Supplement of Hydrol. Earth Syst. Sci., 27, 1891–1908, 2023
https://doi.org/10.5194/hess-27-1891-2023-supplement

Hydrology and Earth System Sciences
Open Access

Supplement of

A general model of radial dispersion with wellbore mixing and skin effects

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Supplementary Materials

S1. Derivation of Eqs. (14a) - (15b)

The dimensionless parameters are defined as: $C_{m1D}=\frac{C_{m1}}{C_0}$, $C_{im1D}=\frac{C_{im1}}{C_0}$, $C_{m2D}=\frac{C_{m2}}{C_0}$, $C_{im2D}=\frac{C_{im2}}{C_0}$, $C_{wD}=\frac{C_w}{C_0}$, $C_{inj,D}=\frac{C_{inj}}{C_0}$, $C_{cha,D}=\frac{C_{cha}}{C_0}$, $t_D=\frac{|A|t}{\alpha_2^2R_{m1}}$, $t_{inj,D}=\frac{|A|\,t_{inj}}{\alpha_2^2R_{m1}}$, $r_D=\frac{r}{\alpha_2}$, $r_{wD}=\frac{r_w}{\alpha_2}$, $r_{sD}=\frac{r_s}{\alpha_2}$, $r_{0D}=\frac{r_0}{\alpha_2}$, $\mu_{m1D}=\frac{\alpha_2^2\mu_{m1}}{A}$, $\mu_{im1D}=\frac{\alpha_2^2R_{m1}\mu_{im1}}{R_{im1}A}$, $\mu_{m2D}=\frac{\alpha_2^2\mu_{m2}R_{m1}}{AR_{m2}}$, $\mu_{im2D}=\frac{\alpha_2^2R_{m1}\mu_{im2}}{R_{im2}A}$ and $A=\frac{Q}{2\pi B\theta_{m1}}$. After the dimensionless transform, the governing equations become

$$\frac{\partial C_{m1D}}{\partial t_D}=\frac{\lambda}{r_D}\frac{\partial^2 C_{m1D}}{\partial r_D^2}-\frac{1}{r_D}\frac{\partial C_{m1D}}{\partial r_D}-\varepsilon_{m1}(C_{m1D}-C_{im1D})$$

$$-\mu_{m1D}C_{m1D}, r_{wD}<r_D\le r_{sD} \tag{S1a}$$

$$\frac{\partial C_{im1D}}{\partial t_D}=\varepsilon_{im1}(C_{m1D}-C_{im1D})-\mu_{im1D}C_{im1D}, r_{wD}<r_D\le r_{sD}, \tag{S1b}$$

$$\frac{\partial C_{m2D}}{\partial t_D}=\frac{\eta}{r_D}\frac{\partial^2 C_{m2D}}{\partial r_D^2}-\frac{\eta}{r_D}\frac{\partial C_{m2D}}{\partial r_D}-\varepsilon_{m2}(C_{m2D}-C_{im2D})-\mu_{m2D}C_{m2D}, r_D>r_{sD}, \tag{S1c}$$

$$\frac{\partial C_{im2D}}{\partial t_D}=\varepsilon_{im2}(C_{m2D}-C_{im2D})-\mu_{im2D}C_{im2D}, r_D>r_{sD}, \tag{S1d}$$

where $\varepsilon_{m1}=\frac{\omega_1\alpha_2^2}{A\theta_{m1}}$, $\varepsilon_{im1}=\frac{\omega_1\alpha_2^2R_{m1}}{A\theta_{im1}R_{im1}}$, $\varepsilon_{m2}=\frac{\omega_2\alpha_2^2R_{m1}}{A\theta_{m2}R_{m2}}$, $\varepsilon_{im2}=\frac{\omega_2\alpha_2^2R_{m1}}{A\theta_{im2}R_{im2}}$, $\eta=\frac{\theta_{m1}R_{m1}}{\theta_{m2}R_{m2}}$ and $\lambda=\frac{\alpha_1}{\alpha_2}$.

As for the boundary conditions at the well screen, a Heaviside step function will be employed to combine them at the injection and chasing phases:

$$C_w(r_w,t)=C_{inj}\left[H(t)-H\left(t-t_{inj}\right)\right]+C_{cha}H\left(t-t_{inj}\right), t>0, \tag{S2}$$

where $H(t)$ is the Heaviside step function, $C_w(r_w,t)$ is concentration [ML^{-3}] in the wellbore.

The dimensionless initial conditions and dimensionless boundary conditions are

$$C_{m1D}(r_D,t_D)|_{t_D=0}=C_{im1D}(r_D,t_D)|_{t_D=0}=C_{m2D}(r_D,t_D)|_{t_D=0}$$

$$=C_{im2D}(r_D,t_D)|_{t_D=0}=0, r_D>r_{wD}, \tag{S3a}$$

$$C_{m2D}(r_D,t_D)|_{r_D\to\infty} = C_{im2D}(r_D,t_D)|_{r_D\to\infty} = 0,\, t_D > 0, \tag{S3b}$$

$$\left[C_{m1D}(r_D,t_D) - \lambda\frac{\partial C_{m1D}(r_D,t_D)}{\partial r_D}\right]\Big|_{r_D=r_{wD}} = C_{inj,D}(t_D),\, 0 < t_D \le t_{inj,D}, \tag{S4a}$$

$$\left[C_{m1D}(r_D,t_D) - \lambda\frac{\partial C_{m1D}(r_D,t_D)}{\partial r_D}\right]\Big|_{r_D=r_{wD}} = C_{cha,D}(t_D),\, t_D > t_{inj,D}, \tag{S4b}$$

$$C_{\mathrm{w}D}(r_{wD},t_D) = C_{inj,D}\left[H(t_D) - H\left(t_D - t_{inj,D}\right)\right] + C_{cha,D}H\left(t_D - t_{inj,D}\right). \tag{S4c}$$

The dimensionless forms of Eqs. (7) - (8) are

$$\beta_{inj}\frac{dC_{inj,D}(t_D)}{dt_D} = 1 - C_{inj,D}(t_D),\, 0 < t_D \le\ t_{inj,D}, \tag{S5a}$$

$$\beta_{cha}\frac{dC_{cha,D}(t_D)}{dt_D} = -C_{cha,D}(t_D),\, t_D > t_{inj,D}, \tag{S5b}$$

where $\beta_{inj} = \frac{V_{w,inj}r_{wD}}{\xi R_{m1}\alpha_2}$ and $\beta_{cha} = \frac{V_{w,cha}r_{wD}}{\xi R_{m1}\alpha_2}$.

The dimensionless forms of Eqs. (12) - (13) are

$$C_{m1D}(r_{sD},t_D) = C_{m2D}(r_{sD},t_D),\, t_D > 0, \tag{S6a}$$

$$\left[\lambda\frac{\partial C_{m1D}(r_D,t_D)}{\partial r_D}\right]\Big|_{r_D=r_{sD}} = \left[\frac{\partial C_{m2D}(r_D,t_D)}{\partial r_D}\right]\Big|_{r_D=r_{sD}},\, t_D > 0, \tag{S6b}$$

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

$$s\bar{C}_{m1D} = \frac{\lambda}{r_D}\frac{\partial^2\bar{C}_{m1D}}{\partial r_D^2} - \frac{1}{r_D}\frac{\partial\bar{C}_{m1D}}{\partial r_D} - \varepsilon_{m1}(\bar{C}_{m1D} - \bar{C}_{im1D}) - \mu_{m1D}\bar{C}_{m1D}, \tag{S7a}$$

$$s\bar{C}_{im1D} = \varepsilon_{im1}(\bar{C}_{m1D} - \bar{C}_{im1D}) - \mu_{im1D}\bar{C}_{im1D}, \tag{S7b}$$

where the over bar represents the variable in Laplace domain; s is the Laplace transform parameter in respect to the dimensionless time t_D.

Substituting Eq. (S7b) into Eq. (S7a), one has

$$\frac{\lambda}{r_D}\frac{\partial^2\bar{C}_{m1D}}{\partial r_D^2} - \frac{1}{r_D}\frac{\partial\bar{C}_{m1D}}{\partial r_D} - E_1\bar{C}_{m1D} = 0,\, r_{wD} < r_D \le r_{sD}, \tag{S8}$$

where $E_1 = s + \varepsilon_{m1} + \mu_{m1D} - \frac{\varepsilon_{m1}\varepsilon_{im1}}{s+\varepsilon_{im1}+\mu_{im1D}}$.

Conducting Laplace transform to Eqs. (S1c) - (S1d), one has

$$s\bar{C}_{m2D} = \frac{\eta}{r_D}\frac{\partial^2 \bar{C}_{m2D}}{\partial r_D^2} - \frac{\eta}{r_D}\frac{\partial \bar{C}_{m2D}}{\partial r_D} - \varepsilon_{m2}(\bar{C}_{m2D} - \bar{C}_{im2D}) - \mu_{m2D}\bar{C}_{m2D}, \tag{S9a}$$

$$s\bar{C}_{im2D} = \varepsilon_{im2}(\bar{C}_{m2D} - \bar{C}_{im2D}) - \mu_{im2D}\bar{C}_{im2D}. \tag{S9b}$$

Substituting Eq. (S9b) into Eq. (S9a), one has

$$\frac{1}{r_D}\frac{\partial^2 \bar{C}_{m2D}}{\partial r_D^2} - \frac{1}{r_D}\frac{\partial \bar{C}_{m2D}}{\partial r_D} - E_2\bar{C}_{m2D} = 0, r_D > r_{sD}, \tag{S10}$$

where $E_2 = \frac{1}{\eta}\left(s + \varepsilon_{m2} + \mu_{m2D} - \frac{\varepsilon_{m2}\varepsilon_{im2}}{s+\varepsilon_{im2}+\mu_{im2D}}\right)$.

The boundary conditions in the Laplace domain are

$$\left[\bar{C}_{m1D}(r_D, s) - \lambda\frac{\partial \bar{C}_{m1D}(r_D,s)}{\partial r_D}\right]\Big|_{r_D=r_{wD}} = \frac{1}{s(s\beta_{inj}+1)}, 0 < t_D \leq\ t_{inj,D}, \tag{S11a}$$

$$\left[\bar{C}_{m1D}(r_D, s) - \lambda\frac{\partial \bar{C}_{m1D}(r_D,s)}{\partial r_D}\right]\Big|_{r_D=r_{wD}} = \frac{\beta_{cha}c_{inj,D}(r_{wD},t_{inj,D})}{(s\beta_{cha}+1)}, t_D > t_{inj,D}, \tag{S11b}$$

$$\bar{C}_{m1D}(r_{sD}, s) = \bar{C}_{m2D}(r_{sD}, s), t_D > 0, \tag{S11c}$$

$$\lambda\left[\frac{\partial \bar{C}_{m1D}(r_D,s)}{\partial r_D}\right]\Big|_{r_D=r_{sD}} = \left[\frac{\partial \bar{C}_{m2D}(r_D,s)}{\partial r_D}\right]\Big|_{r_D=r_{sD}}, t_D > 0, \tag{S11d}$$

$$\bar{C}_{m2D}(r_D, s)|_{r_D\to\infty} = 0, t_D > 0, \tag{S11e}$$

The general solutions of Eq. (S8) and Eq. (S10) are respectively

$$\bar{C}_{m1D} = N_1\,exp\left(\frac{r_D}{2\lambda}\right)A_i(y_1) + N_2 exp\ \left(\frac{r_D}{2\lambda}\right)B_i(y_1), r_{wD} < r_D \leq r_{sD}, \tag{S12a}$$

$$\bar{C}_{m2D} = N_3\,exp\left(\frac{r_D}{2}\right)A_i(y_2) + N_4 exp\ \left(\frac{r_D}{2}\right)B_i(y_2), r_D > r_{sD}, \tag{S12b}$$

where $y_1 = \left(\frac{E_1}{\lambda}\right)^{1/3}\left(r_D + \frac{1}{4\lambda E_1}\right)$; $y_2 = (E_2)^{1/3}\left(r_D + \frac{1}{4E_2}\right)$; N_1, N_2, N_3 and N_4 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.

