



Stepwise superposition approximation approach for analytical solutions with non-zero initial concentration using existing solutions of zero initial concentration in contaminate transport

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Abstract

Analytical solutions for contaminant transport are widely used for both theoretical and practical purposes. However, many existing solutions are obtained subject to an initial condition of zero concentration, which is often unrealistic in many practical cases. This article proposed a stepwise superposition approximation approach to solve the non-zero initial concentration problem for first-type and third-type boundary conditions by using the existing zero initial concentration solution. Theoretical examples showed that the approach was highly efficient if a proper superposition scheme with relative concentration increments was constructed. The key parameter that controlled the convergence speed was the time increment (Δt) multiplied by the rate constant (λ). The approach served also as an alternative way to make a convenient concentration calculation even if the non-zero initial concentration solution of a problem was known.

Key words: analytical solution; contaminate transport; non-zero initial concentration; superposition approximation; relative concentration increment

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Introduction

Analytical solutions for contaminant transport are useful tools for studying the mechanisms of contaminant transport phenomena, estimating transport parameters from laboratory or field experiments, verifying numerical models, and predicting concentration distributions in simple conditions. As the significance of the issues, many researchers have developed analytical solutions to suit different conditions (Wang and Wu, 2009; Guerrero et al., 2009; Kumar et al., 2010).

Most analytical transport solutions are subject to a homogenous initial condition (zero initial concentration, ZIC), i.e., $C|_{t=0} = 0$ (Wilson and Miller, 1978; Sauty and Pierre, 1980; Batu, 1989, 1993; Leij et al., 2000; Chen et al., 2002; Srivastava et al., 2004; Huang and Goltz, 2006; Leij and Bradford, 2009; Wang and Wu, 2009; Zhan et al., 2009). Only a few are subject to an inhomogeneous initial condition, $C|_{t=0} \neq 0$ (van Genuchten, 1981; Leij and Dane, 1990; Chao and Stephens, 1995; Srinivasan and Clement, 2008; Guerrero et al., 2009). There are two main reasons for this: (1) ZIC solutions can be applied

easily to solve corresponding problems with a non-zero initial concentration (NZIC), such as those of non-reactive transport; hence, no special attention need be given, and (2) NZIC solution is very difficult to achieve as the complexity of the problems, if not impossible. In addition, analytical solutions often become more complex if NZIC condition is applied (Leij et al., 1991; Toride et al., 1999) and hence are more inconvenient for practitioners to use. However, the NZIC problems occur frequently in practical applications. For instance, common geochemical components, such as ions of calcium, magnesium, sulfate, chloride, exist universally in groundwater. Oxidants such as oxygen may have a background distribution before they are injected into the ground in the contaminated site remediation. Groundwater contains many organic pollutants before new sources of pollutants leak into the aquifers. In all these cases, the concentrations of the objective subjects (ions, oxidants and organic pollutants) must be considered as the initial conditions if their transport are simulated by using the analytical solutions. Therefore, it is significant in finding a general method to solve the NZIC problems if their ZIC solutions are known.

This article presents a method that can be used to calculate the concentration distribution of a NZIC problem when

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its corresponding analytical solution of the ZIC problem is known. Specifically, a stepwise superposition approximation approach is proposed to solve reactive transport problems subject to boundary conditions of the first type (concentration distribution) and the third type (hydrodynamic dispersion flux). For the situations in which the NZIC solutions are known, the approach is also usable as an alternative if the NZIC solutions are inconvenient to be employed.

1 Theory

The most commonly used initial condition for the analytical solution of contaminant transport is of a constant concentration type expressed as $C|_{t=0} = C_i$, where C_i is the initial concentration constant. Hence, the solutions subject to this type of initial condition will be discussed in detail. Let us take the one-dimensional transport problem as an example. Two- and three-dimensional transport issues can be similarly handled in reference to the procedure presented for the one-dimensional transport problem, and this is demonstrated in Section 2.

Our purpose is to obtain the analytical solution for governing equation:

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} - \lambda C + \frac{\gamma}{\theta} \quad (1)$$

subject to the NZIC of:

$$C(x, t)|_{t=0} = C_i \quad (2)$$

with various boundary conditions stated below, under the condition that the corresponding solution for Eq. (1) with a ZIC of:

$$C(x, t)|_{t=0} = 0 \quad (3)$$

is known as

$$C(x, t) = f(x, t) \quad (4)$$

where, C (mg/L) is the contaminant concentration; C_i (mg/L) is the initial concentration constant; γ (mg/(L·day)) is the source term; v (m/day) is the pore velocity of the fluid; D_L (m²/day) is the longitudinal dispersion coefficients; θ is the porosity for a saturated medium or the moisture content for an unsaturated medium; λ (1/day) is the first order rate constant; $f(x, t)$ represents the known ZIC solution; x (m) is the location of the calculation point; and t (day) is the calculation time.

