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Analytical solutions of the one-dimensional advection–dispersion solute transport equation subject to time-dependent boundary conditions

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HIGHLIGHTS

- We extend the Duhamel theorem to the case of advective–dispersive solute transport.
- Analytical formulas relate exact solutions to time-independent auxiliary solutions.
- Explicit analytical expressions are developed for selected particular cases.
- Results are compared with other specific solutions from the literature.

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ABSTRACT

Analytical solutions of the advection–dispersion solute transport equation remain useful for a large number of applications in science and engineering. In this paper we extend the Duhamel theorem, originally established for diffusion type problems, to the case of advective–dispersive transport subject to transient (time-dependent) boundary conditions. Generalized analytical formulas are established which relate the exact solutions to corresponding time-independent auxiliary solutions. Explicit analytical expressions were developed for the instantaneous pulse problem formulated from the generalized Dirac delta function for situations with first-type or third-type inlet boundary conditions of both finite and semi-infinite domains. The developed generalized equations were evaluated computationally against other specific solutions available from the literature. Results showed the consistency of our expressions.

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1. Introduction

Analyses of many contaminant transport problems require the use of mathematical models commensurate with the application. While many field problems require comprehensive numerical models simulating transient fluid flow and solute transport, many transport problems may well be addressed using simplified one- or multi-dimensional analytical models. As pointed out in several studies [1–5], analytical models are useful for providing initial or approximate studies of alternative pollution scenarios, conducting sensitivity analyses to investigate the effects of various parameters or processes on contaminant transport, extrapolating results over large times and spatial scales where numerical solutions become impractical, serving as screening models, estimating transport parameters from laboratory or well-defined field experiments, providing benchmark solutions for more complex transport processes that cannot be solved analytically, and for verifying more comprehensive numerical solutions of the governing transport equations.

The literature contains many analytical solutions for advection–dispersion type transport problems in one and multiple dimensions, including solutions for sequential decay chains, non-equilibrium transport problems and finite and infinite domains (e.g. [2,6–15]). Most or all of these solutions are for boundary conditions that are constant in time or change in only a very simple manner with time (e.g., step or exponential functions). By contrast, very few analytical solutions are available when the boundary conditions are arbitrary functions of time. Still, it is known from the heat conduction literature that Duhamel's theorem provides a convenient approach for developing solutions to heat conduction problems with time-dependent boundary conditions, and/or for time-dependent energy generation scenarios by utilizing the

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solution to the same problem with time-independent energy sources [16,17].

The objective of the present work is to apply Duhamel's theorem to one-dimensional advection–dispersion solute transport problems with boundary conditions that are dependent upon time. A general framework is provided to obtain the desired solutions from known solutions of cases having time-independent boundary conditions. The equations developed in this paper hence may be used to extend existing solutions to situations where the boundary conditions are time-dependent.

2. Problem formulation

Contaminant transport in homogeneous porous media is generally modeled by assuming a constant average transport velocity, linear equilibrium sorption, and first-order decay. For a finite (of length L_0) or semi-infinite medium, this problem can be formulated as:

$$R\frac{\partial c(x,t)}{\partial t} = Lc(x,t) \tag{1a}$$

where L is a linear operator of the form:

$$L \equiv D\frac{\partial^2}{\partial x^2} - v\frac{\partial}{\partial x} - \mu \tag{1b}$$

which is to be solved here subject to the following initial and boundary conditions:

$$c(x,0) = 0 \tag{2}$$

$$c(0,t) = g(t) \tag{3a}$$

or

$$-D\frac{\partial c(0,t)}{\partial x} + vc(0,t) = vg(t) \tag{3b}$$

$$\frac{\partial c(L_0,t)}{\partial x} = 0 \tag{4a}$$

or

$$\frac{\partial c(\infty,t)}{\partial x} = 0 \tag{4b}$$

where $c(x, t)$ is the dimensional concentration [M L^{-3}] as a function of distance x [L] and time t [T], $g(t)$ is some known time-dependent function representing the inlet concentration [M L^{-3}], R is a constant retardation coefficient [−], v is a constant average pore water velocity [L T^{-1}], μ is a constant first-order decay constant [T^{-1}], and D is a constant dispersion coefficient [L^2 T^{-1}].

Eqs. (3a) and (3b) describe two possible formulations of the inlet boundary condition at $x = 0$, generally referred to as first-type (or Dirichlet) and third-type (or Cauchy) boundary conditions, respectively. Boundary condition (4a) for a finite transport domain is often referred to as the Danckwerts outlet condition [18]. The physical basis and applicability of these conditions are discussed in great detail elsewhere [8,19,20].