Substituting Eq. (S12b) into Eq. (S11e), one has

$$N_4 = 0. \tag{S13}$$

Substituting Eq. (S12a) into Eq. (S11a), one has

$$N_1 exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}A_i(y_w) - \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} A_i'(y_w)\right] + N_2 exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}B_i(y_w) - \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} exp\left(\frac{r_{wD}}{2}\right) B_i'(y_w)\right] = F_1, \tag{S14a}$$

where $y_w = \left(\frac{E_1}{\lambda}\right)^{1/3}\left(r_{wD} + \frac{1}{4\lambda E_1}\right)$, and $F_1 = \frac{1}{s(s\beta_{inj}+1)}$.

Substituting Eq. (S12a) into Eq. (S11b), one has

$$N_1 exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}A_i(y_w) - \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} A_i'(y_w)\right] + N_2 exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}B_i(y_w) - \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} exp\left(\frac{r_{wD}}{2}\right) B_i'(y_w)\right] = F_2, \tag{S14b}$$

where $F_2 = \frac{\beta_{cha} C_{inj,D}(r_{wD}, t_{inj,D})}{(s\beta_{cha}+1)}$.

Conducting Laplace transform on Eq. (S4c), one has

$$\bar{C}_{wD}(r_{wD}, s) = C_{inj,D}\frac{1-exp(-t_{inj,D}s)}{s} + C_{cha,D}\frac{exp(-t_{inj,D}s)}{s}, r_D = r_{wD}, \tag{S14c}$$

Thus, Eqs. (S14a) - (S14c) could be combined as the following equation

$$N_1 exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}A_i(y_w) - \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} A_i'(y_w)\right] + N_2 exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}B_i(y_w) - \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} exp\left(\frac{r_{wD}}{2}\right) B_i'(y_w)\right] = F, \tag{S14d}$$

where $F = C_{inj,D}\frac{1-exp(-t_{inj,D}s)}{s} + C_{cha,D}\frac{exp(-t_{inj,D}s)}{s}$.

Substituting Eqs. (S12a) - (S12b) into Eq. (S11c), one has

$$N_1\, exp\left(\frac{r_{sD}}{2\lambda}\right) A_i(y_{1s}) + N_2 ex\,p\left(\frac{r_{sD}}{2\lambda}\right) B_i(y_{1s}) = N_3\, exp\left(\frac{r_{sD}}{2}\right) A_i(y_{2s}), \tag{S15}$$

where $y_{1s} = \left(\frac{E_1}{\lambda}\right)^{1/3}\left(r_{sD} + \frac{1}{4\lambda E_1}\right)$; $y_{2s} = (E_2)^{1/3}\left(r_{sD} + \frac{1}{4E_2}\right)$.

Substituting Eqs. (S12a) - (S12b) into Eq. (S11d) yields

$$N_1 exp\left(\frac{r_{sD}}{2\lambda}\right)\left[\frac{1}{2}A_i(y_{1s}) + \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} A_i'(y_{1s})\right] + N_2 exp\left(\frac{r_{sD}}{2\lambda}\right)\left[\frac{1}{2}B_i(y_{1s}) + \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} B_i'(y_{1s})\right] = N_3 exp\left(\frac{r_{sD}}{2}\right)\left[\frac{1}{2}A_i(y_{2s}) + (E_2)^{1/3}A_i'(y_{2s})\right], \quad \text{(S16)}$$

where $A_i'(\cdot)$ and $B_i'(\cdot)$ are the derivative of the Airy functions of the first kind and second kind, respectively.

The values of N_1, N_2, and N_3 could be determined by solving Eqs. (S14d) - (S16):

$$N_1 = \frac{F - H_2 N_2}{H_1},$$

$$N_2 = \frac{H_3 H_8 F - H_5 H_6 F}{H_1 H_5 H_7 + H_2 H_3 H_8 - H_2 H_5 H_6 - H_1 H_4 H_8},$$

$$N_3 = \frac{H_3 F}{H_1 H_5} - \frac{H_2 H_3 N_2}{H_1 H_5} + \frac{H_4 N_2}{H_5},$$

where $H_1 = exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}A_i(y_w) - \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} A_i'(y_w)\right]$,

$$H_2 = exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}B_i(y_w) - \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} exp\left(\frac{r_{wD}}{2}\right) B_i'(y_w)\right],$$

$$H_3 = exp\left(\frac{r_{sD}}{2\lambda}\right) A_i(y_{1s}),\ H_4 = exp\left(\frac{r_{sD}}{2\lambda}\right) B_i(y_{1s}),\ H_5 = exp\left(\frac{r_{sD}}{2}\right) A_i(y_{2s}),$$

$$H_6 = exp\left(\frac{r_{sD}}{2\lambda}\right)\left[\frac{1}{2}A_i(y_{1s}) + \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} A_i'(y_{1s})\right],$$

$$H_7 = exp\left(\frac{r_{sD}}{2\lambda}\right)\left[\frac{1}{2}B_i(y_{1s}) + \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} B_i'(y_{1s})\right],$$

$$H_8 = exp\left(\frac{r_{sD}}{2}\right)\left[\frac{1}{2}A_i(y_{2s}) + (E_2)^{1/3}A_i'(y_{2s})\right],$$

and $F = C_{inj,D}\frac{1-exp(-t_{inj,D}s)}{s} + C_{cha,D}\frac{exp(-t_{inj,D}s)}{s}$. Substituting the expressions of N_1, N_2, N_3, and N_4 into Eqs. (S12a) - (S12b), one could get the solutions of Eq. (14a) and Eq. (15a).

Substituting Eqs. (S12a) - (S12b) into Eq. (S7b) and Eq. (S9b), one could get the solutions of Eq. (14b) and Eq. (15b)

$$\bar{C}_{im1D} = \frac{\varepsilon_{im1}}{s+\varepsilon_{im1}+\mu_{im1D}}\bar{C}_{m1D}, r_{wD} \le r_D \le r_{sD}, \tag{S17a}$$

$$\bar{C}_{im2D} = \frac{\varepsilon_{im2}}{s+\varepsilon_{im2}+\mu_{im2D}}\bar{C}_{m2D}, r_D > r_{sD}. \tag{S17b}$$

In the injection phase, the values of N_1 and N_2 are modified into N_1' and N_2' as follows

$N_1' = \frac{F_1 - H_2 N_2'}{H_1'}$ and $N_2' = \frac{H_3 H_8 F_1 - H_5 H_6 F_1}{H_1' H_5 H_7 + H_2 H_3 H_8 - H_2 H_5 H_6 - H_1' H_4 H_8}$, where $H_1' = exp\left(\frac{r_{wD}}{2\lambda}\right) A_i(y_w)$.

Substituting N_1' and N_2' into Eq. (S12a), one has

$$\bar{C}_{inj,D} = N_1' \, exp\left(\frac{r_D}{2\lambda}\right) A_i(y_1) + N_2' exp\left(\frac{r_D}{2\lambda}\right) B_i(y_1), r_D = r_{wD}, \tag{S18}$$

In the chasing phase, the values of N_1 and N_2 are modified into N_1'' and N_2'' as follows

$N_1'' = \frac{F_2 - H_2 N_2''}{H_1'}$, $N_2'' = \frac{H_3 H_8 F_2 - H_5 H_6 F_2}{H_1' H_5 H_7 + H_2 H_3 H_8 - H_2 H_5 H_6 - H_1' H_4 H_8}$, and substituting N_1'' and N_2'' into Eq. (S12a), one has

$$\bar{C}_{cha,D} = N_1'' \, exp\left(\frac{r_D}{2\lambda}\right) A_i(y_1) + N_2'' exp\left(\frac{r_D}{2\lambda}\right) B_i(y_1), r_D = r_{wD}, \tag{S19}$$

S2. Model with scale-dependent dispersivity: Derivation of Eqs. (17a) - (18b)

Substituting Eq. (16) into Eq. (1c), the dimensionless form of the governing equations become

$$\frac{\partial C_{m2D}}{\partial t_D} = \frac{k\eta \partial^2 C_{m2D}}{\partial r_D^2} + \frac{k\eta - \eta}{r_D}\frac{\partial C_{m2D}}{\partial r_D} - \varepsilon_{m2}(C_{m2D} - C_{im2D}) - \mu_{m2D} C_{m2D}, r_{sD} \le r_D \le r_{0D}, \tag{S20a}$$

$$\frac{\partial C_{m2D}}{\partial t_D} = \frac{\eta}{r_D}\frac{\partial^2 C_{m2D}}{\partial r_D^2} - \frac{\eta}{r_D}\frac{\partial C_{m2D}}{\partial r_D} - \varepsilon_{m2}(C_{m2D} - C_{im2D}) - \mu_{m2D} C_{m2D}, r_D \ge r_{0D}. \tag{S20b}$$

Similarly, one could obtain the dimensionless initial conditions and dimensionless boundary conditions, the expressions of the dimensionless initial conditions and dimensionless boundary conditions are the same with Eqs. (S3a) - (S6b), except that

$$\left[\lambda \frac{\partial C_{m1D}(r_D, t_D)}{\partial r_D}\right]\Bigg|_{r_D = r_{sD}} = \left[k \frac{\partial C_{m2D}(r_D, t_D)}{\partial r_D}\right]\Bigg|_{r_D = r_{sD}}. \tag{S21}$$

In the formation zone, we could obtain the boundary condition at $r_D = r_{0D}$

$$kr_D \frac{\partial C_{m2D}(r_D,t_D)}{\partial r_D} = \frac{\partial C_{m2D}(r_D,t_D)}{\partial r_D}, r_D = r_{0D}, \tag{S22}$$

Then conducting Laplace transform to Eqs. (S20a)- (S20b), one has

$$s\bar{C}_{m2D} = k\eta \frac{\partial^2 \bar{C}_{m2D}}{\partial r_D^2} + \frac{k\eta - \eta}{r_D}\frac{\partial \bar{C}_{m2D}}{\partial r_D} - \varepsilon_{m2}(\bar{C}_{m2D} - \bar{C}_{im2D}) - \mu_{m2D}\bar{C}_{m2D}, r_{sD} \leq r_D \leq r_{0D}, \tag{S23a}$$

$$s\bar{C}_{m2D} = \frac{\eta}{r_D}\frac{\partial^2 \bar{C}_{m2D}}{\partial r_D^2} - \frac{\eta}{r_D}\frac{\partial \bar{C}_{m2D}}{\partial r_D} - \varepsilon_{m2}(\bar{C}_{m2D} - \bar{C}_{im2D}) - \mu_{m2D}\bar{C}_{m2D}, r_D \geq r_{0D} \tag{S23b}$$

Substituting Eq. (S9b) into Eqs. (S23a) - (S23b), one has

$$\frac{\partial^2 \bar{C}_{m2D}}{\partial r_D^2} + \frac{n}{r_D}\frac{\partial \bar{C}_{m2D}}{\partial r_D} - \varepsilon_1^2 \bar{C}_{m2D} = 0, r_{sD} \leq r_D \leq r_{0D}, \tag{S24a}$$

$$\frac{1}{r_D}\frac{\partial^2 \bar{C}_{m2D}}{\partial r_D^2} - \frac{1}{r_D}\frac{\partial \bar{C}_{m2D}}{\partial r_D} - \varepsilon_1^2 \bar{C}_{m2D} = 0, r_D > r_{0D}. \tag{S24b}$$

where $n = 1 - \frac{1}{k}$ and $\varepsilon_1 = \sqrt{\frac{E_2}{k\eta}}$.