The source term, γ , can be divided into four categories: (1) $\gamma = \text{constant}$, indicating a uniform source strength over the entire domain (van Genuchten, 1981; Toride et al., 1999; Islam and Singhal, 2002); (2) $\gamma = M\delta$, indicating an instantaneous source at the source location (Sauty and Pierre 1980; Leij et al., 2000; Wang and Wu, 2009), where M is the mass instantaneously released per unit source area, and δ is the Dirac Delta function defined as

$$\delta = \begin{cases} 1, & \text{for } x \in \text{source and } t = 0 \\ 0, & \text{otherwise} \end{cases}$$

(3) $\gamma = \gamma_c \delta$, indicating a continuous source at the source location (Hunt, 1978; Wilson and Miller, 1978; Park and Zhan, 2001; Wang and Wu, 2009), where γ_c is the mass released per unit time per unit source area, and

$$\delta = \begin{cases} 1, & \text{for } x \in \text{source} \\ 0, & \text{otherwise} \end{cases}$$

(4) $\gamma = 0$, indicating that there is no source inside the domain (Domenico, 1987; Chen, 2007). Aside from term γ , a source may also be located on the boundary and can be expressed as a boundary condition (Sagar, 1982; Chao and Stephens, 1995; Park and Zhan, 2001; Guerrero et al., 2009).

1.1 Solutions for infinitive boundary conditions

Equation (1) is solved subject to NZIC (Eq. (2)) and the boundary conditions of:

$$C(x, t)|_{x \rightarrow \pm\infty} = C_i \exp(-\lambda t) \quad \text{and/or} \quad \frac{\partial C}{\partial x} \Big|_{x \rightarrow \pm\infty} = 0 \quad (5)$$

whereas the ZIC solution to Eq. (1) with homogenous boundary conditions of:

$$C(x, t)|_{x \rightarrow \pm\infty} = 0 \quad \text{and/or} \quad \frac{\partial C}{\partial x} \Big|_{x \rightarrow \pm\infty} = 0 \quad (6)$$

is known as presented in Eq. (4). Many known solutions are obtained subject to the infinitive boundary conditions given by Eq. (6) (Wilson and Miller 1978; Leij et al., 2000; Park and Zhan, 2001; Wang and Wu, 2009).

To obtain the solution to Eq. (1), the following substitution is made:

$$G(x, t) = C(x, t) - C_i \exp(-\lambda t) \quad (7)$$

Differentiating G with respect to t and x , respectively, leads to:

$$\frac{\partial G}{\partial t} = \frac{\partial C}{\partial t} + \lambda C_i \exp(-\lambda t) \quad \text{and} \quad \frac{\partial G}{\partial x} = \frac{\partial C}{\partial x} \quad (8)$$

Substituting G for C in Eqs. (1), (2), and (5) yields:

$$\frac{\partial G}{\partial t} = D_L \frac{\partial^2 G}{\partial x^2} - v \frac{\partial G}{\partial x} - \lambda G + \frac{\gamma}{\theta} \quad (9)$$

$$G(x, t)|_{t=0} = 0 \quad (10)$$

$$G(x, t)|_{x \rightarrow \pm\infty} = 0 \quad \text{and/or} \quad \frac{\partial G}{\partial x} \Big|_{x \rightarrow \pm\infty} = 0 \quad (11)$$

This mathematical model is clearly the same as that consisting of Eqs. (1), (3), and (6). Hence, the solution must be identical, that is, $G(x, t) = f(x, t)$ in reference to Eq. (4). Thus, the solution to Eq. (1) subject to initial condition Eq. (2) and boundary condition Eq. (5) is:

$$C(x, t) = f(x, t) + C_i \exp(-\lambda t) \quad (12)$$

where, $f(x, t)$ is the corresponding ZIC solution given by Eq. (4). Equation (12) indicates that for an infinitive boundary condition with the source located inside the domain, the NZIC solution is equal to the ZIC solution plus a term $C_i \exp(-\lambda t)$.

1.2 Solutions for a first-type boundary condition

Suppose the source is located at the upstream boundary. The first-type boundary condition at source is:

$$C(x, t)|_{x=0} = C_0 \quad (13)$$

and the infinitive boundary is:

$$C(x, t)|_{x \rightarrow \infty} = C_i \exp(-\lambda t) \text{ or } \left. \frac{\partial C}{\partial x} \right|_{x \rightarrow \infty} = 0 \quad (14)$$

In this case, Eq. (1) is solved subject to Eqs. (2), (13), and (14) (Hunt, 1978; Sauty and Pierre, 1980; van Genuchten, 1981; Domenico, 1987; Sagar, 1982; Batu, 1989; Leij and Dane, 1990; Toride et al., 1999; Leij et al., 2000; Srivastava et al., 2004; Srinivasan and Clement, 2008; Leij and Bradford, 2009; Zhan et al., 2009; Kumar et al., 2010).

