



## A note on the solution to one-dimensional advection-dispersion-reaction problems

Marko V. Lubarda<sup>a</sup>, and Vlado A. Lubarda<sup>b</sup>

<sup>a</sup>Department of Mechanical and Aerospace Engineering, UC San Diego, San Diego, California, USA; <sup>b</sup>Department of Nano and Chemical Engineering, UC San Diego, San Diego, California, USA

### ABSTRACT

The series representation of the reactant concentration in one-dimensional advection-dispersion-reaction problems within a container of finite length is derived in a compact and computationally less complex form than other representations found in the literature. The initial concentration of the reactant is assumed to be uniform ( $C_0$ ), while the boundary conditions are assumed to be a constant reactant flux ( $UC_e$ ) at the inlet and a zero concentration gradient at the outlet of the container, where  $U$  is the average fluid velocity. The concentration is expressed in terms of the introduced constants  $a$  and  $b$  for the steady-state part, and  $I_n$ ,  $J_n$  and  $K_n$  for the transient part of the response. The derived solution to the advection-dispersion-reaction problem can be readily generalized to include a uniform source/sink term (zero-order production rate  $\sigma$ ) by making the replacements of  $C_0$  and  $C_e$  with  $C_0 - \sigma/k$  and  $C_e - \sigma/k$ , where  $k$  is the reaction rate constant, and by adding the particular solution  $\sigma/k$ . A simple form of the solution to the advection-dispersion equation with a source term is also derived; its transient part is expressed in terms of the integrals  $I_n$  and  $K_n$  only. The formulation of the analysis is cast in such a way that the same eigenfunctions and the same eigenvalue condition apply to all three considered cases, advection-dispersion-reaction with and without a source-term, and advection-dispersion with a source term, independently of the values of  $k$  and  $\sigma$ .

### KEYWORDS

Advection; concentration; dispersion; eigenfunctions; partial differential equations; Péclet number; reaction; transport

### Introduction

We derive a compact form of the series-type solution to the one-dimensional advection-dispersion-reaction equation described by the partial differential equation for the reactant concentration  $C$ ,

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - U \frac{\partial C}{\partial x} - kC, \quad (1.1)$$

where  $x$  is the longitudinal coordinate and  $t$  is the time. The average fluid velocity is  $U$ , the dispersion coefficient characterizing the degree of back-mixing due to the velocity fluctuations around the plug-flow uniform velocity is  $D$ , and  $k$  is the reaction rate constant, all assumed to be position and time independent. The initial concentration is considered to be uniform throughout the reaction zone of length  $L$ ,

$$C(x, t = 0) = C_0. \quad (1.2)$$

The boundary conditions are a constant reactant flux at the inlet, and a zero reactant concentration gradient at the outlet of the container. Because the concentration flux in one-dimensional advection-dispersion is defined by  $j_x = UC - D\partial C/\partial x$ , the boundary conditions are

$$\left( UC - D \frac{\partial C}{\partial x} \right)_{x=0^+} = UC_e, \quad \left( \frac{\partial C}{\partial x} \right)_{x=L^-} = 0. \quad (1.3)$$

Due to forward dispersion, the concentration across the inlet boundary experiences a discontinuity  $C(0^+, t) - C_e = (\partial C/\partial x)_{x=0^+}$ . The zero concentration gradient at the outlet follows from the assumption that  $C(L^+, t) = C(L^-, t)$  and that there is no dispersion immediately after the exit of the container. The boundary conditions (1.3) were independently proposed by Langmuir (1908) and Danckwerts (1953), and are commonly referred to as the Danckwerts boundary

conditions. In Langmuir's original work, it was assumed that the container (heated reactor) is sharply bounded at the inlet and outlet by thin porous plugs through whose pores the gases move so fast that the reacting substance is predominantly carried by convection with negligible diffusion. On the sides of the plugs not facing the reactor, the diffusion coefficients  $D_l$  and  $D_r$  could be different from zero, but since we assumed that the inlet concentration  $C_e$  is constant in time, we must take  $D_l = 0$  to eliminate the time-dependence of  $C(x = 0^-, t)$ .

An alternative interpretation of the considered boundary conditions can be made if the process zone of length  $L$  is considered to be a model for a series connection of infinitely thin batch reactors, each having a stirring-induced uniform concentration in the radial direction, while the longitudinal change of concentration between adjacent batch reactors is due to a chemical reaction with the rate coefficient  $k$  and axial dispersion with an effective dispersion coefficient  $D$  (e.g., Fogler 2005; Conesa 2020). The "closed-closed" type of boundary conditions can then be visualized by considering a fluid mixture entering the first batch and exiting from the last batch reactor. The inclusion of axial dispersion makes the governing differential equation second-order, enabling the imposition and fulfillment of the second boundary condition (at  $x=L$ ), which in many cases reduces to the condition of zero concentration gradient at the outlet of the reactor.