Similar to Eqs. (S11a) - (S11e) and Eq. (S21), the boundary conditions at wellbore and infinity in the Laplace domain are

$$\left[\bar{C}_{m1D}(r_D,s) - \lambda \frac{\partial \bar{C}_{m1D}(r_D,s)}{\partial r_D}\right]\Big|_{r_D=r_{wD}} = \frac{1}{s(s\beta_{inj}+1)}, \tag{S25a}$$

$$\left[\bar{C}_{m1D}(r_D,s) - \lambda \frac{\partial \bar{C}_{m1D}(r_D,s)}{\partial r_D}\right]\Big|_{r_D=r_{wD}} = \frac{\beta_{cha} C_{inj,D}(r_{wD}, t_{inj,D})}{(s\beta_{cha}+1)}, \tag{S25b}$$

$$\bar{C}_{m1D}(r_{sD},s) = \bar{C}_{m2D}(r_{sD},s), \tag{S25c}$$

$$\left[\lambda \frac{\partial \bar{C}_{m1D}(r_D,s)}{\partial r_D}\right]\Big|_{r_D=r_{sD}} = \left[k \frac{\partial \bar{C}_{m2D}(r_D,s)}{\partial r_D}\right]\Big|_{r_D=r_{sD}}, \tag{S25d}$$

$$\left[kr_D \frac{\partial \bar{C}_{m2D}(r_D,s)}{\partial r_D}\right]\Big|_{r_D=r_{0D}} = \left[\frac{\partial \bar{C}_{m2D}(r_D,s)}{\partial r_D}\right]\Big|_{r_D=r_{0D}}, \tag{S25e}$$

$$\bar{C}_{m2D}(r_{0D},s) = \bar{C}_{m2D}(r_{0D},s), \tag{S25f}$$

$$\bar{C}_{m2D}(r_D,s)|_{r_D\to\infty} = 0. \tag{S25g}$$

The general solutions of Eq. (S8) and Eq. (S23) are respectively

$$\bar{C}_{m1D} = \mathcal{T}_1\, exp\left(\frac{r_D}{2\lambda}\right) A_i(y_1) + \mathcal{T}_2 exp\ \left(\frac{r_D}{2\lambda}\right) B_i(y_1), r_{wD} < r_D \le r_{sD}, \tag{S26a}$$

$$\bar{C}_{m2D} = \mathcal{T}_3 r_D^m K_m(\varepsilon_1 r_D) + \mathcal{T}_4 r_D^m I_m(\varepsilon_1 r_D), r_{sD} \le r_D \le r_{0D}, \tag{S26b}$$

$$\bar{C}_{m2D} = \mathcal{T}_5\, exp\left(\frac{r_D}{2}\right) A_i(y_3) + \mathcal{T}_6 exp\ \left(\frac{r_D}{2}\right) B_i(y_3), r_D > r_{0D}, \tag{S26c}$$

where $m = \frac{1}{2k}$; $y_3 = (\varepsilon_1)^{1/3}\left(r_D + \frac{1}{4\varepsilon_1}\right)$; $\mathcal{T}_1$, $\mathcal{T}_2$, $\mathcal{T}_3$, $\mathcal{T}_4$, $\mathcal{T}_5$ and $\mathcal{T}_6$ are constants which could be determined by the boundary conditions; $I_m$and K_m are the m^{th}-order modified Bessel functions of the first kind and second kind, respectively.

Substituting Eq. (S6f) into Eq. (S26c), one has

$$\mathcal{T}_6 = 0. \tag{S27}$$

Substituting Eq. (S26a) into Eq. (S25a), one has

$$\mathcal{T}_1 exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}A_i(y_w) - \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} A_i'(y_w)\right] + \mathcal{T}_2 exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}B_i(y_w) - \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} exp\left(\frac{r_{wD}}{2}\right) B_i'(y_w)\right] = F_1. \tag{S28}$$

Substituting Eq. (S26a) into Eq. (S25b), one has

$$\mathcal{T}_1 exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}A_i(y_w) - \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} A_i'(y_w)\right] + \mathcal{T}_2 exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}B_i(y_w) - \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} exp\left(\frac{r_{wD}}{2}\right) B_i'(y_w)\right] = F_2, \tag{S29a}$$

Similar to the treatment of Eq. (S14d), Eqs. (S28) - (S29a) could be combined as the following equation

$$\mathcal{T}_1 exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}A_i(y_w) - \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} A_i'(y_w)\right] + \mathcal{T}_2 exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}B_i(y_w) - \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} exp\left(\frac{r_{wD}}{2}\right) B_i'(y_w)\right] = F, \tag{S29b}$$

where $F = C_{inj,D}\frac{1-exp(-t_{inj,D}s)}{s} + C_{cha,D}\frac{exp(-t_{inj,D}s)}{s}$.

Substituting Eqs. (S26a) - (S26b) into Eq. (S25c), one has

$$\mathcal{T}_1\, exp\left(\frac{r_{sD}}{2\lambda}\right) A_i(y_{1s}) + \mathcal{T}_2\, ex\,p\left(\frac{r_{sD}}{2\lambda}\right) B_i(y_{1s}) = \mathcal{T}_3 r_{sD}^m K_m(\varepsilon_1 r_{sD}) + \mathcal{T}_4 r_D^m I_m(\varepsilon_1 r_D), \qquad \text{(S30)}$$

Substituting Eqs. (B7a) - (B7b) into Eq. (B6d) yields

$$\mathcal{T}_1 exp\left(\frac{r_{sD}}{2\lambda}\right)\left[\frac{1}{2}A_i(y_{1s}) + \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} A_i'(y_{1s})\right] + \mathcal{T}_2 exp\left(\frac{r_{sD}}{2\lambda}\right)\left[\frac{1}{2}B_i(y_{1s}) + \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} B_i'(y_{1s})\right] =$$

$$-\mathcal{T}_3 k\varepsilon_1 r_{sD}^{m+1} K_{m-1}(\varepsilon_1 r_{sD}) + \mathcal{T}_4 k\{m r_{sD}^{m-1} I_m(\varepsilon_1 r_D) + 0.5\varepsilon_1 r_{sD}^m [I_{m-1}(\varepsilon_1 r_D) + I_{m+1}(\varepsilon_1 r_D)]\}, \qquad \text{(S31)}$$

where $K_{m-1}(\cdot)$ is the derivative of the m^{th}-order modified Bessel function of the second kind, $I_{m-1}(\cdot)$ and $I_{m+1}(\cdot)$ are the derivatives of the m^{th}-order modified Bessel function of the first kind.

Substituting Eqs. (S26b) - (S26c) into Eq. (S25e) and Eq. (S25f) yields

$$-\mathcal{T}_3 k\varepsilon_1 r_{0D}^{m+2} K_{m-1}(\varepsilon_1 r_{0D}) + \mathcal{T}_4 k\{m r_{0D}^m I_m(\varepsilon_1 r_{0D}) + 0.5\varepsilon_1 r_{0D}^{m+1}[I_{m-1}(\varepsilon_1 r_{0D}) +$$

$$I_{m+1}(\varepsilon_1 r_{0D})]\} = \mathcal{T}_5\left[0.5 exp\left(\frac{r_D}{2}\right) A_i(y_4) + \varepsilon_1^{1/3}\, exp\left(\frac{r_D}{2}\right) A_i'(y_4)\right], \qquad \text{(S32)}$$

$$\mathcal{T}_3 r_{0D}^m K_m(\varepsilon_1 r_{0D}) + \mathcal{T}_4 r_{0D}^m I_m(\varepsilon_1 r_{0D}) = \mathcal{T}_5\, exp\left(\frac{r_{0D}}{2}\right) A_i(y_4), \qquad \text{(S33)}$$

where $y_4 = (\varepsilon_1)^{1/3}\left(r_{0D} + \frac{1}{4\varepsilon_1}\right)$.

The values of $\mathcal{T}_1$, $\mathcal{T}_2$, $\mathcal{T}_3$, $\mathcal{T}_4$, $\mathcal{T}_5$ and $\mathcal{T}_6$ could be determined by solving Eqs. (S27) - (S33), one has

$$\mathcal{T}_1 = \frac{F - W_2\mathcal{T}_2}{W_1},$$

$$\mathcal{T}_2 = \frac{W_1W_5}{W_1W_4 - W_2W_3}\mathcal{T}_3 + \frac{W_1W_6}{W_1W_4 - W_2W_3}\mathcal{T}_4 - \frac{W_3F}{W_1W_4 - W_2W_3},$$

$$\mathcal{T}_3 = \frac{W_{13}W_{15} - W_{12}W_{16}}{W_{11}W_{16} - W_{13}W_{14}}\mathcal{T}_4,$$

$$\mathcal{T}_4 = \frac{W_3F(W_1W_8 - W_2W_7) - W_7F(W_1W_4 - W_2W_3)}{(W_1W_5\Theta + W_1W_6)(W_1W_8 - W_2W_7) - (W_1W_9\Theta - W_1W_{10})(W_1W_4 - W_2W_3)} \text{ and } \mathcal{T}_5 = \frac{W_{14}}{W_{16}}\mathcal{T}_3 + \frac{W_{15}}{W_{16}}\mathcal{T}_4.$$

where $W_1 = exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}A_i(y_w) - \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} A_i'(y_w)\right]$,

$$W_2 = exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}B_i(y_w) - \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} exp\left(\frac{r_{wD}}{2}\right)B_i'(y_w)\right],$$

$$W_3 = exp\left(\frac{r_{sD}}{2\lambda}\right)A_i(y_{1s}),\ ex\,p\left(\frac{r_{sD}}{2\lambda}\right)B_i(y_{1s}),\ W_5 = r_{sD}^m K_m(\varepsilon_1 r_{sD}),\ W_6 = r_D^m I_m(\varepsilon_1 r_D),$$

$$W_7 = exp\left(\frac{r_{sD}}{2\lambda}\right)\left[\frac{1}{2}A_i(y_{1s}) + \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} A_i'(y_{1s})\right],$$

$$W_8 = exp\left(\frac{r_{sD}}{2\lambda}\right)\left[\frac{1}{2}B_i(y_{1s}) + \lambda\left(\frac{E_1}{\lambda}\right)^{1/3} B_i'(y_{1s})\right],$$

$$W_9 = -k\varepsilon_1 r_{sD}^{m+1}K_{m-1}(\varepsilon_1 r_{sD}),$$

$$W_{10} = k\{m r_{sD}^{m-1} I_m(\varepsilon_1 r_D) + 0.5\varepsilon_1 r_{sD}^m [I_{m-1}(\varepsilon_1 r_D) + I_{m+1}(\varepsilon_1 r_D)]\},$$

$$W_{11} = -k\varepsilon_1 r_{0D}^{m+2}K_{m-1}(\varepsilon_1 r_{0D}),$$

$$W_{12} = k\{m r_{0D}^m I_m(\varepsilon_1 r_{0D}) + 0.5\varepsilon_1 r_{0D}^{m+1}[I_{m-1}(\varepsilon_1 r_{0D}) + I_{m+1}(\varepsilon_1 r_{0D})]\},$$

$$W_{13} = 0.5exp\left(\frac{r_D}{2}\right)A_i(y_4) + \varepsilon_1^{1/3} exp\left(\frac{r_D}{2}\right)A_i'(y_4),$$

$W_{14} = r_{0D}^m K_m(\varepsilon_1 r_{0D})$, $W_{15} = r_{0D}^m I_m(\varepsilon_1 r_{0D})$, $W_{16} = exp\left(\frac{r_{0D}}{2}\right)A_i(y_4)$ and $\Theta = \frac{W_{13}W_{15} - W_{12}W_{16}}{W_{11}W_{16} - W_{13}W_{14}}$

In the injection phase, the values of $\mathcal{T}_1$ and $\mathcal{T}_2$ are modified into $\mathcal{T}_1'$ and $\mathcal{T}_2'$ as follows

$$\mathcal{T}_1' = \frac{F_1 - W_2'\mathcal{T}_2'}{W_1'},\ \mathcal{T}_2' = \frac{W_1'W_5}{W_1'W_4 - W_2'W_3}\mathcal{T}_3' + \frac{W_1'W_6}{W_1'W_4 - W_2'W_3}\mathcal{T}_4' - \frac{W_3F_1}{W_1'W_4 - W_2'W_3},$$

where $W_1' = exp\left(\frac{r_{wD}}{2\lambda}\right)A_i(y_w)$, $W_2' = exp\left(\frac{r_{wD}}{2\lambda}\right)B_i(y_w)$, $\mathcal{T}_3' = \frac{W_{13}W_{15} - W_{12}W_{16}}{W_{11}W_{16} - W_{13}W_{14}}\mathcal{T}_4'$, and $\mathcal{T}_4' = \frac{W_3F_1(W_1'W_8 - W_2'W_7) - W_7F_1(W_1'W_4 - W_2'W_3)}{(W_1'W_5\Theta + W_1'W_6)(W_1'W_8 - W_2'W_7) - (W_1'W_9\Theta - W_1'W_{10})(W_1'W_4 - W_2'W_3)}$.