Similarly, substituting Eq. (7) into Eqs. (1) and (2) will produce Eqs. (9) and (10), respectively, and Eqs. (13) and (14) become:

$$G(x, t)|_{x=0} = C_0 - C_i \exp(-\lambda t) \quad (15)$$

$$G(x, t)|_{x \rightarrow \infty} = 0 \text{ or } \left. \frac{\partial G}{\partial x} \right|_{x \rightarrow \infty} = 0 \quad (16)$$

In the case where chemical reaction is not considered during the transport (non-reactive transport, $\lambda = 0$), we have $G(x, t)|_{x=0} = C_0 - C_i = \text{constant}$. The ZIC solution is clearly directly applicable. Suppose it can be expressed as:

$$C(x, t) = f(x, t) = C_0 F(x, t) \quad (17)$$

then the NZIC solution is:

$$C(x, t) = C_i + (C_0 - C_i)F(x, t) \quad (18)$$

This equation indicates that for a non-reactive transport with an upstream first-type boundary condition, the NZIC solution is obtained by changing the ZIC solution of $C_0 F(x, t)$ to $C_i + (C_0 - C_i)F(x, t)$.

However, in the case of reactive transport, the ZIC solution is not directly applicable any more because the boundary concentration, as given by Eq. (15), is not a constant but a function of time. To use the ZIC solution, we propose a novel stepwise superposition approach to obtain the approximate solution. Our purpose is to obtain the solution of Eq. (1) subject to the first-type boundary condition given by Eq. (13). After the substitution by using Eq. (7), the problem becomes to obtain the solution of Eq. (9) subject to boundary condition Eq. (15). If $G(x, t)|_{x=0} = \text{constant}$, the ZIC solution can be used directly to obtain the

NZIC solution. Since the inflow concentration given by Eq. (15) is a function of time, the ZIC solution cannot be used directly but we can divide the inflow change into discrete time steps. In each step, function $\exp(-\lambda t)$ in Eq. (15) is approximated by a constant. This constant is evaluated by its average value over the time step length. As the inflow function $G(x, t)|_{x=0}$ is approximated as a set of stepwise constants, the ZIC solution is applicable. Based on the superposition principle (Zheng and Bennett, 2002), we know that the total concentration change is equal to the sum of concentration increments contributed in each time step. In this way, the NZIC solution is obtained. This is the basic idea of the stepwise superposition approximation approach.

Based on the idea of the aforementioned approach, we discretize $0-t$ into N time-steps with the step length of $\Delta t = t/N$. For each time step, function $\exp(-\lambda t)$ in Eq. (15) is approximated by its average value, E , over the length of the step, Δt . Replacing $\exp(-\lambda t)$ by E , we have the approximate solution about G as:

$$G(x, t) \approx (C_0 - C_i E)F(x, t) \quad (19)$$

Define the relative concentration increment (RCI) as:

$$S(x, t) = \frac{1}{C_i} [C_0 F(x, t) - G(x, t)] = EF(x, t) \quad (20)$$

For the first time step, $k = 1$, the RCI contribution made by the boundary concentration change in this step lasts continuously from the initial time ($t = 0$) to time t and is expressed as:

$$\Delta S_1 = S_1(x, t) - S_0(x, t = 0) = \Delta E_1 F(x, t) \quad (21)$$

where, $S_0 = 0$; ΔE_1 is the average value of $\exp(-\lambda t)$ over $0 - \Delta t$ and is estimated as:

$$\Delta E_1 = E_1 - E_0 = \frac{1 - \exp(-\lambda \Delta t)}{\lambda \Delta t} \quad (22)$$

where, $E_0 = 0$. Similarly, for the k th time step, the RCI contribution by the boundary concentration change in this step lasts from time $(k-1)\Delta t$ to time t . Thus, we have the following Eq. (23):

$$\Delta S_k = \Delta E_k F[(x, t - (k-1)\Delta t)] \quad (23)$$

where,

$$\Delta E_k = E_k - E_{k-1} = \frac{2 \exp[-(k-1)\lambda \Delta t] - \exp(-k\lambda \Delta t) - \exp[-(k-2)\lambda \Delta t]}{\lambda \Delta t} \quad (24)$$

$k = 2, 3, \dots, N$

The total increment of S is the sum of the individual RCI contributions in each time step and is hence equal to:

$$S = \frac{1 - \exp(-\lambda \Delta t)}{\lambda \Delta t} F(x, t) + \sum_{k=2}^N \Delta E_k F(x, t - (k-1)\Delta t) \quad (25)$$

By substituting Eq. (7) into Eq. (20) for $G(x,t)$ with S expressed in Eq. (25), we have:

$$C(x,t) = C_0 F(x,t) + C_i [\exp(-\lambda t) - S] \quad (26)$$

This is the final approximate solution for the first-type boundary condition when C_i = constant.