3. Solutions using Duhamel's theorem

Our solution follows the methodology outlined by Ozisik [16] for heat conduction problems. We first give the general solution for any arbitrary transient function of the inlet concentration, $g(t)$, and then present the solutions for two special cases: an instantaneous pulse described by the Dirac delta function (Section 3.2) and a finite pulse input function (Section 3.3).

3.1. General Duhamel solution

Let $\Phi(x, t; \tau)$ [M L^{-3}], be the auxiliary solution of the following problem where τ is a parameter (but not the time variable):

$$R\frac{\partial \Phi(x,t;\tau)}{\partial t} = L\Phi(x,t;\tau) \tag{5}$$

$$\Phi(x,0;\tau) = 0 \tag{6}$$

$$\Phi(0,t;\tau) = g(\tau) \tag{7a}$$

or

$$-D\frac{\partial \Phi(0,t;\tau)}{\partial x} + v\Phi(0,t;\tau) = vg(\tau) \tag{7b}$$

$$\frac{\partial \Phi(L_0,t;\tau)}{\partial x} = 0 \tag{8c}$$

or

$$\frac{\partial \Phi(\infty,t;\tau)}{\partial x} = 0 \tag{8d}$$

Duhamel's theorem relates $c(x, t)$ of Eqs. (1–4) to the solution $\Phi(x, t; \tau)$ of Eqs. (5–8) by means of the following integral expression:

$$c(x,t) = \frac{\partial}{\partial t}\int_0^t \Phi(x,t-\tau;\tau)d\tau \tag{9}$$

The proof of the extended Duhamel's theorem for the advection–dispersion equation is not shown here, but can be easily obtained by applying Laplace transforms to Eqs. (1–4) and (5–8) and by considering the definition of the generalized convolution as defined by Bartels and Churchill [21]. Because the initial condition (Eq. 6) is zero, one obtains

$$c(x,t) = \int_0^t \frac{\partial}{\partial t}\Phi(x,t-\tau;\tau)\, d\tau \tag{10}$$

We now adopt the following substitution:

$$\Phi(x,t;\tau) = \varphi(x,t)g(\tau) \tag{11}$$

in which $\varphi(x, t)$ is dimensionless [−] and $g(\tau)$ has the same dimension as before for the concentration [M L^{-3}]. Substituting Eq. (11) into Eqs. (5) through (8) leads to

$$R\frac{\partial \varphi(x,t)}{\partial t} = L\varphi(x,t) \tag{12}$$

$$\varphi(x,0) = 0 \tag{13}$$

$$\varphi(0,t) = 1 \tag{14a}$$

or

$$-D\frac{\partial \varphi(0,t)}{\partial x} + v\varphi(0,t) = v \tag{14b}$$

$$\frac{\partial \varphi(L_0,t)}{\partial x} = 0 \tag{15a}$$

or

$$\frac{\partial \varphi(\infty,t)}{\partial x} = 0 \tag{15b}$$

whereas $c(x, t)$ given by Eq. (10) becomes:

$$c(x,t) = \int_0^t g(\tau)\frac{\partial}{\partial t}\varphi(x,t-\tau)d\tau \tag{16}$$

By noting that $\frac{\partial}{\partial t}\varphi(x,t-\tau)=-\frac{\partial}{\partial\tau}\varphi(x,t-\tau)$, the last equation also can alternatively be written as:

$$c(x,t)=-\int_0^t g(\tau)\frac{\partial}{\partial\tau}\varphi(x,t-\tau)d\tau = g(0)\varphi(x,t)+\int_0^t\varphi(x,t-\tau)\frac{dg(\tau)}{d\tau}d\tau \tag{17}$$

3.2. Special case: instantaneous pulse

Assume that $g(t)$ is an instantaneous pulse of the form $g(t) = m_0\,\delta(t)$, where m_0 [M L^{-3} T] is the amount of injected mass over a certain cross-sectional area divided by the volumetric water flux through that same area, and $\delta(t)$ is the generalized Dirac delta function [T^{-1}]. Eq. (16) then reduces to

$$c(x,t)=m_0\int_0^t\delta(\tau)\frac{\partial}{\partial t}\varphi(x,t-\tau)d\tau \tag{18}$$

