Green's function , one has:

$$P_1A_i\left(y_{ext}|_{r_D=\varepsilon^+}\right)+P_2B_i\left(y_{ext}|_{r_D=\varepsilon^+}\right)=P_3A_i\left(y_{ext}|_{r_D=\varepsilon^-}\right). \tag{S81}$$

$$\left[P_3\zeta^{1/3}A_i'(y_{ext})\right]_{r_D=\varepsilon^-}-\left[P_1\zeta^{\frac{1}{3}}A_i'(y_{ext})+P_2\zeta^{\frac{1}{3}}B_i'(y_{ext})\right]_{r_D=\varepsilon^+}=-1. \tag{S82}$$

The values of P_1, P_2 and P_3 could be determined by Eqs. (S69) - (S71), namely:

$$P_1=-\frac{\pi A_i\left(y_{ext}|_{r_D=\varepsilon^+}\right)}{\zeta^{1/3}}W\ ,\ \ P_2=\frac{\pi A_i\left(y_{ext}|_{r_D=\varepsilon^+}\right)}{\zeta^{1/3}},$$

$$P_3=\frac{\pi A_i\left(y_{ext}|_{r_D=\varepsilon^+}\right)}{\zeta^{1/3}}\left[\frac{B_i\left(y_{ext}|_{r_D=\varepsilon^+}\right)}{A_i\left(y_{ext}|_{r_D=\varepsilon^+}\right)}-W\right].$$

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S2. Numerical simulations

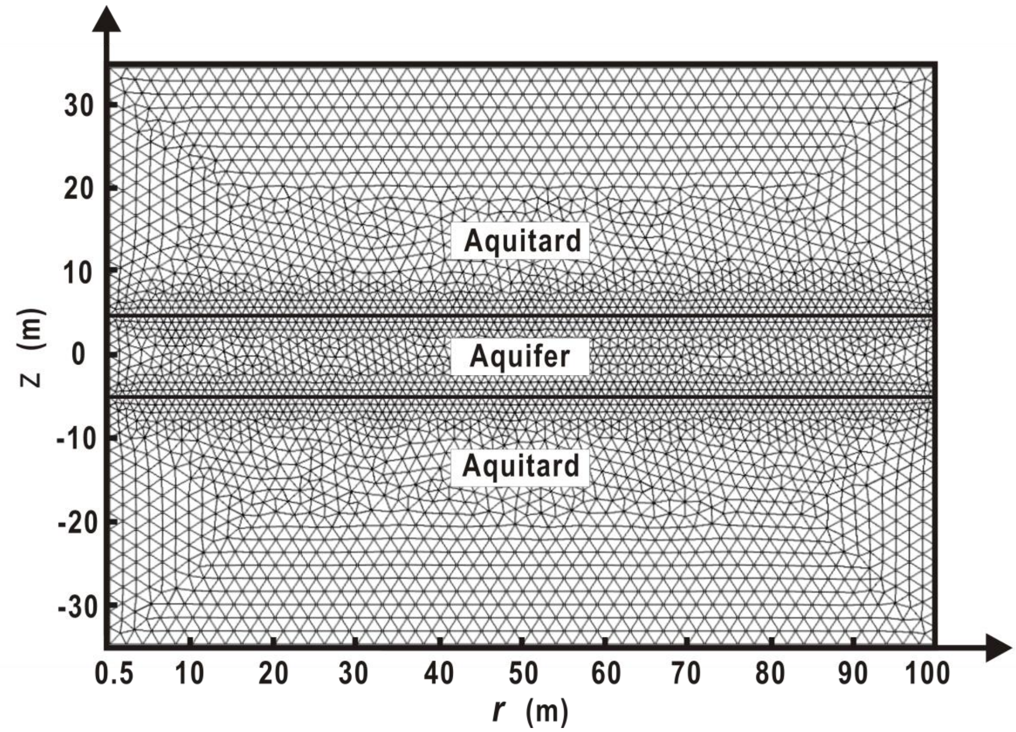

Figure S1. The grid mesh of the aquifer-aquitard system used in the Galerkin finite element program using COMSOL Multiphysics.

S3. References for Table 4

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