1.3 Solutions for a second-type boundary condition

In the case of a second-type boundary condition, the contaminant enters the domain by dispersion through the upstream inlet boundary with a flux as:

$$-D_L \frac{\partial C}{\partial x} \Big|_{x=0} = \frac{s}{\theta} \quad (27)$$

The infinitive boundary condition is the same as in Eq. (14), where, s (mg/(m²·day)) is the boundary dispersion flux (Leij et al., 2000; Chen, 2007). In this case, the solution for an NZIC problem is the same as in Eq. (12).

1.4 Solutions for a third-type boundary condition

In the case of a third-type boundary condition, Eq. (1) is solved subject to initial condition Eq. (2), infinitive boundary condition Eq. (14), and inlet boundary condition of the hydrodynamic dispersion flux as:

$$\left(-D_L \frac{\partial C}{\partial x} + vC \right) \Big|_{x=0} = \frac{g}{\theta} \quad (28)$$

where, g (mg/(m²·day)) is the boundary hydrodynamic dispersion flux (e.g., Leij et al., 1991, 2000; Batu, 1993; Srivastava et al., 2004; Huang and Goltz, 2006; Srinivasan and Clement, 2008; Guerrero et al., 2009; Kumar et al., 2010).

Substituting G for C again, Eq. (1) becomes Eq. (9). The initial and infinitive boundary conditions of Eqs. (2) and (14) are homogenized to become Eqs. (10) and (16). The flux boundary condition (28) becomes:

$$\left(-D_L \frac{\partial G}{\partial x} + vG \right) \Big|_{x=0} = \frac{g}{\theta} - vC_i \exp(-\lambda t) \quad (29)$$

Similarly, for non-reactive transport, $\lambda = 0$, Eq. (29) becomes:

$$\left(-D_L \frac{\partial G}{\partial x} + vG \right) \Big|_{x=0} = \frac{g}{\theta} - vC_i = \text{constant} \quad (30)$$

Clearly, the NZIC solution for this case is identical to the corresponding ZIC solution, but $\frac{g}{\theta}$ is replaced by $\frac{g}{\theta} - vC_i$, and C_i is added to the solution. For instance, if the ZIC solution can be expressed as:

$$C(x,t) = \frac{g}{\theta v} F(x,t) \quad (31)$$

the solution for the corresponding NZIC problem is:

$$C(x,t) = C_i + \left(\frac{g}{\theta v} - C_i \right) F(x,t) \quad (32)$$

In the reactive transport, the third-type boundary condition (Eq. (29)) is not constant. In this case, a similar

superposition approximation approach is applied again as discussed in Section 1.2. Suppose its ZIC solution is Eq. (31). This time, the RCI is defined as:

$$S(x,t) = \frac{1}{C_i} \left[\frac{g}{\theta v} F(x,t) - G(x,t) \right] = EF(x,t) \quad (33)$$

where, E is the average value of $\exp(-\lambda t)$. For N time steps, the total increment of S is:

$$S = \frac{1 - \exp(-\lambda \Delta t)}{\lambda \Delta t} F(x,t) + \sum_{k=2}^N \Delta E_k F(x,t - (k-1)\Delta t) \quad (34)$$

where, ΔE_k is given by Eq. (24). Hence, the final approximate NZIC solution for the third-type boundary condition is:

$$C(x,t) = \frac{g}{\theta v} F(x,t) + C_i [\exp(-\lambda t) - S] \quad (35)$$

2 Test and solution examples

2.1 Test of the approach with van Genuchten solution for first-type boundary condition

The purpose of this section is to test theoretically the correctness of the proposed approach by using the van Genuchten (1981) solution with a non-zero initial concentration. First, the concentration distribution is calculated by the van Genuchten solution for C_i = constant. Then, the same parameters are used again to make the calculation for C_i = constant by using the stepwise superposition approximation approach based on the ZIC van Genuchten solution (that is, C_i is set to zero in the van Genuchten solution). Finally, the results of these two calculations are compared. If the approach is correct, the two solutions should produce similar results.