Using the property [22]:

$$\int\delta(\xi-\sigma)F(\xi)d\xi=F(\sigma) \tag{19}$$

Eq. (18) simplifies to

$$c(x,t)=m_0\frac{\partial\varphi(x,t)}{\partial t} \tag{20}$$

3.3. Special case: Finite pulse

In this case, the function $g(t)$ is defined as a finite pulse of the form

$$g(t)=\begin{cases} f(t) & 0<t\leqslant t_0\\ 0 & t>t_0\end{cases} \tag{21}$$

Using Eqs. (17) and (21), and separating the integral at the discontinuity ($t = t_0$) into two parts leads to

$$c(x,t)=\begin{cases} f(0)\varphi(x,t)+\int_0^t\varphi(x,t-\tau)\frac{df(\tau)}{d\tau}d\tau & t\leqslant t_0\\ f(0)\varphi(x,t)-f(t_0)\varphi(x,t-t_0)+\int_0^{t_0}\varphi(x,t-\tau)\frac{df(\tau)}{d\tau}d\tau & t>t_0\end{cases} \tag{22}$$

4. Specific solutions for the instantaneous pulse

In the following we give solutions for the case of an instantaneous pulse for a solute transport scenario described by Eqs. (1–4). The expressions were developed using Eq. (20), together with equations compiled by van Genuchten and Alves [23] serving as the auxiliary solution, $\varphi(x, t)$, of Eqs. (12–15) for the various types of boundary conditions (BCs). The solutions are relatively routine, but shown here to illustrate the implementation of Duhamel's theorem. More involved examples are given in Section 5.

4.1. Instantaneous pulse, first type inlet BC; semi-infinite domain

The auxiliary solution $\varphi(x, t)$ is given by Case C5 of van Genuchten and Alves [23]. Differentiation of that solution with respect to time as indicated by Eq. (20) leads to the well-known solution (e.g., Skaggs and Leij [20]; Table 6.1–3):

$$\frac{c(x,t)}{C_0}=\frac{DR^2x\exp\left[-\frac{(tv-Rx)^2}{4DRt}-\frac{\mu t}{R}\right]}{2\sqrt{\pi}(DRt)^{3/2}} \tag{23}$$

4.2. Instantaneous pulse, third type inlet BC; semi-finite domain

The auxiliary solution $\varphi(x, t)$ is given by Case C6 of van Genuchten and Alves [23]. Differentiation versus time gives (e.g., Skaggs and Leij [20]; Table 6.1–3):

$$\frac{c(x,t)}{C_0}=\frac{v\exp\left[-\frac{(tv-Rx)^2}{4DRt}-\frac{\mu t}{R}\right]}{\sqrt{\pi}(DRt)^{1/2}}-\frac{v^2\exp(\frac{vx}{D}-\frac{\mu t}{R})}{2DR}erfc\left[\frac{tv+Rx}{2(DRt)^{1/2}}\right] \tag{24}$$

4.3. Instantaneous pulse, first-type inlet BC; finite domain

The auxiliary solution $\varphi(x, t)$ is given by Case C7 of van Genuchten and Alves [23], which if differentiated versus time leads immediately to

$$\frac{c(x,t)}{C_0}=\sum_{m=1}^{\infty}E_{12}(\beta_m,x)\left[\frac{v^2}{4DR}+\frac{\beta_m^2D}{L_0^2R}\right]\exp\left(\frac{vx}{2D}-\frac{\mu t}{R}-\frac{v^2t}{4DR}-\frac{\beta_m^2Dt}{L_0^2R}\right) \tag{25a}$$

$$E_{12}(\beta_m,x)=\frac{2\beta_m\sin\left(\frac{\beta_mx}{L_0}\right)}{\beta_m^2+\left(\frac{vL_0}{2D}\right)^2+\frac{vL_0}{2D}} \tag{25b}$$

in which the eigenvalues β_m are roots of the following transcendental equation:

$$\beta_m\cot(\beta_m)+\frac{vL_0}{2D}=0 \tag{26}$$

4.4. Instantaneous pulse, third type inlet BC; finite domain

The auxiliary solution $\varphi(x, t)$ is now given by Case C8 of van Genuchten and Alves [23]. Differentiation versus time of that solution gives

$$\frac{c(x,t)}{C_0}=\sum_{m=1}^{\infty}E_{32}(\beta_m,x)\left(\frac{v^2}{4DR}+\frac{\beta_m^2D}{L_0^2R}\right)\exp\left(\frac{vx}{2D}-\frac{\mu t}{R}-\frac{v^2t}{4DR}-\frac{\beta_m^2Dt}{L_0^2R}\right) \tag{27a}$$