Substituting $\mathcal{T}_1'$ and $\mathcal{T}_2'$ into Eq. (S26a), one has

$$\bar{C}_{inj,D}(r_{wD}, \mathrm{s}) = \mathcal{T}_1' \,exp\left(\frac{r_D}{2\lambda}\right)A_i(y_1) + \mathcal{T}_2' exp\left(\frac{r_D}{2\lambda}\right)B_i(y_1), \tag{S34}$$

In the chasing phase, the values of $\mathcal{T}_1$ and $\mathcal{T}_2$ are changed into $\mathcal{T}_1''$ and $\mathcal{T}_2''$ as follows

$$\mathcal{T}_1'' = \frac{F_2 - W_2'\mathcal{T}_2''}{W_1'},\ \mathcal{T}_2'' = \frac{W_1'W_5}{W_1'W_4 - W_2'W_3}\mathcal{T}_3'' + \frac{W_1'W_6}{W_1'W_4 - W_2'W_3}\mathcal{T}_4'' - \frac{W_3F_2}{W_1'W_4 - W_2'W_3},$$

where $\mathcal{T}_3'' = \frac{W_{13}W_{15}-W_{12}W_{16}}{W_{11}W_{16}-W_{13}W_{14}}\mathcal{T}_4''$, $\mathcal{T}_4'' = \frac{W_3F_2(W_1'W_8-W_2'W_7)-W_7F_2(W_1'W_4-W_2'W_3)}{(W_1'W_5\Theta+W_1'W_6)(W_1'W_8-W_2'W_7)-(W_1'W_9\Theta-W_1'W_{10})(W_1'W_4-W_2'W_3)}$.

Substituting $\mathcal{T}_1''$ and $\mathcal{T}_2''$ into Eq. (S29a), one has

$$\bar{C}_{cha,D}(r_{wD},\mathrm{s}) = \mathcal{T}_1''\,exp\left(\frac{r_D}{2\lambda}\right)A_i(y_1) + \mathcal{T}_2''exp\,\left(\frac{r_D}{2\lambda}\right)B_i(y_1), \tag{S35}$$

Substituting Eqs. (S25a) - (S25c) into Eq. (S1b) and Eq. (S1d), one has

$$\bar{C}_{im1D} = \frac{\varepsilon_{im1}}{s+\varepsilon_{im1}+\mu_{im1D}}\bar{C}_{m1D}, r_{wD} \le r_D \le r_{sD}, \tag{S36a}$$

$$\bar{C}_{im2D} = \frac{\varepsilon_{im2}}{s+\varepsilon_{im2}+\mu_{im2D}}\bar{C}_{m2D}, r_D > r_{sD}. \tag{S36b}$$

S3. The MIM model and solution in an aquifer-aquitard system

S3.1 Mathematical model

Assuming that advection, dispersion and sorption involved in the solute transport in the aquifer-aquitard system, the governing equations are

$$\theta_{m1}R_{m1}\frac{\partial C_{m1}}{\partial t} = \frac{\theta_{m1}}{r}\frac{\partial}{\partial r}\left(r\alpha_1|v_{a1}|\frac{\partial C_{m1}}{\partial r}\right) - \theta_{m1}v_{a1}\frac{\partial C_{m1}}{\partial r} - \omega_1(C_{m1}-C_{im1})$$

$$-\theta_m\mu_{m1}C_{m1} - \frac{\theta_{um}D_u}{2b}\frac{\partial C_{um}}{\partial z}\bigg|_{z=b} + \frac{\theta_{lm}D_l}{2b}\frac{\partial C_{lm}}{\partial z}\bigg|_{z=-b}, r_w \le\ r \le r_s, \tag{S37a}$$

$$\theta_{im1}R_{im1}\frac{\partial C_{im1}}{\partial t} = \omega_1(C_{m1}-C_{im1}) - \theta_{im1}\mu_{im1}C_{im1}, r_w \le\ r \le r_s, \tag{S37b}$$

$$\theta_{m2}R_{m2}\frac{\partial C_{m2}}{\partial t} = \frac{\theta_{m2}}{r}\frac{\partial}{\partial r}\left(r\alpha_2|v_{a2}|\frac{\partial C_{m2}}{\partial r}\right) - \theta_{m2}v_{a2}\frac{\partial C_{m2}}{\partial r} - \omega_2(C_{m2}-C_{im2})$$

$$-\theta_{m2}\mu_{m2}C_{m2} - \frac{\theta_{um}D_u}{2b}\frac{\partial C_{um}}{\partial z}\bigg|_{z=b} + \frac{\theta_{lm}D_l}{2b}\frac{\partial C_{lm}}{\partial z}\bigg|_{z=-b}, r > r_s, \tag{S37c}$$

$$\theta_{im2}R_{im2}\frac{\partial C_{im2}}{\partial t} = \omega_2(C_{m2}-C_{im2}) - \theta_{im2}\mu_{im2}C_{im2}, r\ > r_s, \tag{S37d}$$

$$\theta_{um}R_{um}\frac{\partial C_{um}}{\partial t} = \theta_{um}D_u\frac{\partial^2 C_{um}}{\partial z^2} - \omega_u(C_{um}-C_{uim}) - \theta_{um}\mu_{um}C_{um}, z \ge b, \tag{S38a}$$

$$\theta_{uim}R_{uim}\frac{\partial C_{uim}}{\partial t} = \omega_u(C_{um}-C_{uim}) - \theta_{uim}\mu_{uim}C_{uim}, z \ge b \tag{S38b}$$

$$\theta_{lm}R_{lm}\frac{\partial C_{lm}}{\partial t} = \theta_{lm}D_l\frac{\partial^2 C_{lm}}{\partial z^2} - \omega_l(C_{lm}-C_{lim}) - \theta_{lm}\mu_{lm}C_{lm}, z \le -b, \tag{S39a}$$

$$\theta_{lim} R_{lim} \frac{\partial C_{lim}}{\partial t} = \omega_l (C_{lm} - C_{lim}) - \theta_{lim} \mu_{lim} C_{lim}, z \leq -b, \quad \text{(S39b)}$$

where the subscripts "u" and "l" refer to the parameters in the upper and lower aquitard, respectively; the subscripts "m" and "im" refer to the parameters in the mobile and immobile regions, respectively; the subscripts ''1'' and "2" refer to the parameters in the skin and formation regions, respectively; C_{m1} and C_{im1} are the mobile and immobile concentrations [ML^{-3}] of the skin zone, respectively; C_{m2} and C_{im2} are the mobile and immobile concentrations [ML^{-3}] of the formation zone, respectively; C_{um} and C_{uim} are the mobile and immobile concentrations [ML^{-3}] of the upper aquitard, respectively; C_{lm} and C_{lim} are the mobile and immobile concentrations [ML^{-3}] of the upper aquitard, respectively; t is time [T]; r is the radial distance [L] from the center of the well; r_w is radius of the well [L]; r_s is the radial distance [L] from the center of the well to the outer radius of the skin zone; z represents the vertical distance [L]; b is the half of the aquifer thickness [L]; α_1 and α_2 represent the longitudinal dispersivities [L] in the skin and formation zones, respectively; D_u and D_l are the vertical dispersion coefficients [L^{2}T^{-1}] of the upper and lower aquitards, respectively; v_{a1} and v_{a2} represent the average radial pore velocity [LT^{-1}] of the skin and formation zones, respectively; and $v_{a1} = \frac{u_1}{\theta_{m1}}$ and $v_{a1} = \frac{u_2}{\theta_{m2}}$; u_1 and u_2 represent Darcian velocity [LT^{-1}] of the skin and formation zones, respectively; μ_{m1},μ_{im1}, μ_{m2}, μ_{im2} μ_{um}, μ_{uim}, μ_{lm} and μ_{lim} are reaction rates for first-order biodegradation, or radioactive decay, or the first-order reaction rate [T^{-1}], respectively; θ_{m1}, θ_{im1}, θ_{m2} and θ_{im2} are the mobile and immobile porosities [dimensionless] , respectively; θ_{um},θ_{uim}, θ_{lm} and θ_{lim} are the mobile and immobile porosities [dimensionless], respectively; $R_{m1} = 1 + \frac{\rho_b K_d}{\theta_{m1}}$ and $R_{im1} = 1 + \frac{\rho_b K_d}{\theta_{im1}}$ are regarded as retardation factors [dimensionless] for the mobile and immobile regions of the skin zone, respectively; $R_{m2} = 1 + \frac{\rho_b K_d}{\theta_{m2}}$ and $R_{im2} = 1 + \frac{\rho_b K_d}{\theta_{im2}}$ are regarded as retardation factors [dimensionless] for the mobile and immobile regions of the aquifer, respectively; $R_{um} = 1 + \frac{\rho_b K_d}{\theta_{um}}$ and $R_{uim} = 1 + \frac{\rho_b K_d}{\theta_{uim}}$ are regarded as retardation factors [dimensionless] for the mobile and immobile regions of the upper aquitard, respectively; $R_{lm} = 1 + \frac{\rho_b K_d}{\theta_{lm}}$ and $R_{lim} = 1 + \frac{\rho_b K_d}{\theta_{lim}}$ could be regarded as retardation factors [dimensionless] for the mobile and immobile regions in the lower aquitard, respectively; K_d is the equilibrium distribution coefficient for the linear sorption process [$M^{-1}L^{3}$]; ρ_b is the bulk density [ML^{-3}] of the aquifer material; ω_a, ω_u and ω_l are the first-order mass transfer coefficients [T^{-1}] of the aquifer, upper aquitard, and lower aquitard, respectively.

Subject to the following initial and boundary conditions

$$C_{m1}(r,t)|_{t=0} = C_{im1}(r,t)|_{t=0} = C_{m2}(r,t)|_{t=0} = C_{im2}(r,t)|_{t=0} = C_{um}(r,z,t)|_{t=0} = C_{uim}(r,z,t)|_{t=0} = C_{lm}(r,z,t)|_{t=0} = C_{lim}(r,z,t)|_{t=0} = 0, r \geq r_w, \quad \text{(S40)}$$

$$C_{m2}(r,t)|_{r\to\infty} = C_{im2}(r,t)|_{r\to\infty} = C_{um}(r,z,t)|_{r\to\infty} = C_{uim}(r,z,t)|_{r\to\infty} = C_{lm}(r,z,t)|_{r\to-\infty} = C_{lim}(r,z,t)|_{r\to-\infty} = 0, r \geq r_w, \quad \text{(S41)}$$

$$C_{m1}(r,t) = C_{um}(r,z=b,t), r_w \leq r \leq r_s, \quad \text{(S42a)}$$

$$C_{m2}(r,t) = C_{um}(r,z=b,t), r > r_s, \quad \text{(S42b)}$$

$$C_{m1}(r,t) = C_{lm}(r,z=-b,t), r_w \leq r \leq r_s, \quad \text{(S43a)}$$

$$C_{m2}(r,t) = C_{lm}(r,z=-b,t), r > r_s. \quad \text{(S43b)}$$

The flux concentration continuity is applied in boundary condition of the wellbore, and one has

$$\left[v_{a1,inj} C_{m1}(r,t) - \alpha_1 |v_{a1,inj}| \frac{\partial C_{m1}(r,t)}{\partial r}\right]\Big|_{r=r_w} = \left[v_{a1,inj} C_{inj}(t)\right]\Big|_{r=r_w}, 0 < t \leq t_{inj}, \quad \text{(S44a)}$$

$$\left[v_{a1,cha} C_{m1}(r,t) - \alpha_1 |v_{a1,cha}| \frac{\partial C_{m1}(r,t)}{\partial r}\right]\Big|_{r=r_w} = \left[v_{a1,cha} C_{cha}(t)\right]\Big|_{r=r_w}, t > t_{inj}, \quad \text{(S44b)}$$

where $C_{inj}(t)$ and $C_{cha}(t)$ represent the wellbore concentrations [ML^{-3}] of tracer in the injection and chasing phases, respectively.