For an NZIC problem of:

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} - \lambda C \quad (36)$$

$$C(x,t)|_{t=0} = C_i \quad (37)$$

$$C(x,t)|_{x=0} = C_0 \quad (38)$$

$$\frac{\partial C}{\partial x} \Big|_{x \rightarrow \infty} = 0 \quad (39)$$

van Genuchten (1981) derived an analytical solution using the Laplace transform techniques. The solution is:

$$C(x,t) = C_0 H(x,t) + M(x,t) \quad (40)$$

where,

$$H(x,t) = \frac{1}{2} \exp \left[\frac{(v-u)x}{2D_L} \right] \operatorname{erfc} \left(\frac{x-ut}{2\sqrt{D_L t}} \right) + \frac{1}{2} \exp \left[\frac{(v+u)x}{2D_L} \right] \operatorname{erfc} \left(\frac{x+ut}{2\sqrt{D_L t}} \right) \quad (41)$$

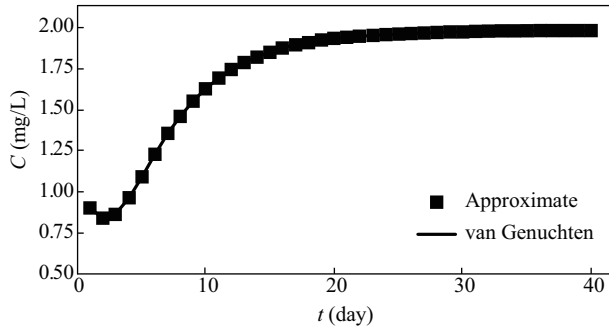


Fig. 1 Comparison of the concentration distributions determined by the stepwise superposition approximation presented in Eq. (45) and the solution of van Genuchten (1981) in Eq. (40) for a first-type boundary condition of $C_i = 1$ mg/L, $C_0 = 6$ mg/L and $\lambda = 0.1$ day $^{-1}$.

$$M(x, t) = C_i \exp(-\lambda t) \left[1 - \frac{1}{2} \operatorname{erfc} \left(\frac{x-vt}{2\sqrt{D_L t}} \right) - \frac{1}{2} \exp \left(\frac{vx}{D_L} \right) \operatorname{erfc} \left(\frac{x+vt}{2\sqrt{D_L t}} \right) \right] \quad (42)$$

in which erfc is the complementary error function, and

$$u = \sqrt{v^2 + 4\lambda D_L} \quad (43)$$

With $C_i = 0$ in Eq. (37), we can obtain its corresponding ZIC solution as:

$$C(x, t) = C_0 H(x, t). \quad (44)$$

In using the stepwise superposition approximation approach presented in this article for the solution of the NZIC problem, considering $F(x, t) = H(x, t)$ in this case, Eq. (26) becomes:

$$C(x, t) = C_0 H(x, t) + C_i [\exp(-\lambda t) - S] \quad (45)$$

where, S is given by Eq. (25) with $F(x, t)$ replaced by $H(x, t)$.

Figure 1 shows the comparative curves of the calculated results obtained by Eq. (45) and the van Genuchten solution (Eq. (40)). The calculation parameters are as follows: $C_0 = 6$ mg/L, $C_i = 1$ mg/L, $\lambda = 0.1$ day $^{-1}$, $D_L = 0.4$ m 2 /day, $v = 0.25$ m/day, $x = 4$ m, and $t = 1, 2, \dots, 40$ day(s). For the approximate solution, $\Delta t = 1$ day. As can be seen from Fig. 1, the results agree very well with each other, indicating that the superposition approximation approach is correct. The calculation error is primarily controlled by parameter $\lambda \Delta t$ and calculation position x . In general, a smaller $\lambda \Delta t$ value and a larger x value result in fewer errors. Figure 2 shows the change in the maximum relative error σ_{\max} (defined as $\sigma_{\max} = \operatorname{Max} \operatorname{abs}(C_e - C_a) \times 100 / C_e$, where, C_e and C_a are the exact and approximate concentrations, respectively) with parameter $\lambda \Delta t$. For $x \geq 0.1$ m, σ_{\max} is less than 1% if $\lambda \Delta t < 0.25$. Since the value of the reaction rate constant λ is typically small, convergence to the exact solution is relatively fast.