Equation (1.1) with the initial and boundary conditions (1.2) and (1.3), or their alternatives, has been used as a mathematical model to describe a wide variety of advective-dispersive-reaction problems, including chemical reactors (Carberry 1976; Salmi and Romanainen 1995; Fogler 2005; Ziskind et al. 2011; Mott and Green 2015; Conesa 2020), nutrient or contaminant transport in groundwater through porous columns (Schnoor 1996; Delgado 2006; Masters and Ela 2008), flow-through systems for drug delivery (Mohd Mahali et al. 2014; McGinty 2014), etc. The time dependence of the inlet boundary condition and the position dependence of the initial condition have also been studied in great detail, as well as the incorporation of the position-dependent dispersion coefficient and the time and position dependent source term (Kumar

et al. 2009; Pérez Guerrero and Skaggs 2010; Pérez Guerrero et al. 2009, 2013; Chen and Liu 2011; Chen et al. 2017; Ahmed et al. 2017; Sridharan and Hein 2019; Abbasi et al. 2021; Kumar et al. 2022). The Laplace transform was frequently used with respect to time and the generalized integral transform with respect to position. Most recently, the Green's-function-based analytical solution to the one-dimensional convection-diffusion-reaction-source equation was presented by Parhizi et al. (2022), with time-dependent boundary conditions, position-dependent initial condition, and the source/sink term dependent on time and position. This work was in the context of a heat-transfer problem, but the analysis applies to other transport phenomena, as well. Mathematical theory with applications of reaction-diffusion equations have been presented by Grindrod (1996), while numerical methods for solving advection-dispersion-reaction equations have been summarized by Hundsdoerfer and Verwer (2003).

By using the non-dimensional position and time variables  $\xi = x/L$  and  $\tau = Ut/L$ , equations (1.1)–(1.3) can be rewritten as

$$\frac{\partial C}{\partial \tau} = \frac{1}{\text{Pe}} \frac{\partial^2 C}{\partial \xi^2} - \frac{\partial C}{\partial \xi} - \kappa C, \quad (1.4)$$

$$C(\xi, 0) = C_0, \quad (1.5)$$

$$\left( C - \frac{1}{\text{Pe}} \frac{\partial C}{\partial \xi} \right)_{\xi=0} = C_e, \quad \left( \frac{\partial C}{\partial \xi} \right)_{\xi=1} = 0, \quad (1.6)$$

where

$$\text{Pe} = \frac{UL}{D}, \quad \kappa = \frac{kL}{U}. \quad (1.7)$$

The Péclet number  $\text{Pe}$  represents the ratio of the advection and dispersion (diffusion) contributions to solute transport (its reciprocal  $1/\text{Pe}$  being referred to as the Bodenstein number), and  $\kappa$  is the product of the reaction rate constant  $k$  and the advection time scale  $L/U$ . The nondimensional number  $\kappa$  also represents a variant of the Damköhler number ( $\text{Da}_I = kL/U$ , Damköhler group I; Catchpole and Fulford 1966; Deen 2012), defined in a dimensional sense by the ratio of the reaction rate ( $kC$ ) and the advection rate ( $U\partial C/\partial x$ ).

We derive in this paper an appealing compact representation for the series solution for the reactant concentration in one-dimensional advection-dispersion-reaction problems within a domain of

finite length, which is computationally less complex than other representations found in the literature. This is accomplished by a compact representation of the Fourier-type coefficients for the transient part of the solution, which are expressed in terms of the introduced integrals  $I_n$ ,  $J_n$  and  $K_n$ . The derived solution to the advection-dispersion-reaction equation is then extended to include the effect of uniform source/sink term by inspection, without performing additional analysis. A simple form of the solution to the advection-dispersion-growth equation, which includes a source term but not a reaction (decay) term is also presented. The analysis is cast by using the same eigenfunctions and the same eigenvalue condition in all three considered cases, advection-dispersion-reaction with and without a source-term, and advection-dispersion with a source term, independently of the values of the reaction rate constant  $k$  and the growth term  $\sigma$  (Figure 1).

### Advection-dispersion-reaction equation

The solution to the advection-dispersion-reaction equation (1.4), with the initial condition (1.5) and the boundary conditions (1.6), can be sought as the sum of the steady-state solution  $\varphi = \varphi(\xi)$  and the remaining transient part. This is commonly expressed as (Brenner 1962)

$$C(\xi, \tau) = \varphi(\xi) + e^{(\text{Pe}\xi/2) - q\tau} \phi(\xi, \tau), \quad q = \kappa + \text{Pe}/4. \quad (2.1)$$

The function  $\varphi(\xi)$  is the solution to the boundary-value problem

$$\frac{1}{\text{Pe}} \frac{d^2 \varphi}{d\xi^2} - \frac{d\varphi}{d\xi} - \kappa \varphi = 0, \quad (2.2)$$

$$\left( \varphi - \frac{1}{\text{Pe}} \frac{d\varphi}{d\xi} \right)_{\xi=0} = C_e, \quad \left( \frac{d\varphi}{d\xi} \right)_{\xi=1} = 0, \quad (2.3)$$

and is given by

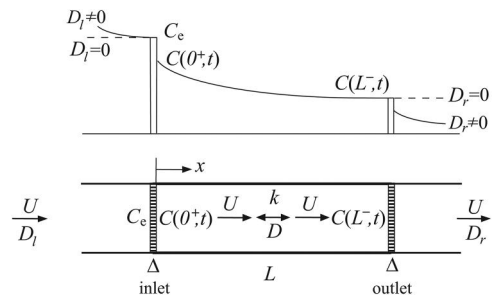
$$\varphi(\xi) = C_e [a e^{(1+\alpha)\text{Pe}\xi/2} + b e^{(1-\alpha)\text{Pe}\xi/2}], \quad (2.4)$$

$$\alpha = (1 + 4\kappa/\text{Pe})^{1/2},$$

where the integration constants  $a$  and  $b$  are

$$a = \frac{2(1-\alpha)}{(1-\alpha)^2 - (1+\alpha)^2 e^{\alpha\text{Pe}}}, \quad (2.5)$$

$$b = -\frac{2(1+\alpha) e^{\alpha\text{Pe}}}{(1-\alpha)^2 - (1+\alpha)^2 e^{\alpha\text{Pe}}}.$$