Considering the mixing effect of the injected tracer with the original water in the wellbore, the variations of concentration in the injection and chasing phases could be described as

$$V_{w,inj}\frac{dC_{inj}}{dt} = -\xi v_{a1,inj}(r_w)\left[C_{inj}(t) - C_0\right], 0 < t \le t_{inj}, \tag{S45a}$$

$$V_{w,cha}\frac{dC_{cha}}{dt} = -\xi v_{a1,cha}(r_w)[C_{cha}(t)], t > t_{inj}. \tag{S45b}$$

3.2 Derivation of the analytical solutions

The dimensionless parameters are defined as: $C_{m1D} = \frac{C_{m1}}{C_0}$, $C_{im1D} = \frac{C_{im1}}{C_0}$, $C_{m2D} = \frac{C_{m2}}{C_0}$, $C_{im2D} = \frac{C_{im2}}{C_0}$, $C_{wD} = \frac{C_w}{C_0}$, $C_{inj,D} = \frac{C_{inj}}{C_0}$, $C_{cha,D} = \frac{C_{cha}}{C_0}$, $C_{umD} = \frac{C_{um}}{C_0}$, $C_{uimD} = \frac{C_{uim}}{C_0}$, $C_{lmD} = \frac{C_{lm}}{C_0}$, $C_{limD} = \frac{C_{lim}}{C_0}$, $t_D = \frac{|A|t}{\alpha_2^2 R_{m1}}$, $t_{inj,D} = \frac{|A|t_{inj}}{\alpha_2^2 R_{m1}}$, $r_D = \frac{r}{\alpha_2}$, $r_{wD} = \frac{r_w}{\alpha_2}$, $z_D = \frac{z}{B}$, $\mu_{m1D} = \frac{\alpha_2^2\mu_{m1}}{A}$, $\mu_{im1D} = \frac{\alpha_2^2 R_{m1}\mu_{im1}}{R_{im1}A}$, $\mu_{m2D} = \frac{\alpha_2^2\mu_{m2}}{A}$, $\mu_{im2D} = \frac{\alpha_2^2 R_{m1}\mu_{im2}}{R_{im2}A}$, $\mu_{umD} = \frac{\alpha_2^2 R_m\mu_m}{R_{um}A}$, $\mu_{uimD} = \frac{\alpha_2^2 R_m\mu_{im}}{R_{um}A}$, $\mu_{lmD} = \frac{\alpha_2^2 R_m\mu_m}{AR_{lm}}$, $\mu_{limD} = \frac{\alpha_2^2 R_m\mu_{im}}{R_{lm}A}$ and $A = \frac{Q}{4\pi B\theta_{m1}}$. The dimensionless forms of the governing equation could be rewritten as

$$\frac{\partial C_{m1D}}{\partial t_D} = \frac{\lambda}{r_D}\frac{\partial^2 C_{m1D}}{\partial r_D^2} - \frac{1}{r_D}\frac{\partial C_{m1D}}{\partial r_D} - \varepsilon_{m1}(C_{m1D} - C_{im1D}) - \mu_{m1D}C_{m1D} - \frac{\theta_{um}\alpha_2^2 D_u}{2A\theta_{m1}b^2}\frac{\partial C_{umD}}{\partial z_D}\bigg|_{z=1} + \frac{\theta_{lm}\alpha_2^2 D_l}{2Ab^2\theta_{m1}}\frac{\partial C_{lmD}}{\partial z_D}\bigg|_{z=-1}, r_{wD} \le r_D \le r_{sD}, \tag{S46a}$$

$$\frac{\partial C_{im1D}}{\partial t_D} = \varepsilon_{im1}(C_{m1D} - C_{im1D}) - \mu_{im1D}C_{im1D}, r_{wD} \le r_D \le r_{sD}, \tag{S46b}$$

$$\frac{\partial C_{m2D}}{\partial t_D} = \frac{1}{r_D}\frac{\partial^2 C_{m2D}}{\partial r_D^2} - \frac{1}{r_D}\frac{\partial C_{m2D}}{\partial r_D} - \varepsilon_{m2}(C_{m2D} - C_{im2D}) - \mu_{m2D}C_{m2D} - \frac{\theta_{um}\alpha_2^2 D_u}{2A\theta_{m2}\mathrm{b}^2}\frac{\partial C_{umD}}{\partial z_D}\bigg|_{z=1} + \frac{\theta_{lm}\alpha_2^2 D_l}{2Ab^2\theta_{m2}}\frac{\partial C_{lmD}}{\partial z_D}\bigg|_{z=-1}, r_D > r_{sD}, \tag{S46c}$$

$$\frac{\partial C_{im2D}}{\partial t_D} = \varepsilon_{im2}(C_{m2D} - C_{im2D}) - \mu_{im2D}C_{im2D}, r_D > r_{sD}, \tag{S46d}$$

$$\frac{\partial C_{umD}}{\partial t_D} = \frac{R_{m1}\alpha_2^2 D_u}{Ab^2 R_{um}}\frac{\partial^2 C_{umD}}{\partial z_D^2} - \varepsilon_{um}(C_{umD} - C_{uimD}) - \mu_{umD}C_{umD}, z_D \geq 1, t_D > 0, \tag{S47a}$$

$$\frac{\partial C_{uimD}}{\partial t_D} = \varepsilon_{uim}(C_{umD} - C_{uimD}) - \mu_{uimD}C_{uimD},\ z_D \geq 1,\ t_D > 0 \tag{S47b}$$

$$\frac{\partial C_{lmD}}{\partial t_D} = \frac{R_{m1}\alpha_2^2 D_l}{Ab^2 R_{lm}}\frac{\partial^2 C_{lmD}}{\partial z_D^2} - \varepsilon_{lm}(C_{lmD} - C_{limD}) - \mu_{lmD}C_{lmD}, z_D \leq -1, t_D > 0, \tag{S48a}$$

$$\frac{\partial C_{uimD}}{\partial t_D} = \varepsilon_{lim}(C_{lmD} - C_{limD}) - \mu_{limD}C_{limD},\ z_D \leq -1,\ t_D > 0, \tag{S48b}$$

where $\varepsilon_{m1} = \frac{\omega_1\alpha_2^2}{A\theta_{m1}}$, $\varepsilon_{im1} = \frac{\omega_1\alpha_2^2 R_{m1}}{A\theta_{im1}R_{im1}}$, $\varepsilon_{m2} = \frac{\omega_2\alpha_2^2}{A\theta_{m2}}$, $\varepsilon_{im2} = \frac{\omega_2\alpha_2^2 R_{m1}}{A\theta_{im2}R_{im2}}$, $\varepsilon_{um} = \frac{\omega_u\alpha_2^2 R_{m1}}{A\theta_{um}R_{um}}$, $\varepsilon_{uim} = \frac{\omega_u\alpha_2^2 R_{m1}}{A\theta_{uim}R_{uim}}$, $\varepsilon_{lm} = \frac{\omega_l\alpha_2^2 R_{m1}}{A\theta_{lm}R_{lm}}$, $\varepsilon_{lim} = \frac{\omega_l\alpha_2^2 R_{m1}}{A\theta_{lim}R_{lim}}$.

Substituting the dimensionless parameters into Eqs. (S40) - (S43), one has

$$C_{m1D}(r_D,t_D)|_{t_D=0} = C_{im1D}(r_D,t_D)|_{t_D=0} = C_{m2D}(r_D,t_D)|_{t_D=0} = C_{im2D}(r_D,t_D)|_{t_D=0} = C_{umD}(r_D,z_D,t_D)|_{t_D=0} = C_{uimD}(r_D,z_D,t_D)|_{t_D=0} = C_{lmD}(r_D,z_D,t_D)|_{t_D=0} = C_{limD}(r_D,z_D,t_D)|_{t_D=0} = 0, \tag{S49}$$

$$C_{m2D}(r_D,t_D)|_{r_D\to\infty} = C_{im2D}(r_D,t_D)|_{r_D\to\infty} = C_{umD}(r_D,z_D,t_D)|_{z_D\to\infty} = C_{uimD}(r_D,z_D,t_D)|_{z_D\to\infty} = C_{lmD}(r_D,z_D,t)|_{z_D\to-\infty} = C_{limD}(r_D,z_D,t_D)|_{z_D\to-\infty} = 0, \tag{S50}$$

$$C_{m1D}(r_D,t_D) = C_{umD}(r_D,z_D = 1,t_D), r_{wD} \leq\ r_D \leq r_{sD}, \tag{S51a}$$

$$C_{m2D}(r_D,t_D) = C_{umD}(r_D,z_D = 1,t_D), r_{wD} \leq\ r_D \leq r_{sD}, \tag{S51b}$$

$$C_{m2D}(r_D,t_D) = C_{lmD}(r_D,z_D = -1,t_D), r_D > r_{sD}, \tag{S51c}$$

$$C_{m2D}(r_D,t_D) = C_{lmD}(r_D,z_D = -1,t_D), r_D > r_{sD}. \tag{S51d}$$

Conducting Laplace transform to Eqs. (S47a) - (S47b), one has:

$$s\bar{C}_{umD} = \frac{R_{m1}\alpha_2^2 D_u}{AB^2 R_{um}}\frac{\partial^2 \bar{C}_{umD}}{\partial z_D^2} - (\varepsilon_{um} + \mu_{umD})\bar{C}_{umD} + \varepsilon_{um}\bar{C}_{uimD}, z_D \geq 1, \tag{S52a}$$

$$s\bar{C}_{uimD} = \varepsilon_{uim}(\bar{C}_{umD} - \bar{C}_{uimD}) - \mu_{uimD}\bar{C}_{uimD},\ z_D \geq 1. \tag{S52b}$$

Substituting Eq. (S52b) into Eq. (S52a), Eq. (S52a) could be rewritten as

$$\frac{R_{m1}\alpha_2^2 D_u}{Ab^2 R_{um}}\frac{\partial^2 \bar{C}_{umD}}{\partial z_D^2} - \left(s + \varepsilon_{um} + \mu_{umD} - \frac{\varepsilon_{um}\varepsilon_{uim}}{s+\mu_{uimD}+\varepsilon_{uim}}\right)\bar{C}_{umD} = 0, z_D \geq 1. \quad \text{(S53)}$$

Similarly, Eqs. (S48a) - (S48b) become:

$$\frac{R_{m1}\alpha_2^2 D_l}{Ab^2 R_{lm}}\frac{\partial^2 \bar{C}_{lmD}}{\partial z_D^2} - \left(s + \varepsilon_{lm} + \mu_{lmD} - \frac{\varepsilon_{lm}\varepsilon_{lim}}{s+\mu_{limD}+\varepsilon_{lim}}\right)\bar{C}_{lmD} = 0, z_D \leq -1. \quad \text{(S54)}$$

Eqs. (S49) - (S51d) and Eq. (S53) compose a model of the second-order ordinary differential equation (ODE) with boundary conditions, and the general solution of the Eq. (S53) is

$$\bar{C}_{umD} = A_1 e^{a_1 z_D} + B_1 e^{a_2 z_D}, z_D \geq 1. \quad \text{(S54a)}$$

Similarly, the general solution of Eq. (S54) is

$$\bar{C}_{lmD} = A_2 e^{b_1 z_D} + B_2 e^{b_2 z_D}, z_D \leq -1, \quad \text{(S54b)}$$

where $a_1 = \sqrt{s + \varepsilon_{um} + \mu_{umD} - \frac{\varepsilon_{um}\varepsilon_{uim}}{s+\mu_{uimD}+\varepsilon_{uim}}}$, $a_2 = -\sqrt{s + \varepsilon_{um} + \mu_{umD} - \frac{\varepsilon_{um}\varepsilon_{uim}}{s+\mu_{uimD}+\varepsilon_{uim}}}$, $b_1 = \sqrt{s + \varepsilon_{lm} + \mu_{lmD} - \frac{\varepsilon_{lm}\varepsilon_{lim}}{s+\mu_{limD}+\varepsilon_{lim}}}$ and $b_2 = -\sqrt{s + \varepsilon_{lm} + \mu_{lmD} - \frac{\varepsilon_{lm}\varepsilon_{lim}}{s+\mu_{limD}+\varepsilon_{lim}}}$.