2.2 Test with the van Genuchten solution for a third-type boundary condition

This case is the same as the previous one, except that the first-type boundary condition (Eq. (38)) is replaced by

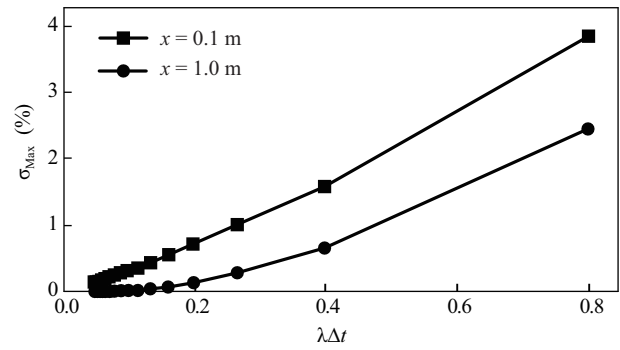


Fig. 2 Variations of the maximum relative error, σ_{\max} with parameter $\lambda \Delta t$ at $x = 0.1$ m and 1.0 m, respectively, for a first-type boundary condition.

a third-type boundary condition:

$$\left(-D_L \frac{\partial C}{\partial x} + vC \right) \Big|_{x=0} = \frac{g}{\theta} \quad (46)$$

van Genuchten (1981) gave the solution for this problem as:

$$C(x, t) = \frac{g}{\theta v} A(x, t) + C_i \exp(-\lambda t) [1 - B(x, t)] \quad (47)$$

where

$$A(x, t) = \frac{v}{v+u} \exp \left[\frac{(v-u)x}{2D_L} \right] \operatorname{erfc} \left(\frac{x-ut}{2\sqrt{D_L t}} \right) + \frac{v}{v-u} \exp \left[\frac{(v+u)x}{2D_L} \right] \operatorname{erfc} \left(\frac{x+ut}{2\sqrt{D_L t}} \right) + \frac{v^2}{2\lambda D_L} \exp \left(\frac{vx}{D_L} - \lambda t \right) \operatorname{erfc} \left(\frac{x+vt}{2\sqrt{D_L t}} \right) \quad (48)$$

$$B(x, t) = \frac{1}{2} \operatorname{erfc} \left(\frac{x-vt}{2\sqrt{D_L t}} \right) + \sqrt{\frac{v^2 t}{\pi D_L}} \exp \left[-\frac{(x-vt)^2}{4D_L t} \right] - \frac{1}{2} \left(1 + \frac{vx}{D_L} + \frac{v^2 t}{D_L} \right) \exp \left(\frac{vx}{D_L} \right) \operatorname{erfc} \left(\frac{x+vt}{2\sqrt{D_L t}} \right) \quad (49)$$

and u is the same as in Eq. (43). In this case, the corresponding ZIC solution is:

$$C(x, t) = \frac{g}{\theta v} A(x, t). \quad (50)$$

For this NZIC problem, substituting $A(x, t)$ for $F(x, t)$ in Eq. (35), we have the following solution:

$$C(x, t) = \frac{g}{\theta v} A(x, t) + C_i [\exp(-\lambda t) - S] \quad (51)$$

where, S is given by Eq. (34) with $F(x, t)$ replaced by $A(x, t)$.

Figure 3 compares the calculation results obtained respectively by Eq. (51) and the van Genuchten solution (Eq. (47)). The parameters are $g = 100$ mg/(m 2 ·day), $\theta = 0.2$, $t = 5$ day, $\Delta t = 0.5$ day, $x = 0, 0.1, \dots, 4$ m, and the rest are the same as in the previous case. Again, a good agreement exists here. When $\lambda \Delta t$ is set to 0.25 and 0.1, σ_{\max} is 1.528% and 0.389%, respectively (Fig. 4).

2.3 Solution examples

In the following part, two examples are given for the application of the approach. The first one is the NZIC solution of a three-dimensional transport of contaminant released continuously from an inner patch source. The mathematical model for this example is (Fig. 5):

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - v \frac{\partial C}{\partial x} - \lambda C + \frac{\gamma}{\theta} \delta \quad (52)$$

$$C(x, y, z, t)|_{t=0} = C_i \quad (53)$$

$$C(x, y, z, t)|_{x,y \rightarrow \pm\infty} = C_i \exp(-\lambda t) \quad (54)$$

$$\left. \frac{\partial C}{\partial z} \right|_{z=0} = \left. \frac{\partial C}{\partial z} \right|_{z=b} = 0 \quad (55)$$

where, γ (mg/day) is the source strength (mass released from the source per unit time); D_x , D_y and D_z are the principal values of the hydrodynamic dispersion coefficient, respectively; b (m) is the thickness of the aquifer; and δ (m^{-3}) is Delta function:

$$\delta = \begin{cases} 1, & (x, y, z) \in \text{source} \\ 0, & \text{otherwise} \end{cases}$$

From Eq. (12), we know that the solution of the above model is:

$$C(x, y, z, t) = f(x, y, z, t) + C_i \exp(-\lambda t) \quad (56)$$

where, $f(x, y, z, t)$ is the ZIC solution of the problem (Park and Zhan, 2001; Wang and Wu, 2009).