$$E_{32}(\beta_m,x)=\frac{\frac{2vL_0}{D}\beta_m\left[\beta_m\cos\left(\frac{\beta_mx}{L_0}\right)+\frac{vL_0}{2D}\sin\left(\frac{\beta_mx}{L_0}\right)\right]}{\left[\beta_m^2+\left(\frac{vL_0}{2D}\right)^2+\frac{vL_0}{D}\right]\left[\beta_m^2+\left(\frac{vL_0}{2D}\right)^2\right]} \tag{27b}$$

in which the eigenvalues β_m are obtained from:

$$\beta_m\cot(\beta_m)-\frac{\beta_m^2D}{vL_0}+\frac{vL_0}{4D}=0 \tag{28}$$

5. Example applications

The solutions listed in the previous section are relatively standard and could be obtained easily without application of Duhamel's theorem. Here we show two additional solutions implemented within a more general Duhamel framework, and compare them with previously developed exact solutions.

5.1. Example 1: Exponential inlet distribution; decay

We solve the transport problem for a semi-infinite medium subject to a third-type inlet boundary condition. The governing equations are given by Eqs. (1) and (2) subject to Eqs. (3b) and (4b), along with the following data set: $g(t) = C_a + C_b\exp(-\lambda t)$, $R = 1$, $\mu = 0.3\ \mathrm{day}^{-1}$, $D = 0.7\ \mathrm{m^2/day}$, $v = 0.3$ m/day, $C_a = 1\ \mathrm{kg/m^3}$,

Table 1
Concentration values $c(x, t)$ at $t = 0.1$ and $t = 1.0$ day (example 1).

x	$c(x, 0.1)$ Eq. (16)	$c(x, 0.1)$ Eq. (17)	$c(x, 0.1)$ C14, Eq. (29)	$c(x, 1)$ Eq. (16)	$c(x, 1)$ Eq. (17)	$c(x, 1)$ C14, Eq. (29)
0	0.345747–4.14732E-11 i	0.345747–2.95659E-28 i	0.345747	0.636578	0.636578	0.636578
1	0.00129972	0.00129972	0.00129972	0.239872	0.239872	0.239872
2	1.11677E-8	1.11677E-8	1.11677E-8	0.0533083	0.0533083	0.0533083
3	1.14162E-16	1.14162E-16	1.14162E-16	0.00658916	0.00658916	0.00658916
4	1.12897E-27	1.12897E-27	1.12897E-27	0.000436546	0.000436546	0.000436546
5	9.93261E-42	9.93261E-42	9.93261E-42	1.51316E-05	1.51316E-05	0.0000151316
6	7.46131E-59	7.46131E-59	7.46131E-59	2.69961E-7	2.69961E-7	2.69961E-7
7	4.67686E-79	4.67686E-79	4.67686E-79	2.45109E-9	2.45109E-9	2.45109E-9
8	2.41191E-102	2.41191E-102	2.41191E-102	1.12344E-11	1.12344E-11	1.12344E-11
9	1.01396E-128	1.01396E-128	1.01396E-128	2.58411E-14	2.58411E-14	2.58411E-14
10	3.45271E-158	3.45271E-158	3.45271E-158	2.96977E-17	2.96977E-17	2.96977E-17

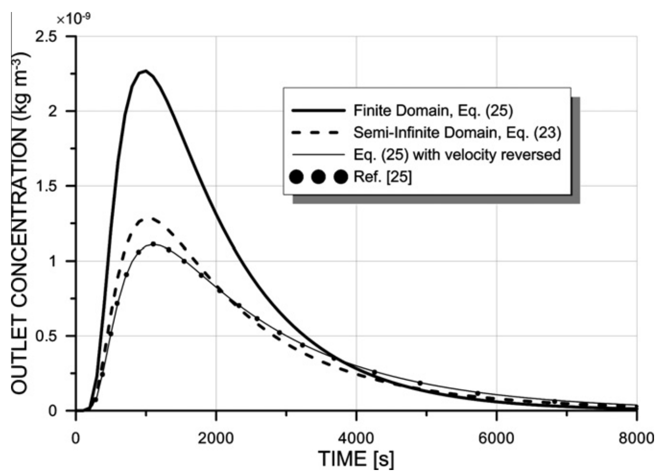

Fig. 1. Outlet concentration for a finite domain (Eq. (25)) and semi-infinite (Eq. (23)) domain. Also, the concentration computed for a finite domain with the velocity reversed ("flow against dispersion").