Substituting Eqs. (S54a) - (S54b) into Eqs. (S51a) - (S51d), one has

$$\bar{C}_{umD} = B_1 e^{a_2 z_D}, z_D \geq 1, \quad \text{(S55a)}$$

$$\bar{C}_{lmD} = A_2 e^{b_1 z_D}, z_D \leq -1, \quad \text{(S55b)}$$

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, the solutions of the aquitards are

$$\bar{C}_{umD} = \bar{C}_{m1D} exp\ (a_2 z_D - a_2), r_{wD} \leq r_D \leq r_{sD}, \quad \text{(S56a)}$$

$$\bar{C}_{umD} = \bar{C}_{m2D} exp\ (a_2 z_D - a_2), r_D > r_{sD}, \quad \text{(S56b)}$$

$$\bar{C}_{uimD} = \frac{\varepsilon_{uim}}{s+\varepsilon_{uim}+\mu_{uimD}}\bar{C}_{umD}, r_D \geq r_{wD}, \quad \text{(S56c)}$$

$$\bar{C}_{lmD} = \bar{C}_{m1D} exp\ (b_1 z_D + b_1), r_{wD} \leq r_D \leq r_{sD}, \quad \text{(S57a)}$$

$$\bar{C}_{lmD} = \bar{C}_{m2D} exp\ (b_1 z_D + b_1), r_D > r_{sD}, \quad \text{(S57b)}$$

$$\bar{C}_{limD} = \frac{\varepsilon_{lim}}{s+\varepsilon_{lim}+\mu_{limD}}\bar{C}_{lmD}, r_D \geq r_{wD}, \tag{S57c}$$

The dimensionless forms of Eqs. (S44a) - (S45b) become

$$\left[C_{m1D} - \lambda\frac{\partial C_{m1D}(r_D,t_D)}{\partial r_D}\right]\Big|_{r=r_{wD}} = C_{inj,D}(t_D), 0 < t_D \leq\ t_{inj,D}, \tag{S58a}$$

$$\left[C_{m1D} - \lambda\frac{\partial C_{m1D}(r_D,t_D)}{\partial r_D}\right]\Big|_{r=r_{wD}} = C_{cha,D}(t_D), t_D > t_{inj,D}, \tag{S58b}$$

$$\beta_{inj}\frac{dC_{inj,D}(t_D)}{dt_D} = 1 - C_{inj,D}(t_D), 0 < t_D \leq t_{inj,D}, \tag{S59a}$$

$$\beta_{cha}\frac{dC_{cha,D}(t_D)}{dt_D} = -C_{cha,D}(t_D), t_D > t_{inj,D}, \tag{S59b}$$

where $\beta_{inj} = \frac{V_{w,inj}r_{wD}}{\xi R_m \alpha_2}$ and $\beta_{cha} = \frac{V_{w,cha}r_{wD}}{\xi R_m \alpha_2}$.

After applying Laplace transform to Eqs. (S46a) - (S46b), one has

$$s\bar{C}_{m1D} = \frac{\lambda}{r_D}\frac{\partial^2 \bar{C}_{m1D}}{\partial r_D^2} - \frac{1}{r_D}\frac{\partial \bar{C}_{m1D}}{\partial r_D} - \varepsilon_{m2}(\bar{C}_{m1D} - \bar{C}_{im1D}) - \mu_{m1D}\bar{C}_{m1D} - \frac{\theta_{um}\alpha_2^2 D_u}{2A\theta_{m1}b^2}\frac{\partial \bar{C}_{umD}}{\partial z_D}\Big|_{z=1} +$$

$$\frac{\theta_{lm}\alpha_2^2 D_l}{2Ab^2\theta_{m1}}\frac{\partial \bar{C}_{lmD}}{\partial z_D}\Big|_{z=-1}, r_{wD} \leq r_D \leq r_{sD}, \tag{S60a}$$

$$s\bar{C}_{im1D} = \varepsilon_{im2}(\bar{C}_{m1D} - \bar{C}_{im1D}) - \mu_{im1D}\bar{C}_{im1D}, r_{wD} \leq r_D \leq r_{sD}. \tag{S60b}$$

Substituting Eq. (S60b) into Eq. (S60a), Eq. (S60a) could be rewritten as

$$\frac{\lambda}{r_D}\frac{\partial^2 \bar{C}_{m1D}}{\partial r_D^2} - \frac{1}{r_D}\frac{\partial \bar{C}_{m1D}}{\partial r_D} - \left(\varepsilon_{m1} + \mu_{m1D} - \frac{\varepsilon_{m1}\varepsilon_{im1}}{s+\mu_{im1D}+\varepsilon_{im1}}\right)\bar{C}_{m1D} - \frac{\theta_{um}\alpha_2^2 D_u}{2A\theta_{m1}b^2}\frac{\partial \bar{C}_{umD}}{\partial z_D}\Big|_{z=1} +$$

$$\frac{\theta_{lm}\alpha_2^2 D_l}{2Ab^2\theta_{m1}}\frac{\partial \bar{C}_{lmD}}{\partial z_D}\Big|_{z=-1}, r_{wD} \leq r_D \leq r_{sD}. \tag{S61}$$

After applying Laplace transform to Eqs. (S46c) - (S46d), the following equations would be obtained

$$s\bar{C}_{m2D} = \frac{\eta}{r_D}\frac{\partial^2 \bar{C}_{m2D}}{\partial r_D^2} - \frac{\eta}{r_D}\frac{\partial \bar{C}_{m2D}}{\partial r_D} - \varepsilon_{m2}(C_{m2D} - C_{im2D}) - \frac{\theta_{um}\alpha_2^2 D_u}{2A\theta_{m2}b^2}\frac{\partial \bar{C}_{umD}}{\partial z_D}\Big|_{z=1} +$$

$$\frac{\theta_{lm}\alpha_2^2 D_l}{2Ab^2\theta_{m2}}\frac{\partial \bar{C}_{lmD}}{\partial z_D}\Big|_{z=-1}, r_D > r_{sD}, \tag{S62a}$$

$$s\bar{C}_{im2D} = \varepsilon_{im2}(\bar{C}_{m2D} - \bar{C}_{im2D}) - \mu_{im2D}\bar{C}_{im2D}, r_D > r_{sD}. \tag{S62b}$$

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

$$s\bar{C}_{m2D} = \frac{\eta}{r_D}\frac{\partial^2 \bar{C}_{m2D}}{\partial r_D^2} - \frac{\eta}{r_D}\frac{\partial \bar{C}_{m2D}}{\partial r_D} - \left(\varepsilon_{m2} + \mu_{m2D} - \frac{\varepsilon_{m2}\varepsilon_{im2}}{s+\mu_{im2D}+\varepsilon_{im2}}\right)\bar{C}_{m2D} -$$

$$\frac{\theta_{um}\alpha_2^2 D_u}{2A\theta_{m2}b^2}\frac{\partial \bar{C}_{umD}}{\partial z_D}\bigg|_{z=1} + \frac{\theta_{lm}\alpha_2^2 D_l}{2Ab^2\theta_{m2}}\frac{\partial \bar{C}_{lmD}}{\partial z_D}\bigg|_{z=-1}, r_D > r_{sD}. \quad \text{(S63)}$$

Substituting Eq. (S56a) and Eq. (S57a) into Eq. (S61), one has

$$\frac{\lambda}{r_D}\frac{\partial^2 \bar{C}_{m1D}}{\partial r_D^2} - \frac{1}{r_D}\frac{\partial \bar{C}_{m1D}}{\partial r_D} - E_3\bar{C}_{m1D} = 0, r_{wD} \le r_D \le r_{sD}, \quad \text{(S64a)}$$

Substituting Eq. (S56b) and Eq. (S57b) into Eq. (S63), one has

$$\frac{1}{r_D}\frac{\partial^2 \bar{C}_{m2D}}{\partial r_D^2} - \frac{1}{r_D}\frac{\partial \bar{C}_{m2D}}{\partial r_D} - E_4\bar{C}_{m2D} = 0, r_D > r_{sD}, \quad \text{(S64b)}$$

where $E_3 = s + \varepsilon_{m1} + \mu_{m1D} - \frac{\varepsilon_{m1}\varepsilon_{im1}}{s+\mu_{im1D}+\varepsilon_{im1}} - \frac{a_2\theta_{um}\alpha_2^2 D_u}{2A\theta_{m1}b^2} + \frac{b_1\theta_{lm}\alpha_2^2 D_l}{2Ab^2\theta_{m1}}$ and $E_4 = \frac{1}{\eta}\left(s + \varepsilon_{m2} + \mu_{m2D} - \frac{\varepsilon_{m2}\varepsilon_{im2}}{s+\mu_{im2D}+\varepsilon_{im2}} - \frac{a_2\theta_{um}\alpha_2^2 D_u}{2A\theta_{m2}b^2} + \frac{b_1\theta_{lm}\alpha_2^2 D_l}{2Ab^2\theta_{m2}}\right)$.

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

$$\left[\bar{C}_{m1D} - \lambda\frac{\partial \bar{C}_{m1D}(r_D,s)}{\partial r_D}\right]\bigg|_{r_D=r_{wD}} = \frac{1}{s(s\beta_{inj}+1)}, 0 < t_D \le t_{inj,D}, \quad \text{(S65a)}$$

$$\left[\bar{C}_{m1D} - \lambda\frac{\partial \bar{C}_{m1D}(r_D,s)}{\partial r_D}\right]\bigg|_{r_D=r_{wD}} = \frac{\beta_{cha}C_{inj,D}(r_{wD},t_{inj,D})}{(s\beta_{cha}+1)}, t_D > t_{inj,D}, \quad \text{(S65b)}$$

$$\bar{C}_{m1D}(r_{sD},s) = \bar{C}_{m2D}(r_{sD},s), \quad \text{(S65c)}$$

$$\lambda\frac{\partial \bar{C}_{m1D}(r_D,s)}{\partial r_D}\bigg|_{r_D=r_{sD}} = \frac{\partial \bar{C}_{m2D}(r_D,s)}{\partial r_D}\bigg|_{r_D=r_{sD}}, \quad \text{(S65d)}$$

$$\bar{C}_{m2D}(r_D,s)|_{r_D\to\infty} = 0. \quad \text{(S65e)}$$

Therefore, the general solutions of Eq. (S65a) and Eq. (S65b) are

$$\bar{C}_{m1D} = T_1\, exp\left(\frac{r_D}{2\lambda}\right)A_i(\varphi_1) + T_2 exp\left(\frac{r_D}{2\lambda}\right)B_i(\varphi_1), r_{wD} \le r_D \le r_{sD}, \quad \text{(S66a)}$$

$$\bar{C}_{m2D} = T_3\, exp\left(\frac{r_D}{2}\right)A_i(\varphi_2) + T_4 exp\left(\frac{r_D}{2}\right)B_i(\varphi_2), r_D > r_{sD}, \quad \text{(S66b)}$$

where $\varphi_1=\left(\frac{E_3}{\lambda}\right)^{1/3}\left(r_D+\frac{1}{4\lambda E_3}\right)$, $\varphi_2={E_4}^{1/3}\left(r_D+\frac{1}{4E_4}\right)$, T_1, T_2, T_3 and T_4 are constants which could be determined by the boundary conditions.