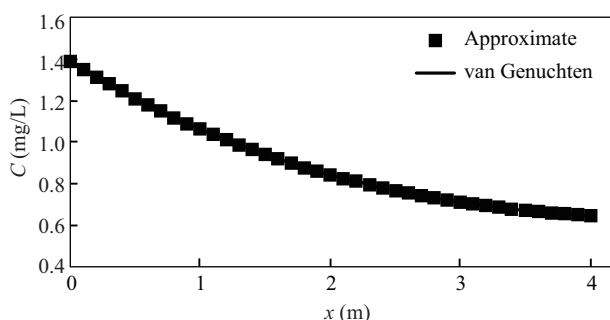


Fig. 3 Comparison of the concentration distributions determined by the stepwise superposition approximation in Eq. (51) with the van Genuchten (1981) solution in Eq. (47) for a third-type boundary condition: $C_i = 1$ mg/L, $g = 100$ $\text{mg}/(\text{m}^2 \cdot \text{day})$ and $\lambda = 0.1$ day^{-1} .

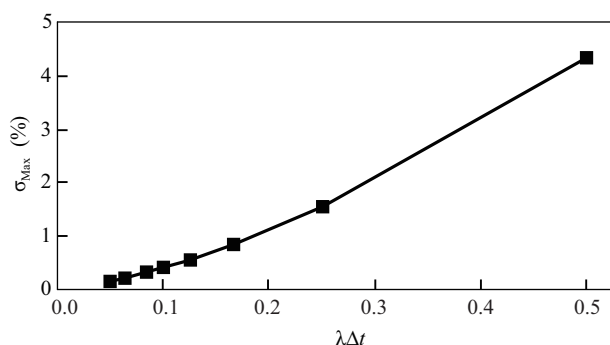


Fig. 4 Variations of the maximum relative error σ_{\max} with parameter $\lambda \Delta t$ for a third-type boundary condition.

$$f(x, y, z, t) = \frac{\gamma}{8\theta y_0(z_1 - z_0)\sqrt{\pi D_x}} \int_0^{\infty} \exp\left[-kt - \frac{(x-w)^2}{4D_x t}\right] \left[\operatorname{erfc}\left(\frac{y-y_0}{2\sqrt{D_y t}}\right) - \operatorname{erfc}\left(\frac{y+y_0}{2\sqrt{D_y t}}\right) \right] \\ \times \left\{ \frac{z_1 - z_0}{b} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_1}{b}\right) - \sin\left(\frac{n\pi z_0}{b}\right) \right] \cos\left(\frac{n\pi z}{b}\right) \exp\left(-\frac{D_z n^2 \pi^2 t}{b^2}\right) \right\} \frac{dw}{\sqrt{\tau}} \quad (57)$$

where, y_0 (m) is the half width of the source patch (Fig. 5), and z_0 (m) and z_1 (m) are the depths of the source top and bottom sides, respectively.

Figure 6 illustrates the concentration calculation results 10 m downstream from the center of the patch source that releases the contaminant continuously at strength of $\gamma = 400$ mg/day with three different initial concentrations of $C_i = 0, 0.15$, and 0.3 mg/L. The other parameters are $D_x = 1$ m^2/day , $D_y = D_z = 0.1$ m^2/day , $\theta = 0.2$, $v = 1$ m/day, $\lambda = 0.006$ day^{-1} , $b = 8$ m, $y_0 = 1$ m, $z_0 = 1$ m, and $z_1 = 2$ m. In Fig. 6, the concentration increases with the increase in time and maintains a steady value in the ZIC case ($C_i = 0$). However, in the two NZIC cases ($C_i = 0.15$ and 0.3 mg/L), the concentration goes up first and then down very slowly.

The second example is similar to the previous one, but the source patch is located on the inlet boundary of the first-type with a constant source concentration, C_0 . Hence, the governing equation is the same as Eq. (52) but without term $\gamma\delta/\theta$. The infinitive boundary condition Eq. (54) is split into three parts:

$$C(x, y, z, t)|_{x=0} = \begin{cases} C_0, & (y, z) \in \text{source} \\ C_i \exp(-\lambda t), & \text{otherwise} \end{cases} \quad (58)$$

$$C(x, y, z, t)|_{x \rightarrow \infty} = C_i \exp(-\lambda t) \quad (59)$$

$$C(x, y, z, t)|_{y \rightarrow \pm\infty} = C_i \exp(-\lambda t) \quad (60)$$

The initial and vertical boundary conditions are the same as in Eqs. (53) and (55).