**Figure 1.** Schematic of a one-dimensional advection-dispersion-reaction process in a container of length  $L$ . The mean velocity of fluid which convects the reactant of concentration  $C(x, t)$  is denoted by  $U$ , the dispersion coefficient accounting for velocity fluctuations is  $D$ , and the rate of reaction is  $k$ . In the “closed-closed” type of plug-flow model with axial dispersion, it is assumed that there is no dispersion immediately upstream from the container, which means that the reactant cannot move backward. Physically, such a condition can be achieved by inserting at the inlet of the container a thin porous plug (of small thickness  $\Delta$ ). If the entry flux  $UC_e$  is to be independent of time, the dispersion coefficient to the left of the first plug must be equal to zero ( $D_l = 0$ ). By conservation of mass, the inlet boundary condition is then  $(UC - D\partial C/\partial x)_{x=0^+} = UC_e$ . Because the reactant concentration at the exit of the container is equal to the concentration inside the pores of the adjacent plug,  $C(L^-, t) = C(L^+, t)$ , the outlet boundary condition is  $(\partial C/\partial x)_{x=L^-} = 0$ . The diffusion coefficient  $D_r$  to the right of the second plug may be different or equal to zero, without affecting the zero concentration gradient condition at the outlet  $x = L^-$ .

The representation of the particular solution (2.4) is equivalent to other well-known representations, such as (33) of Danckwerts (1953), or (50) of Pérez Guerrero et al. (2009), but is cast in a form which is more suitable for extending the solution of the advection-dispersion-reaction problem to the advection-dispersion-reaction-growth problem presented in section “Advection-dispersion-reaction equation with a source term”. The normalized steady-state concentrations  $\varphi(0^+)/C_e$  and  $\varphi(1)/C_e$  are

$$\frac{\varphi(0^+)}{C_e} = \frac{2(1+\alpha)e^{\alpha\text{Pe}/2} - 2(1-\alpha)e^{-\alpha\text{Pe}/2}}{(1+\alpha)^2 e^{\alpha\text{Pe}/2} - (1-\alpha)^2 e^{-\alpha\text{Pe}/2}}, \quad (2.6)$$

$$\frac{\varphi(1)}{C_e} = \frac{4\alpha e^{\text{Pe}/2}}{(1+\alpha)^2 e^{\alpha\text{Pe}/2} - (1-\alpha)^2 e^{-\alpha\text{Pe}/2}},$$

in agreement with the classical results of Wehner and Wilhelm (1956), given by their equations (21) and (22). The normalized steady-state concentration discontinuity across the inlet boundary can be compactly expressed as

$$\frac{\varphi(0^+) - C_e}{C_e} = \frac{1 - \alpha^2}{1 + \alpha^2 + 2\alpha \tanh(\alpha\text{Pe}/2)}. \quad (2.7)$$

After (2.1) is substituted into (1.4), it follows that the function  $\phi(\xi, \tau)$  satisfies the diffusion-type partial differential equation

$$\frac{\partial \phi}{\partial \tau} = \frac{1}{\text{Pe}} \frac{\partial^2 \phi}{\partial \xi^2}, \quad (2.8)$$

with homogeneous boundary conditions

$$\left( \phi - \frac{2}{\text{Pe}} \frac{\partial \phi}{\partial \xi} \right)_{\xi=0} = 0, \quad \left( \phi + \frac{2}{\text{Pe}} \frac{\partial \phi}{\partial \xi} \right)_{\xi=1} = 0, \quad (2.9)$$

and the initial condition

$$\phi(\xi, 0) = [C_0 - \varphi(\xi)] e^{-\text{Pe}\xi/2}. \quad (2.10)$$

The application of separation of variables then gives

$$\phi(\xi, \tau) = \sum_{n=1}^{\infty} A_n g_n(\tau) f_n(\xi), \quad g_n(\tau) = e^{-(\lambda_n^2/\text{Pe})\tau}. \quad (2.11)$$

The utilized eigenfunctions, orthogonal on  $[0, 1]$ , are (Lubarda and Lubarda 2023)

$$f_n(\xi) = \cos(\lambda_n \xi) + \frac{\text{Pe}}{2\lambda_n} \sin(\lambda_n \xi), \quad (2.12)$$

where the eigenvalues  $\lambda_n$  are the positive roots of the transcendental equation

$$\tan \lambda = \frac{4\text{Pe}}{4\lambda^2 - \text{Pe}^2}. \quad (2.13)$$

It is noted that  $f_n(0) = 1$ , while  $f_n(1) = \pm 1$ , alternating from  $+1$  to  $-1$  with increasing  $n$ , beginning with  $f_1(1) = 1$ , because from (2.12) and (2.13) it follows that  $f_n^2(1) = 1$ .