Substituting Eq. (S66b) into Eq. (S65e), one has

$$T_4=0. \tag{S67}$$

Substituting Eq. (S66a) into Eq. (S65a), one has

$$T_1 exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}A_i(\varphi_w)-\lambda\left(\frac{E_3}{\lambda}\right)^{1/3}A_i'(\varphi_w)\right]+T_2 exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}B_i(\varphi_w)-\lambda\left(\frac{E_3}{\lambda}\right)^{1/3}B_i'(\varphi_w)\right]=F_1. \tag{S68a}$$

Substituting Eq. (S66a) into Eq. (S65b), one has

$$T_1 exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}A_i(\varphi_w)-\lambda\left(\frac{E_4}{\lambda}\right)^{1/3}A_i'(\varphi_w)\right]+T_2 exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}B_i(\varphi_w)-\lambda\left(\frac{E_4}{\lambda}\right)^{1/3}B_i'(\varphi_w)\right]=F_2, \tag{S68b}$$

where $\varphi_w=\left(\frac{E_3}{\lambda}\right)^{1/3}\left(r_{wD}+\frac{1}{4\lambda E_3}\right)$, $F_1=\frac{1}{s(s\beta_{inj}+1)}$ and $F_2=\frac{\beta_{cha}c_{inj,D}(r_{wD},t_{inj,D})}{(s\beta_{cha}+1)}$.

Substituting Eqs. (S66a) - (S66b) into Eq. (S65c), one has

$$T_1\, exp\left(\frac{r_{sD}}{2\lambda}\right)A_i(\varphi_{1s})+T_2 ex\,p\left(\frac{r_{sD}}{2\lambda}\right)B_i(\varphi_{1s})=T_3\, exp\left(\frac{r_{sD}}{2}\right)A_i(\varphi_{2s}), \tag{S69}$$

where $\varphi_{1s}=\left(\frac{E_3}{\lambda}\right)^{1/3}\left(r_{sD}+\frac{1}{4\lambda E_3}\right)$, $\varphi_{2s}={E_4}^{1/3}\left(r_D+\frac{1}{4E_4}\right)$.

Substituting Eqs. (S66a) - (S66b) into Eq. (S65d), one has

$$T_1 exp\left(\frac{r_{sD}}{2\lambda}\right)\left[\frac{1}{2}A_i(\varphi_{1s})+\lambda\left(\frac{E_3}{\lambda}\right)^{1/3}A_i'(\varphi_{1s})\right]+T_2 exp\left(\frac{r_{sD}}{2\lambda}\right)\left[\frac{1}{2}B_i(\varphi_{1s})+\lambda\left(\frac{E_3}{\lambda}\right)^{1/3}B_i'(\varphi_{1s})\right]=T_3 exp\left(\frac{r_{sD}}{2}\right)\left[\frac{1}{2}A_i(\varphi_{2s})+{E_4}^{1/3}A_i'(\varphi_{2s})\right]. \tag{S70}$$

The values of T_1, T_2, and T_3 could be determined by solving Eqs. (S68a) - (S70)

$$T_1=\frac{F-G_2T_2}{G_1},$$

$$T_2 = \frac{G_3 G_8 F - G_5 G_6 F}{G_1 G_5 G_7 + G_2 G_3 G_8 - G_2 G_5 G_6 - G_1 G_4 G_8}$$

$$T_3 = \frac{G_3 F}{G_1 G_5} - \frac{G_2 G_3 T_2}{G_1 G_5} + \frac{G_4 T_2}{G_5},$$

where $G_1 = exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}A_i(\varphi_w) - \lambda\left(\frac{E_3}{\lambda}\right)^{1/3} A_i'(\varphi_w)\right]$,

$G_2 = exp\left(\frac{r_{wD}}{2\lambda}\right)\left[\frac{1}{2}B_i(\varphi_w) - \lambda\left(\frac{E_3}{\lambda}\right)^{1/3} B_i'(\varphi_w)\right]$,

$G_3 = exp\left(\frac{r_{sD}}{2\lambda}\right)A_i(\varphi_{1s})$, $G_4 = ex\,p\left(\frac{r_{sD}}{2\lambda}\right)B_i(\varphi_{1s})$, $G_5 = exp\left(\frac{r_{sD}}{2}\right)A_i(\varphi_{2s})$,

$G_6 = exp\left(\frac{r_{sD}}{2\lambda}\right)\left[\frac{1}{2}A_i(\varphi_{1s}) + \lambda\left(\frac{E_3}{\lambda}\right)^{1/3} A_i'(\varphi_{1s})\right]$,

$G_7 = exp\left(\frac{r_{sD}}{2\lambda}\right)\left[\frac{1}{2}B_i(\varphi_{1s}) + \lambda\left(\frac{E_3}{\lambda}\right)^{1/3} B_i'(\varphi_{1s})\right]$,

$G_8 = exp\left(\frac{r_{sD}}{2}\right)\left[\frac{1}{2}A_i(\varphi_{2s}) + {E_4}^{1/3} A_i'(\varphi_{2s})\right]$,

and $F = C_{inj,D}\frac{1-exp(-t_{inj,D}s)}{s} + C_{cha,D}\frac{exp(-t_{inj,D}s)}{s}$.

In the injection phase, the values of T_1 and T_2 are modified into T_1' and T_2' as follows

$$T_1' = \frac{F_1 - G_2' T_2'}{G_1'} \text{ and } T_2' = \frac{G_3 G_8 F_1 - G_5 G_6 F_1}{G_1' G_5 G_7 + G_2' G_3 G_8 - G_2' G_5 G_6 - G_1' G_4 G_8},$$

where $G_1' = \frac{1}{2}exp\left(\frac{r_{wD}}{2\lambda}\right)A_i(\varphi_w)$ and $G_2' = \frac{1}{2}exp\left(\frac{r_{wD}}{2\lambda}\right)B_i(\varphi_w)$.

Substituting T_1' and T_2' into Eq. (S66a), one has

$$\bar{C}_{inj,D}(r_{wD}, \mathrm{s}) = T_1'\, exp\left(\frac{r_{wD}}{2\lambda}\right)A_i(\varphi_w) + T_2' exp\left(\frac{r_{wD}}{2\lambda}\right)B_i(\varphi_w), \quad \text{(S71)}$$

In the chasing phase, the values of T_1 and T_2 are modified into T_1' and T_2' as follows

$$T_1'' = \frac{F_2 - G_2' T_2'}{G_1'} \text{ and } T_2'' = \frac{G_3 G_8 F_2 - G_5 G_6 F_2}{G_1' G_5 G_7 + G_2' G_3 G_8 - G_2' G_5 G_6 - G_1' G_4 G_8}.$$

Substituting T_1'' and T_2'' into Eq. (S66a), one has

$$\bar{C}_{cha,D}(r_{wD}, \mathrm{s}) = T_1''\, exp\left(\frac{r_{wD}}{2\lambda}\right)A_i(\varphi_w) + T_2'' exp\left(\frac{r_{wD}}{2\lambda}\right)B_i(\varphi_w). \quad \text{(S72)}$$

Conducting Laplace transform on Eq. (S4c), one has

$$\bar{C}_{wD}(r_{wD}, s) = C_{inj,D}\frac{1-exp(-t_{inj,D}s)}{s} + C_{cha,D}\frac{exp(-t_{inj,D}s)}{s}, \tag{S73}$$

where $C_{inj,D}$ and $C_{cha,D}$ could be determined by Eqs. (S71) - (S72).

Substituting Eqs. (S66a) - (S66b) into Eqs. (S68a) - (S70) and Eq. (S73), one has

$$\bar{C}_{m1D} = T_1\, exp\left(\frac{r_D}{2\lambda}\right) A_i(\varphi_1) + T_2 exp\ \left(\frac{r_D}{2\lambda}\right) B_i(\varphi_1), r_{wD} < r_D \le r_{sD}, \tag{S74a}$$

$$\bar{C}_{m2D} = T_3\, exp\left(\frac{r_D}{2}\right) A_i(\varphi_2), r_D > r_{sD}. \tag{S74b}$$

S4. Numerical simulation by COMSOL Multiphysics

In this study, the numerical simulation based on the Galerkin finite-element method is conducted in the COMSOL Multiphysics platform to test new solutions.

S4.1 Models of Eqs. (14) – (15): Confined aquifer

In our COMSOL simulation for the radial dispersion in a confined aquifer, triangles in the *r*–*z* plane are used as the elements, and it is easy to refine the elements near both the well and the skin-aquifer interfaces, as shown in Figure S2. The number of mesh points is 759, and the number of triangle elements is 1386. The time step increases linearly, and the initial time step is 5s, with a total simulation time of 1000s. The coefficient of determination (R^2) is employed as a criterion to estimate the simulation results as follows

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(C_{ana}-C_{num})^2}{\sum_{i=1}^{N}(C_{ana}-\bar{C}_{ana})^2}, \tag{S751}$$

where C_{ana} and C_{num} are the concentrations calculated by analytical and numerical solutions, respectively, $\bar{C}_{ana}$ is the average concentrations calculated by analytical solution; *N* is the number of sampling points.

S4.2 Models of Eqs. (19) – (20): Leaky-confined aquifer

The temporal and spatial discretization of the aquifer in the numerical simulation is similar to the one used in Section S4.1. To decrease the numerical errors, the size of triangle cells is smaller around the aquifer-aquitard interface. The number of mesh points is 2885, and the number of triangle elements is 5592. Figure S4 shows the comparison between the analytical and numerical solutions, and the agreement is well. All of the R^2 between the analytical and numerical solutions are greater than 0.98. The parameters of the aquifers used in the numerical simulation are from Section S4.1, while the others are: $R_{um} = R_{uim} = R_{lm} = R_{lim} = 1$, $\omega_u = \omega_l = 0.0001$ s^{-1}, $\theta_{um} = \theta_{lm} = 0.1$, $\theta_{uim} = \theta_{lim} = 0.01$, $\mu_{um} = \mu_{uim} = \mu_{lm} = \mu_{lim} = 10^{-7}$ s^{-1}, $D_u = D_l = 0.0005$ cm^2/s.

S5. The fitness of the experimental data by Chao (1999)

Figures 4a and 4b show that the sensitivity of V_w on BTCs is the least. To answer the question that if the influence of V_w could be ignored, we compare solutions of this study with and without the mixing effect, and the experimental data are also included for the comparison, as shown in Figure S5. The results show that two curves are almost the same. The reason is that the V_w is too small in the experiment of Chao (1999). Different sensitivity of V_w on BTCs has been obtained for field applications in which V_w is significantly greater than that used by Chao (1999).