$C_b = 2$ kg/m^3, and $\lambda = 1$ day^{-1}. The analytical solution for this problem corresponds to the Case C14 in van Genuchten and Alves [23].

Eqs. (16) or (17) can be used together with auxiliary solution C8 of van Genuchten and Alves [23] to obtain the desired solution. Although closed-form expressions can be obtained using appropriate integral transform, Laplace transform or other techniques, we obtain the results here by direct numerical integration. A large number of numerical integration routines could be used for this purpose. In our study we used the very flexible NIntegrate subroutine from the Mathematica software package [24]. This numeric alternative for the integral is appropriate when the exact analytical solution cannot be derived, or when the resulting closed-form expressions are very difficult to evaluate (e.g., by containing integral themselves).

Table 1 shows that results obtained with Eqs. (16) and (17) are the same as the closed form solution given by Case C14 van Genuchten and Alves [23]. For completeness we restate that solution here:

$$c(x,t) = \begin{cases} C_a A(x,t) + C_b B(x,t) & \mu \neq \lambda R \\ C_o A(x,t) + C_b E(x,t) & \mu = \lambda R \end{cases} \tag{29}$$

where

$$\begin{aligned} A(x,t) = {} & \frac{v}{u+v}\exp\left[\frac{(v-u)x}{2D}\right] erfc\left[\frac{Rx-ut}{2\sqrt{DRt}}\right] \\ & - \frac{v}{u-v}\exp\left[\frac{(v+u)x}{2D}\right] erfc\left[\frac{Rx+ut}{2\sqrt{DRt}}\right] \\ & + \frac{v^2}{2\mu D}\exp\left(\frac{vx}{D}-\frac{\mu t}{R}\right) erfc\left[\frac{Rx+vt}{2\sqrt{DRt}}\right] \end{aligned} \tag{30}$$

$$\begin{aligned} B(x,t) = e^{-\lambda t}\Bigg\{ & \frac{v}{w+v}\exp\left[\frac{(v-w)x}{2D}\right] erfc\left[\frac{Rx-wt}{2\sqrt{DRt}}\right] \\ & - \frac{v}{w-v}\exp\left[\frac{(v+w)x}{2D}\right] erfc\left[\frac{Rx+wt}{2\sqrt{DRt}}\right] \\ & + \frac{v^2}{2D(\mu-\lambda R)}\exp\left(\frac{vx}{D}-\frac{\mu t}{R}\right) erfc\left[\frac{Rx+vt}{2\sqrt{DRt}}\right]\Bigg\} \end{aligned} \tag{31}$$

$$\begin{aligned} E(x,t) = e^{-\lambda t}\Bigg\{ & \frac{1}{2} erfc\left[\frac{Rx-vt}{2\sqrt{DRt}}\right] + \sqrt{\frac{v^2 t}{\pi DR}}\exp\left[-\frac{(Rx-vt)^2}{4DRt}\right] \\ & - \frac{1}{2}\left(1+\frac{vx}{D}+\frac{v^2 t}{DR}\right)\exp\left(\frac{vx}{D}\right) erfc\left[\frac{Rx+vt}{2\sqrt{DRt}}\right]\Bigg\} \end{aligned} \tag{32}$$

in which

$$u = \sqrt{v^2 + 4\mu D} \tag{33}$$

$$w = \sqrt{v^2 + 4D(\mu - \lambda R)} \tag{34}$$

5.2. Example 2: instantaneous pulse; flow in the negative x direction ($v < 0$)

Recently Ziskind et al. [25] obtained an analytical solution of the advection–dispersion equation with a decay term for a finite one-dimensional domain with an instantaneous pulse boundary condition modeled using the generalized Dirac delta function. They specified the following initial conditions and boundary conditions:

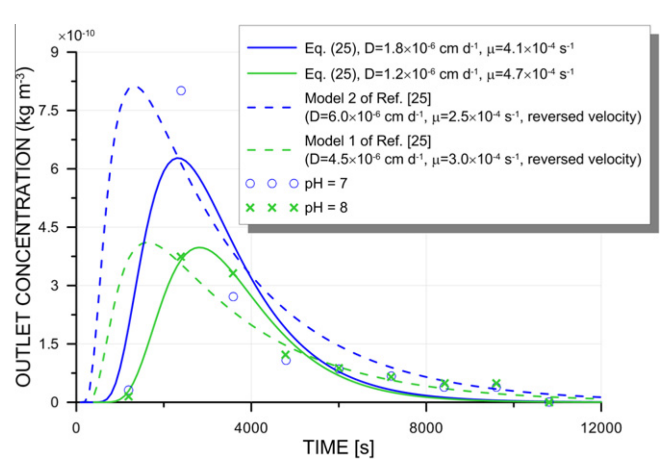

Fig. 2. Re-analysis of transport data presented in Fig. 5 of Ziskind et al. [25]. The model calculations and parameter estimates in [25] were obtained with the velocity reversed (dashed lines). The solid lines show the model fit obtained with the velocity specified in the correct direction.

$$c(\bar{x}, 0) = 0 \tag{35}$$

$$\frac{\partial c(\bar{x} = 0, t)}{\partial \bar{x}} = 0 \tag{36}$$

$$c(\bar{x} = l = L_0, t) = m_0 \delta(t) \tag{37}$$

in which $\bar{x}$ is represents the longitudinal variable used by [25]. The spatial coordinates $\bar{x}$ and x (the latter being the longitudinal position used in our study) are related by $\bar{x} = L_0 - x$. With this relationship the boundary conditions given by Eqs. (36) and (37) are equivalent to Eqs. (4a) and (3a), respectively.

The analytical solution of the above problem is given Eqs. (25) and (26) in Section 4.3, where the velocity values must be considered negative in the equations. It is easily verified that our analytical solution is the same as the solution obtained by [25]. However, the index of summation in our Eq. (25) starts with "m = 1" and not with "m = 0" as specified in Eq. (21) of Ziskind et al. [25].

Numerical evaluations were made for the following data set used in [25]: $R = 1$, $\mu = 3 \times 10^{-4}\ \mathrm{s}^{-1}$, $D = 7 \times 10^{-6}\ \mathrm{m}^2/\mathrm{s}$, $v = 3 \times 10^{-5}$ m/s, $L_0 = 0.23$ m, $m_0 = M_T/Q$ with $M_T = 8 \times 10^{-13}$ kg, and $Q = 8.57 \times 10^{-8}\ \mathrm{m}^3/\mathrm{s}$. Fig. 1 compares the solutions for both a finite domain (Eq. 25) and a semi-infinite-domain (Eq. (23)). The number of summed terms used in Eq. (25) was $N = 20$. Some results presented in [25] were apparently computed, whether intentionally or not, with the velocity reversed, i.e. $v < 0$ in our formulation or $v > 0$ in [25]. Such an arrangement, with flow directed toward the contaminant source boundary, has been termed "flow against dispersion" [26] in the hydrology literature. Fig. 1 also shows results obtained for Eq. (25) with the velocity reversed ($v = -3 \times 10^{-5}$ m/s), along with a few points digitized from a curve presented in Fig. 2 of [25]. Results obtained using the solution developed by [25] were exactly the same as obtained with our Eq. (25), provided the summation is assumed to start with "m = 1".

Fig. 2 presents a re-analysis of bacteriophage transport data from [27] which were analyzed in Fig. 5 of [25]. The dashed lines are a reproduction of the modeling results presented in Fig. 5 of [25]. The dashed lines were computed using Eq. (25) with the D and μ values estimated in [25] (given in Fig. 2), the velocity reversed, and the other model parameter values the same as given above for Fig. 1. The solid lines show the optimal model fit with velocity specified in the correct direction, where the indicated D and μ values were obtained from a new least-squares fit of Eq. (25) to the data. Fig. 2 shows that the obtained fitted model parameters and model agreement with the data differ considerably from those reported in [25]. The model fit for pH = 8 is particularly good.

6. Conclusion

Applications of the Duhamel Theorem were extended to advection–dispersion type solute transport problems in porous media when the boundary conditions are time-dependent. Solutions were obtained from solutions of corresponding non-time dependent auxiliary solutions using very generalized formulas. In this paper we illustrated the approach for relatively standard cases with known exact solutions. In particular, we emphasized cases of instantaneous and finite pulse applications to transport problems in finite and semi-infinite domains. The developed generalized formulas obtained duplicated several specific solutions available in the literature. In this paper we showed applicability to relatively simple one-dimensional equilibrium transport problems, including decay. In future work we intend to show that the general Duhamel approach is equally applicable to more complicated scenarios of transport in multi-dimensional media of solutes subject to non-equilibrium sorption or sequential decay chain reactions.

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