### Expression for coefficients $a_n$

The Fourier-type coefficients  $A_n$  are determined from the initial condition (2.10),

$$\sum_{n=1}^{\infty} A_n f_n(\xi) = C_0 e^{-\text{Pe}\xi/2} - C_e (a e^{\alpha \text{Pe}\xi/2} + b e^{-\alpha \text{Pe}\xi/2}). \quad (2.14)$$

In view of the orthogonality of  $f_n(\xi)$ , the multiplication of (2.14) with  $f_m(\xi)$  and integration gives

$$A_n = \frac{1}{K_n} (C_0 I_n - C_e J_n), \quad (2.15)$$

where

$$I_n = \frac{4\text{Pe}}{\text{Pe}^2 + 4\lambda_n^2}, \quad J_n = \frac{4\text{Pe}}{\alpha^2 \text{Pe}^2 + 4\lambda_n^2}, \quad (2.16)$$

$$K_n = \frac{1}{2} \left[ 1 + \frac{\text{Pe}(4 + \text{Pe})}{4\lambda_n^2} \right],$$

with  $\alpha$  defined in terms of  $\kappa$  and  $\text{Pe}$  by (2.4). In a rather lengthy derivation of (2.15), the eigenvalue condition (2.13) was conveniently incorporated to obtain the compact form of expressions (2.16). The utilized integrals leading to (2.16) are listed in the Appendix. The overall concentration is, therefore,

$$C(\xi, \tau) = \varphi(\xi) + e^{\text{Pe}\xi/2} \sum_{n=1}^{\infty} \frac{1}{K_n} (C_0 I_n - C_e J_n) f_n(\xi) e^{-(\kappa+1/I_n)\tau}. \quad (2.17)$$

In (2.17),  $\xi = x/L$ ,  $\tau = Ut/L$ , and  $\text{Pe}$  and  $\kappa$  are defined by (1.7). The coefficients  $I_n$ ,  $J_n$  and  $K_n$  are given by (2.16), with  $\lambda_n$  as the positive roots of the transcendental equation (2.13), and the eigenfunctions  $f_n(\xi)$  defined by (2.12). The steady-state concentration  $\varphi(\xi)$  is defined by (2.4), with the coefficients  $a$  and  $b$  given by (2.5). The derived expression (2.17) is equivalent but, because of (2.15) and (2.16), more compact expression for the concentration than other expressions found in the literature, e.g., Van Genuchten and Alves (1982), case C8 with  $\gamma = 0$ ). It can be readily used in the design analysis, for example to determine how fast the outlet concentration reaches a desired level, depending on the values of the parameters of the model. In the absence of reaction,  $J_n \equiv I_n$  and (2.15) reduces to

$$A_n = (C_0 - C_e) \frac{I_n}{K_n}, \quad (2.18)$$

$$\frac{I_n}{K_n} = \frac{32\text{Pe} \lambda_n^2}{(\text{Pe}^2 + 4\lambda_n^2)(\text{Pe}^2 + 4\text{Pe} + 4\lambda_n^2)},$$

in agreement with the case A4 from a rich compendium of solutions by Van Genuchten and Alves (1982).

### Numerical results

It is commonly considered that in the range  $0.1 < \text{Pe} < 10$ , the contributions from advection and diffusion (dispersion) are comparable in magnitude; thus for illustrative purposes the

**Table 1.** Eigenvalues  $\lambda_n$  ( $n \leq 16$ ) for  $Pe = 1$ .

$\lambda_1$	$\lambda_2$	$\lambda_3$	$\lambda_4$	$\lambda_5$	$\lambda_6$	$\lambda_7$	$\lambda_8$
0.9602	3.4310	6.4382	9.5296	12.6454	15.7713	18.9024	22.0365
$\lambda_9$	$\lambda_{10}$	$\lambda_{11}$	$\lambda_{12}$	$\lambda_{13}$	$\lambda_{14}$	$\lambda_{15}$	$\lambda_{16}$
25.1725	28.3097	31.4477	34.5864	37.7256	40.8652	44.0050	47.1451

value  $Pe = 1$  is chosen in this section. The lowest sixteen eigenvalues obtained by numerical solution of (2.13) are listed in Table 1. The approximate value  $\lambda_{15} \approx 14\pi$  is within only 0.05% relative error of the numerically determined eigenvalue  $\lambda_{15} = 44.005$ ; the error rapidly decreases further if the approximation  $\lambda_n \approx (n-1)\pi$  is used for all higher values of  $n$ . Thus, we adopt that  $\lambda_n = (n-1)\pi$  for  $n \geq 15$ .

The variation of the normalized concentration  $C(\xi, \tau)/C_e$  for four selected values of  $\tau$  is depicted in Figure 2a and b. If time increases further, the concentration approaches the steady-state profile specified by (2.4). By comparing the plots in Figure 2a and b, it is clear that the increase of the Damköhler number  $\kappa$  decreases the concentration, as expected because of the more pronounced reactant decay (or the lower advection velocity  $U$ , at fixed  $k$  and  $L$ ). Figure 2c and d show the corresponding time-variation of  $C(\xi, \tau)/C_e$  for four selected values of  $\xi$ . For higher values of  $\kappa$ , the steady-state values of the concentration are approached more rapidly; these values are also lower than the corresponding values for the smaller  $\kappa$ . Numerical evaluation easily proceeds for other choices of the Péclet number and the concentration ratio  $C_0/C_e$ .