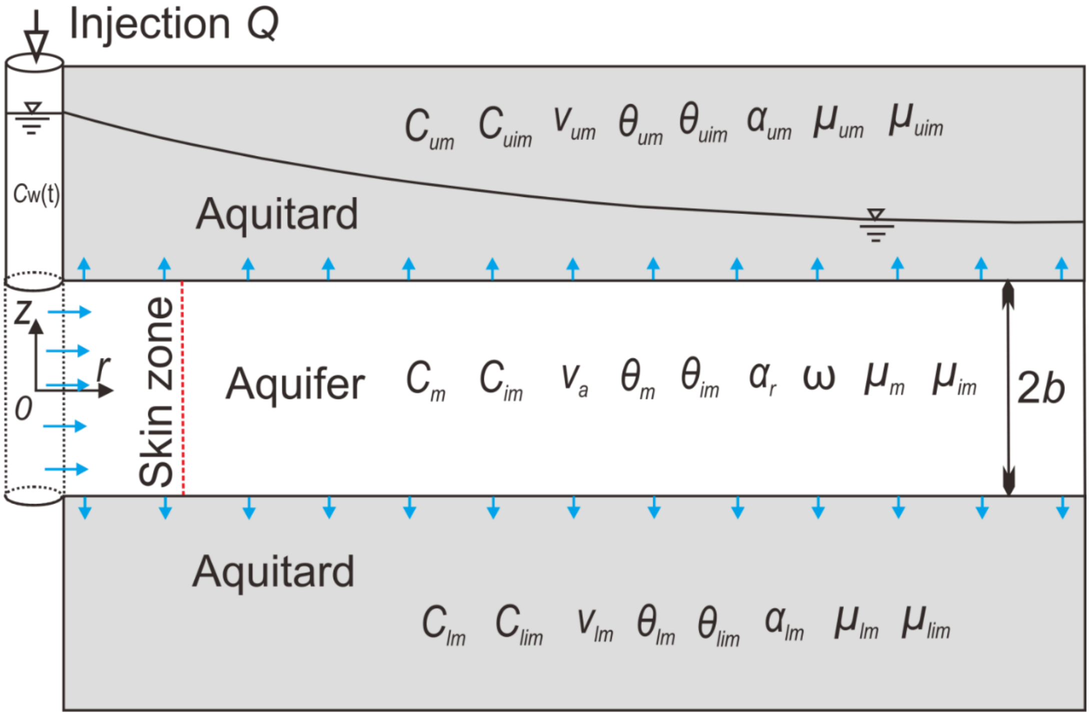


Figure S1. The schematic diagram of the radial dispersion in the aquifer-aquitard system.

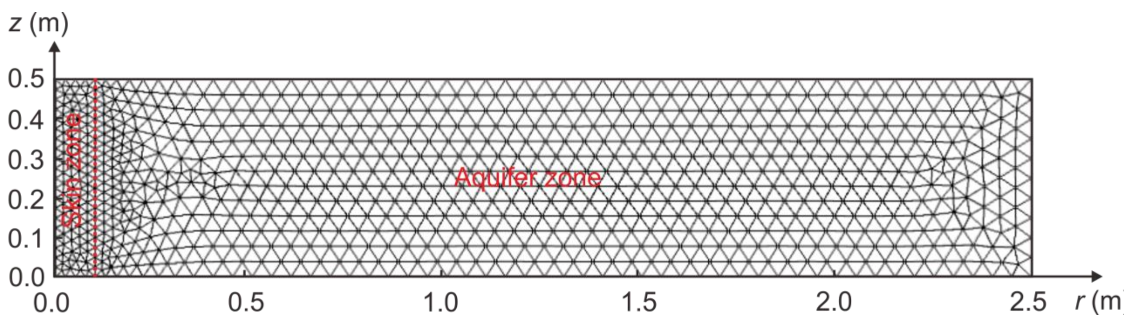


Figure S2. The grid mesh of the skin-aquifer system used in the Galerkin finite-element COMSOL Multiphysics program.

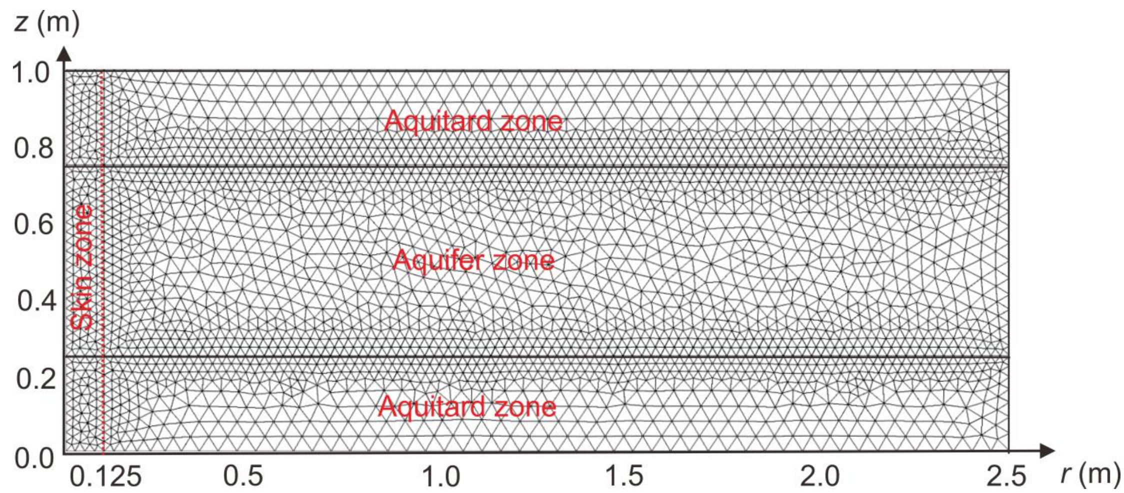
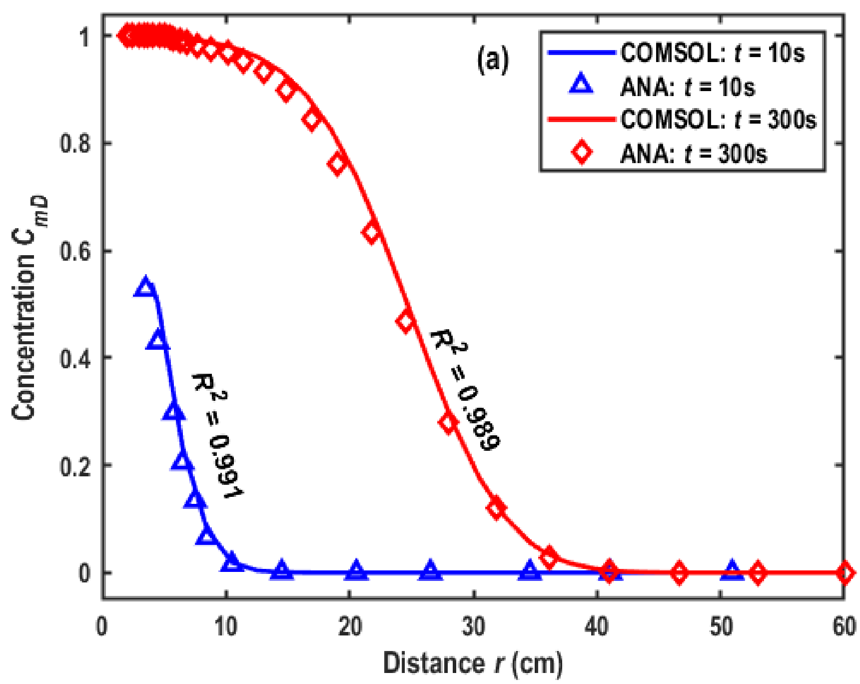


Figure S3. The grid mesh of the skin-aquifer-aquitard system used in the Galerkin finite-element COMSOL Multiphysics program.



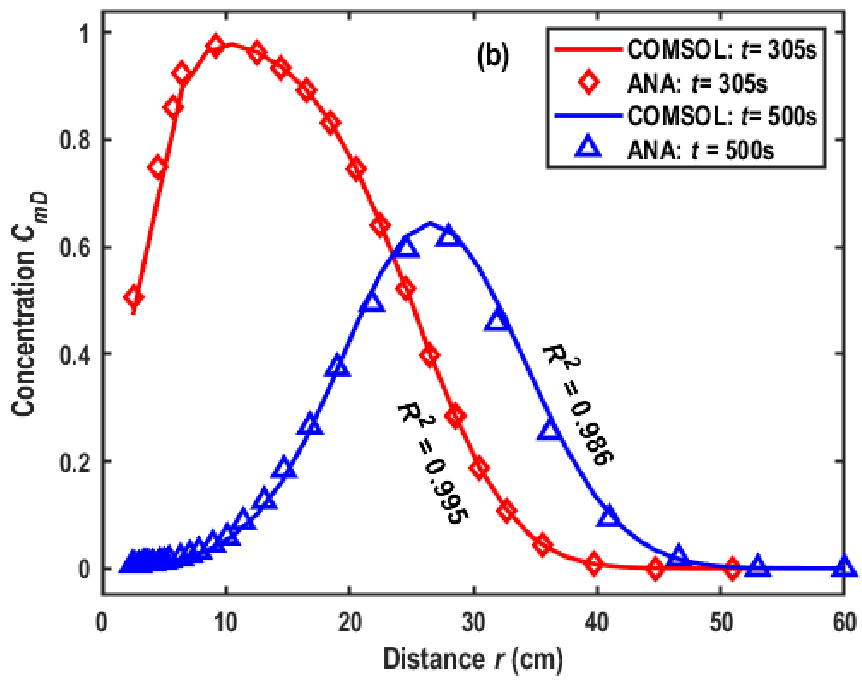


Figure S4. Comparison of the numerical solution by COMSOL Multiphysics and the analytical solution of Eqs. (20) - (23). (a): In the injection phase; (b): In the chasing phase.

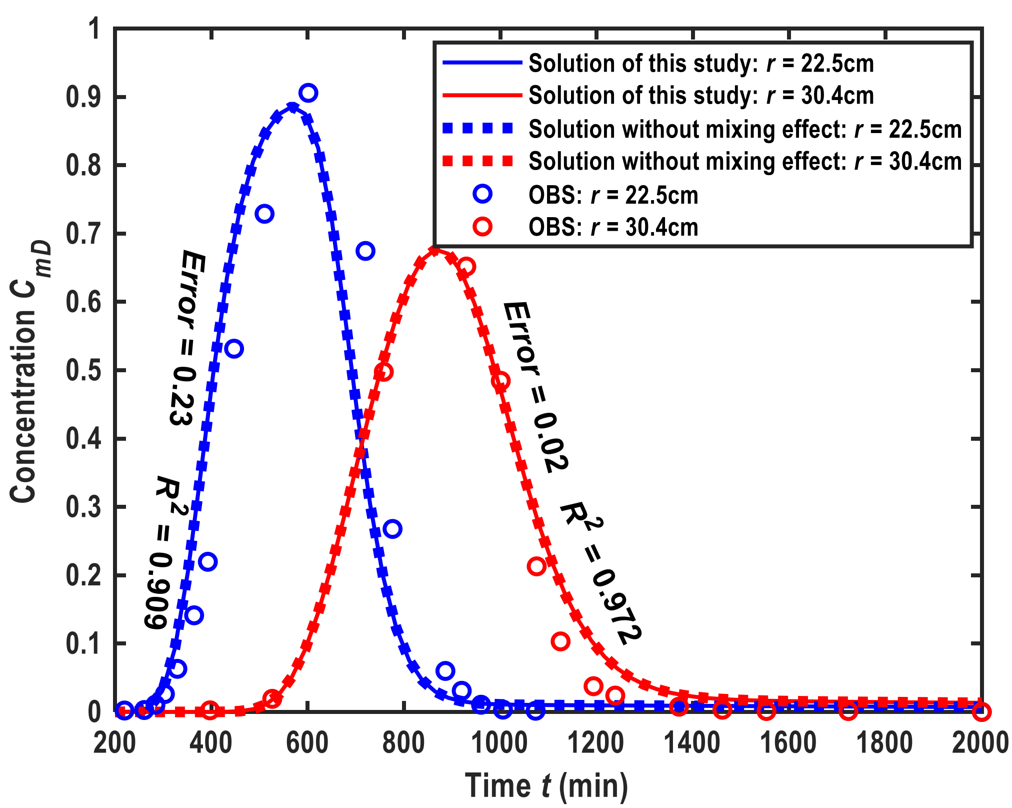


Figure S5. Fitness of observed BTC by the solutions of this study.