In this example, the NZIC solution is in accordance with Eq. (26):

$$C(x, y, z, t) = C_0 F(x, y, z, t) + C_i [\exp(-\lambda t) - S] \quad (61)$$

where, S is given by Eq. (25) with $F(x, t)$ replaced by $F(x, y, z, t)$, and $F(x, y, z, t)$ is the Sagar (1982) solution without C_0 :

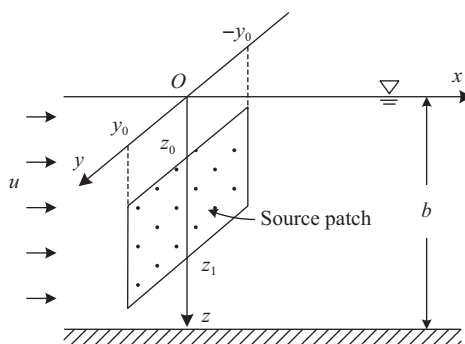


Fig. 5 A schematic diagram of a vertical patch source in three dimensions with parallel non-penetrable upper and lower boundaries.

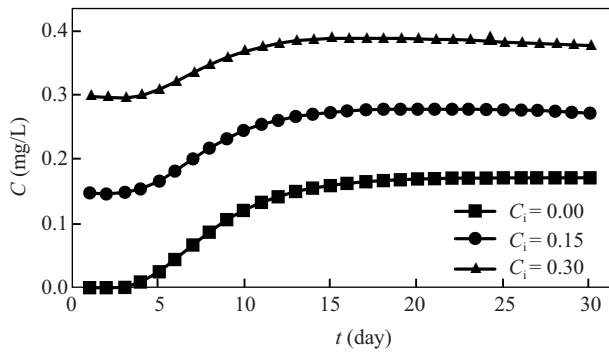


Fig. 6 Theoretical concentrations measured 10 m downstream from the center of the patch source that releases the contaminant continuously at a strength of $\gamma = 400$ mg/day with the initial concentrations of $C_i = 0, 0.15$, and 0.3 mg/L, respectively.

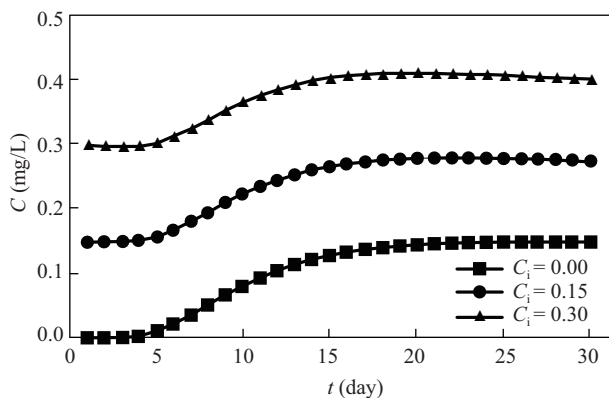


Fig. 7 Theoretical concentrations measured 10 m downstream from the center of the inlet patch source that releases the contaminant continuously at constant concentration of $C_0 = 1$ mg/L with the initial concentrations of $C_i = 0, 0.15$, and 0.3 mg/L, respectively.

$$F(x, y, z, t) = \frac{x}{4\sqrt{\pi D_x}} \int_0^t \exp\left[-\lambda\tau - \frac{(x-v\tau)^2}{4D_x\tau}\right] \left[\operatorname{erfc}\left(\frac{y-y_0}{2\sqrt{D_y\tau}}\right) - \operatorname{erfc}\left(\frac{y+y_0}{2\sqrt{D_y\tau}}\right) \right] \\ \times \left\{ \frac{z_1-z_0}{b} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_1}{b}\right) - \sin\left(\frac{n\pi z_0}{b}\right) \right] \cos\left(\frac{n\pi z}{b}\right) \exp\left(-\frac{D_z n^2 \pi^2 \tau}{b^2}\right) \right\} \frac{d\tau}{\sqrt{\tau^3}} \quad (62)$$

Figure 7 shows the calculation results of the second example with the same parameters as in the previous one, except that the source strength γ is replaced by the constant source concentration of $C_0 = 1$ mg/L. Concentration variations similar to the previous one are found in this example.

3 Conclusions

Obtaining the transport solutions subject to the NZIC condition using the existing solutions of the ZIC is feasible. The approach to determine the NZIC solutions varies with the difference in the original governing equation and boundary conditions. For a first-type or a third-type boundary condition in reactive transport, the proposed stepwise superposition approximation approach is convenient to use with fast convergence speed. It also provides an alternative way to determine the concentration distributions in cases where the original solution is elaborate for making the concentration calculation if the NZIC is considered. Although we have only discussed the transport solutions of a single component, we predict that the approach proposed here can

be similarly applied to multi-component transport cases.

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