To provide an explicit verification of the results plotted in Figure 2 based on the series representation (2.17), we also calculated the normalized concentration  $C(\xi, \tau)/C_e$  for the same values of the parameters as in Figure 2 by using the series representation given as the case C8 (with  $\gamma = 0$ ) of Van Genuchten and Alves (1982), and obtained the same plots. The agreement was further verified analytically, because the latter series representation can be reduced to our representation (2.17) by observing the following relationships between the quantities  $A(\xi, \tau)$ ,  $E(\lambda_n, \xi)$ ,  $B_1(\xi)$ , and  $B_2(\xi, \tau)$  of Van Genuchten and Alves (1982), pages 66–68, and the quantities used in our expression (2.17),

$$A(\xi, \tau) = e^{Pe\xi/2} \sum_{n=1}^{\infty} E(\lambda_n, \xi) e^{-(\kappa+1/I_n)\tau},$$

$$E(\lambda_n, \xi) = \frac{I_n}{K_n} f_n(\xi),$$

$$B_1(\xi) = \frac{1}{C_e} \varphi(\xi),$$

$$B_2(\xi, \tau) = e^{Pe\xi/2} \sum_{n=1}^{\infty} E(\lambda_n, \xi) \frac{J_n}{I_n} e^{-(\kappa+1/I_n)\tau}.$$

### Advection-dispersion-reaction equation with a source term

Having the solution to the advection-dispersion-reaction equation derived, the solution to this equation with the included source/sink term  $\sigma$  in the right-hand side of (1.1) can be deduced immediately. Indeed, if we introduce in (1.4)–(1.6) the concentration  $\hat{C}$  such that  $C = \hat{C} + \sigma/k$  (the sum of the complementary and particular solution), the initial-boundary-value problem for  $\hat{C}$  becomes

$$\frac{\partial \hat{C}}{\partial \tau} = \frac{1}{Pe} \frac{\partial^2 \hat{C}}{\partial \xi^2} - \frac{\partial \hat{C}}{\partial \xi} - \kappa \hat{C}, \quad (3.1)$$

$$\hat{C}(\xi, 0) = C_0 - \frac{\sigma}{k}, \quad (3.2)$$

$$\left( \hat{C} - \frac{1}{Pe} \frac{\partial \hat{C}}{\partial \xi} \right)_{\xi=0} = C_e - \frac{\sigma}{k}, \quad \left( \frac{\partial \hat{C}}{\partial \xi} \right)_{\xi=1} = 0. \quad (3.3)$$

When this is compared with the initial-boundary problem of advection-dispersion-reaction from sections “Introduction” and “Advection-dispersion-reaction equation”, it follows that the solution to (3.1)–(3.3) can be obtained from that solution by making the replacements  $C_e \rightarrow C_e - \sigma/k$  and  $C_0 \rightarrow C_0 - \sigma/k$ . Thus,  $\hat{C}(\xi, \tau) = \hat{\varphi}(\xi) + \exp[(Pe\xi/2) - q\tau]\phi(\xi, \tau)$ , where, from (2.4) and (2.5),

$$\hat{\varphi}(\xi) = (C_e - \sigma/k) [a e^{(1+\alpha)Pe\xi/2} + b e^{(1-\alpha)Pe\xi/2}]. \quad (3.4)$$

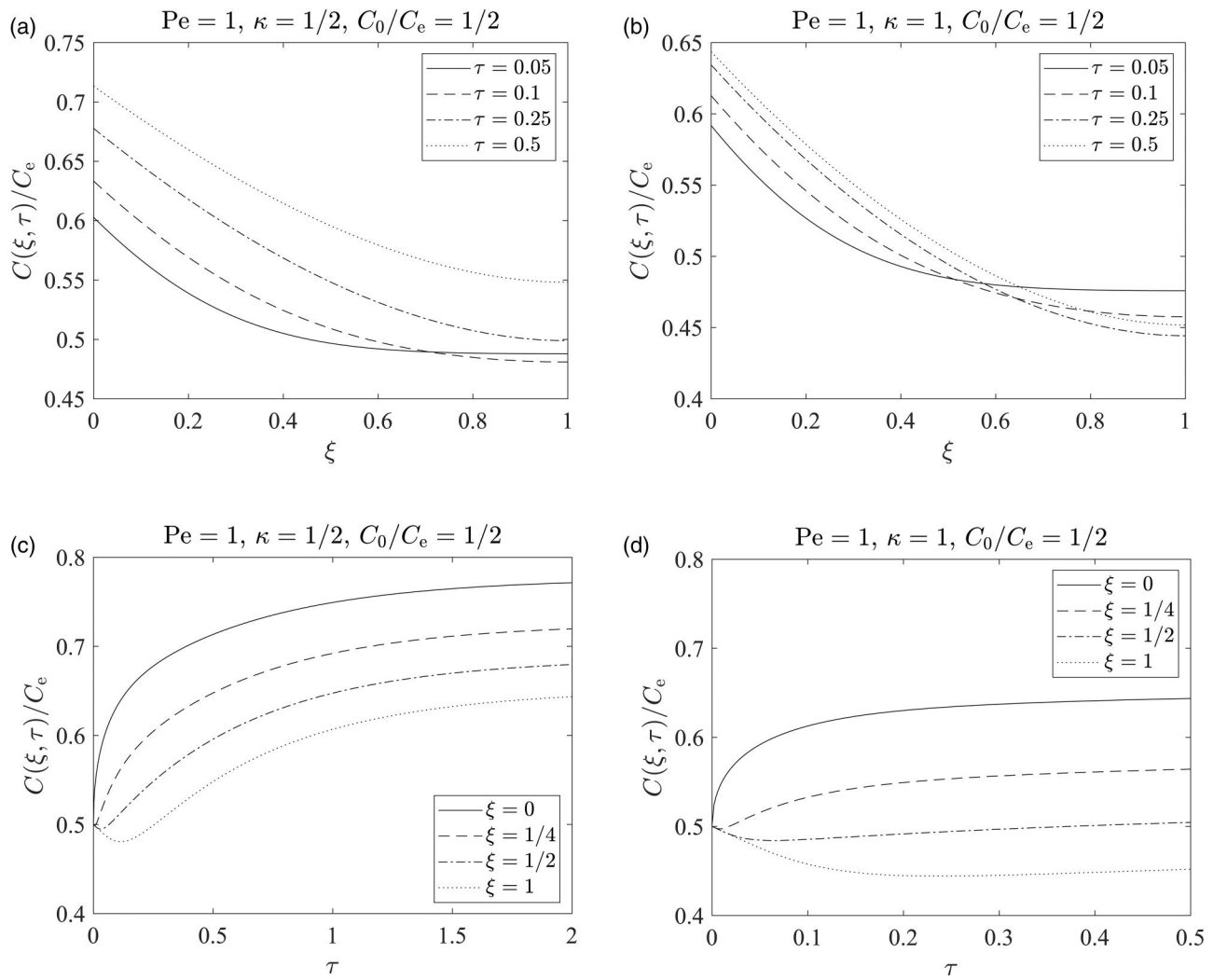
The steady-state concentration is then

$$\varphi(\xi) = \hat{\varphi}(\xi) + \frac{\sigma}{k}. \quad (3.5)$$

The function  $\phi(\xi, \tau)$  appearing in the expression for the transient concentration is given by (2.11), with

$$A_n = \frac{1}{K_n} [(C_0 - \sigma/k)I_n - (C_e - \sigma/k)J_n], \quad (3.6)$$

following directly from (2.15). The integrals  $I_n$ ,  $J_n$  and  $K_n$  are still defined by (2.16). The representation of  $C(\xi, \tau)$  with  $\varphi(\xi)$  and  $A_n$  defined by (3.5)



**Figure 2.** (a) and (b) The variation of the normalized concentration  $C(\xi, \tau)/C_e$  with  $\xi$  for the four shown values of non-dimensional time parameter  $\tau$ . (c) and (d) The variation of the normalized concentration  $C(\xi, \tau)/C_e$  with  $\tau$  for four shown values of  $\xi$ . In parts (a) and (c) the Damköhler number is  $\kappa = 1/2$ , and in parts (b) and (d),  $\kappa = 1$ . The Péclet number in all parts is  $Pe = 1$ , while the ratio  $C_0/C_e = 1/2$ .

and (3.6) is more condensed than other representations given in the literature (e.g., Van Genuchten and Alves (1982), case C8).

In retrospect, one could solve the general advection-dispersion-reaction-growth problem first, for example by expressing the solution from the outset of the analysis as the sum of the complementary and particular solution and by introducing the effective concentrations  $C_0^{\text{eff}} = C_0 - \sigma/k$  and  $C_e^{\text{eff}} = C_e - \sigma/k$ , and then deduce the solution to the advection-dispersion-reaction problem by substituting  $\sigma = 0$  in that solution, but such approach is operationally more involved than the approach presented in sections “Advection-dispersion-reaction equation” and “Advection-dispersion-reaction equation with a source term”.

### Advection-dispersion equation with a source term

The solution to the advection-dispersion equation with a source term, without reaction, can be obtained from the general solution given in section “Advection-dispersion-reaction equation with a source term” in the limit as  $k \rightarrow 0$ , or by deriving the solution from the beginning independently of that solution. In either case, it follows that the steady-state concentration is

$$\varphi(\xi) = C_e + \frac{\sigma L}{U} \left\{ \xi + \frac{1}{Pe} [1 - e^{\text{Pe}(\xi-1)}] \right\}, \quad (4.1)$$

while the coefficients  $A_n$  in the series representation (2.11) of the function  $\phi(\xi, \tau)$  are given by

$$A_n = \frac{I_n}{K_n} \left( C_0 - C_e - \frac{\sigma L}{U} I_n \right). \quad (4.2)$$

The integrals  $I_n$  and  $K_n$  are defined by (2.16), and their ratio is given in (2.18). The overall concentration is

$$C(\xi, \tau) = \varphi(\xi) + e^{\text{Pe}\xi/2} \sum_{n=1}^{\infty} A_n f_n(\xi) e^{-\tau/I_n}, \quad (4.3)$$

which is equivalent to the series representation given by Van Genuchten and Alves (1982), case B8, but cast in a more compact and computationally less complex form. The steady-state exit concentration is  $\varphi(1) = C_e + \sigma L/U$ , as anticipated from the outset of the analysis.

## Conclusion

The series representation of the reactant concentration in one-dimensional advection-dispersion-reaction problems within a domain of finite length is derived in a more compact and computationally less involved form than other representations given in the literature. The initial concentration is assumed to be uniform, while the prescribed boundary conditions are a constant flux at the inlet and a zero concentration gradient at the outlet of the reactor. The solution is conveniently expressed in terms of the introduced constants  $a$  and  $b$  for the steady-state, and  $I_n$ ,  $J_n$  and  $K_n$  for the transient concentration. A generalization of the solution to the advection-dispersion-reaction equation to include a uniform source/sink term is then presented, followed by a simple form of the solution to the advection-dispersion equation with a source term, without reaction. In all three considered cases, the same eigenfunctions  $f_n$  and the same condition for the eigenvalues  $\lambda_n$  apply, which are given by (2.12) and (2.13), for any values of the first-order reaction rate constant  $k > 0$  and the zero-order production rate  $\sigma$ . The reactant concentration in each case is found to be

$$C(\xi, \tau) = \varphi(\xi) + e^{(\text{Pe}\xi/2) - \kappa\tau} \sum_{n=1}^{\infty} A_n f_n(\xi) e^{-\tau/I_n},$$

$$I_n = \frac{4\text{Pe}}{\text{Pe}^2 + 4\lambda_n^2}, \quad (5.1)$$

where the steady-state concentration  $\varphi(\xi)$  and the coefficients  $A_n$  are defined by (2.4) and (2.15) in the case ( $k \neq 0$ ,  $\sigma = 0$ ), (3.5) and (3.6) in the case ( $k \neq 0$ ,  $\sigma \neq 0$ ), and (4.1) and (4.2) in the case ( $k = 0$ ,  $\sigma \neq 0$ ). The corresponding spatial concentration gradient is given by

$$\frac{\partial C}{\partial \xi} = \frac{d\varphi}{d\xi} + \text{Pe} e^{(\text{Pe}\xi/2) - \kappa\tau} \sum_{n=1}^{\infty} A_n \frac{\sin[\lambda_n(1 - \xi)]}{\sin \lambda_n} e^{-\tau/I_n}. \quad (5.2)$$

## Acknowledgements

We thank the anonymous reviewers for their helpful comments and suggestions. Discussions with Professors Justin Opatkiewicz and Aaron Drews related to boundary conditions for chemical reactors are also gratefully acknowledged.

## Disclosure statement

The authors report there are no competing interests to declare.

## References

- Abbasi M, Madani M, Sharifi M, Kazemi A. 2021. Analytical solutions of advection-dispersion-reaction equation with first decay under constant and time-dependent boundary conditions: mass transfer shape factor effects. *Groundw Sustain Dev.* 15:100691. doi:10.1016/j.gsd.2021.100691.
- Ahmed M, Zainab QUA, Qamar S. 2017. Analysis of one-dimensional advection-diffusion model with variable coefficients describing solute transport in a porous medium. *Transp Porous Med.* 118(3):327–344. doi:10.1007/s11242-017-0833-0.
- Brenner H. 1962. The diffusion model of longitudinal mixing in beds of finite length. *Numerical Values. Chem Eng Sci.* 17(4):229–243. doi:10.1016/0009-2509(96)81824-0.
- Catchpole JP, Fulford G. 1966. Dimensionless groups. *Ind Eng Chem.* 58(3):46–60. doi:10.1021/ie50675a012.
- Carberry JJ. 1976. *Chemical and catalytic reaction engineering.* New York (NY): McGraw-Hill.
- Chen J-S, Li LY, Lai K-H, Liang C-P. 2017. Analytical model for advective-dispersive transport involving flexible boundary inputs, initial distributions and zero-order productions. *J Hydrol.* 554:187–199. doi:10.1016/j.jhydrol.2017.08.050.
- Chen J-S, Liu C-W. 2011. Generalized analytical solution for advection-dispersion equation in finite spatial domain with arbitrary time-dependent inlet boundary condition. *Hydrol Earth Syst Sci.* 15(8):2471–2479. doi:10.5194/hess-15-2471-2011.

- Conesa JA. 2020. Chemical reactor design: Mathematical modeling and applications. Weinheim (Germany): Wiley-VCH.
- Danckwerts PV. 1953. Continuous flow systems: distribution of residence times. *Chem Eng Sci.* 2(1):1–13. doi:10.1016/0009-2509(96)81811-2.
- Deen WM. 2012. Analysis of transport phenomena, 2nd ed. New York: oxford Univ Press.
- Delgado JMPQ. 2006. A critical review of dispersion in packed beds. *Heat Mass Transfer.* 42(4):279–310. doi:10.1007/s00231-005-0019-0.
- Fogler HS. 2005. Elements of chemical reaction engineering. Upper Saddle River (NJ): prentice Hall.
- Grindrod P. 1996. The theory and applications of reaction-diffusion equations. Oxford (UK): Oxford Univ Press.
- Hundsdoerfer W, Verwer JG. 2003. Numerical solution of time-dependent advection-diffusion-reaction equations. Berlin (Germany): Springer.
- Kumar A, Jaiswal DK, Kumar N. 2009. Analytical solutions of one-dimensional advection-diffusion equation with variable coefficients in a finite domain. *J Earth Syst Sci.* 118(5):539–549. doi:10.1007/s12040-009-0049-y.
- Kumar R, Chatterjee A, Singh MK, Tsai FT. 2022. Advances in analytical solutions for time-dependent solute transport model. *J Earth Syst Sci.* 131(2):131. doi:10.1007/s12040-022-01858-5.
- Langmuir I. 1908. The velocity of reactions in gases moving through heated vessels and the effect of convection and diffusion. *J Am Chem Soc.* 30(11):1742–1754. doi:10.1021/ja01953a011.
- Lubarda MV, Lubarda VA. 2023. On the proofs of orthogonality of eigenfunctions for heat conduction, wave propagation, and advection-diffusion problems. *Int J Math Educ Sci Technol.* 1–12 (in press). doi:10.1080/0020739X.2023.2184283.
- Masters GM, Ela WP. 2008. Introduction to environmental engineering and science. Upper Saddle River (NJ): Pearson Education, Prentice-Hall.
- McGinty S. 2014. A decade of modelling drug release from arterial stents. *Math Biosci.* 257:80–90. doi:10.1016/j.mbs.2014.06.016.
- Mohd Mahali S, Wang S, Lou X. 2014. Estimation of effective diffusion coefficients of drug delivery devices in a flow-through system. *J Eng Math.* 87:139–152. doi:10.1007/s10665-013-9669-y.
- Mott HV, Green ZA. 2015. Danckwerts' boundary conditions for the plug-flow with dispersion/reaction model. *Chem Eng Commun.* 202(6):739–745. doi:10.1080/00986445.2013.871708.
- Parhizi M, Kilaz G, Ostanek JK, Jain A. 2022. Analytical solution of the convection-diffusion-reaction-source (CDRS) equation using Green's function technique. *Int Comm Heat Mass Transf.* 131:105869. doi:10.1016/j.icheatmasstransfer.2021.105869.
- Pérez Guerrero JS, Pimentel LCG, Skaggs TH, van Genuchten MT. 2009. Analytical solution of the advection-diffusion transport equation using a change-of-variable and integral transform technique. *Int J Heat Mass Transf.* 52(13–14):3297–3304. doi:10.1016/j.ijheatmasstransfer.2009.02.002.
- Pérez Guerrero JS, Pontedeiro EM, van Genuchten MT, Skaggs TH. 2013. Analytical solutions of the one-dimensional advection-dispersion solute transport equation subject to time-dependent boundary conditions. *Chem Eng J.* 221:487–491. doi:10.1016/j.cej.2013.01.095.
- Pérez Guerrero JS, Skaggs TH. 2010. Analytical solution for one-dimensional advection-dispersion transport equation with distance-dependent coefficients. *J Hydrol.* 390(1-2): 57–65. doi:10.1016/j.jhydrol.2010.06.030.
- Salmi T, Romanainen JJ. 1995. A novel exit boundary condition for the axial dispersion model. *Chem Eng Process.* 34(4):359–366. doi:10.1016/0255-2701(94)00531-1.
- Schnoor JL. 1996. Environmental modeling - fate and transport of pollutants in water, air, and soil. New York (NY): Wiley-Interscience.
- Sridharan VK, Hein AM. 2019. Analytical solution of advection-dispersion boundary value processes in environmental flows. *Water Resour Res.* 55(12):10130–10143. doi:10.1029/2019WR025429.
- Van Genuchten M, Alves WJ. 1982. Analytical solutions of one-dimensional convective-dispersive solute transport equations. Technical Bull 1661. Washington (DC): US Department of Agriculture. p. 1–149. doi:10.22004/ag.econ.157268
- Wehner JF, Wilhelm RH. 1956. Boundary conditions of flow reactor. *Chem Eng Sci.* 6(2):89–93. doi:10.1016/0009-2509(96)81814-8.
- Ziskind G, Shmueli H, Gitis V. 2011. An analytical solution of the convection-dispersion-reaction equation for a finite region with a pulse boundary condition. *Chem Eng J.* 167(1):403–408. doi:10.1016/j.cej.2010.11.047.

## Appendix: Utilized integrals

The integrals used in the derivation of the expressions for the coefficients  $A_n$  in sections “Advection-dispersion-reaction equation”, “Advection-dispersion-reaction equation with a source term”, and “Advection-dispersion equation with a source term” are

$$\int_0^1 e^{-\text{Pe}\xi/2} f_n(\xi) d\xi = \frac{4\text{Pe}}{\text{Pe}^2 + 4\lambda_n^2} = I_n,$$

$$\int_0^1 e^{\text{Pe}\xi/2} f_n(\xi) d\xi = \frac{\sin \lambda_n}{\lambda_n} e^{\text{Pe}/2} = L_n,$$

$$\int_0^1 \xi e^{-\text{Pe}\xi/2} f_n(\xi) d\xi = I_n^2 + \frac{1}{\text{Pe}} \left( \frac{\sin \lambda_n}{\lambda_n} e^{-\text{Pe}/2} - I_n \right),$$

$$\int_0^1 f_n^2(\xi) d\xi = \frac{1}{2} \left[ 1 + \frac{\text{Pe}(4 + \text{Pe})}{4\lambda_n^2} \right] = K_n,$$

where  $f_n(x)$  and  $\lambda_n$  are defined by (2.12) and (2.13). We note that  $\sin^2 \lambda_n = I_n^2 \lambda_n^2$ , thus  $f_n^2(1) = 1$ . The condensed form of the expression for  $J_n$  in (2.16) is obtained from  $J_n = aL_n + bI_n$ , where  $a$  and  $b$  are defined by (2.5).