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An analytical method to solve a general class of nonlinear reactive transport models

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ABSTRACT

Three recent papers published in *Chemical Engineering Journal* studied the solution of a model of diffusion and nonlinear reaction using three different methods. Two of these studies obtained series solutions using specialized mathematical methods, known as the Adomian decomposition method and the homotopy analysis method. Subsequently it was shown that the solution of the same particular model could be written in terms of a transcendental function called Gauss' hypergeometric function. These three previous approaches focused on one particular reactive transport model. This particular model ignored advective transport and considered one specific reaction term, $R(C) = \phi^2 C^n$, only. Here we generalize these previous approaches and develop an exact analytical solution for a general class of steady state reactive transport models that incorporate (i) combined advective and diffusive transport and (ii) any sufficiently differentiable reaction term $R(C)$. The new solution is a convergent Maclaurin series. The Maclaurin series solution can be derived without any specialized mathematical methods nor does it necessarily involve the computation of any transcendental function. Applying the Maclaurin series solution to certain case studies shows that the previously published solutions are particular cases of the more general solution outlined here. We also demonstrate the accuracy of the Maclaurin series solution by comparing with numerical solutions for particular cases.

1. Introduction and background

We study the solution of a one-dimensional steady state reactive transport model. The governing differential equation and boundary conditions can be written in dimensional variables as

$$0 = DC'' - VC' - r(C), \quad 0 \le x \le L, \quad C'(0) = 0, \quad C(L) = C_s, \tag{1}$$

where D is the diffusivity, V is the advective velocity, $r(C)$ represents a reaction process and the prime notation represents a derivative with respect to x. This model encodes a number of important engineering processes including several applications in chemical engineering [5,10] and environmental engineering [9,28].

Without loss of generality, we simplify the governing equation by introducing nondimensional quantities $C^* = C/C_s$ and $x^* = x/L$. Substituting these nondimensional quantities into Eq. (1) and introducing a general nondimensional reaction term $R(C^*)$, we omit the asterisk notation and obtain a simplified nondimensional model and boundary conditions that can be written as

$$0 = C'' - PC' - R(C), \quad 0 \le x \le 1, \quad C'(0) = 0, \quad C(1) = 1. \tag{2}$$

The ratio of the timescale of advection to the timescale of diffusion is given by the Péclet number, $P = (VL)/D$. Without advective transport ($P = 0$), Eq. (2) is a model of diffusion and reaction that has been used to study porous catalyst pellets [19]. By including advective transport we have generalized the model so it is now applicable to other problems including tubular reactors and packed-bed reactors [6,22].

Our aim is to construct an analytical solution of Eq. (2). It is instructive at first to discuss some of the options available for obtaining analytical or approximate analytical solutions of nonlinear differential equations. Perturbation techniques are well-known methods to construct approximate analytical solutions of nonlinear problems and require the presence of a small parameter, usually denoted ϵ [7]. The approximate perturbation solution is constructed by expanding in a series involving powers of ϵ. The coefficients in the power series are solved recursively, and the approximation is improved by incorporating more terms in the power series. In many practical applications, the perturbation solution can be remarkably accurate even for a modestly sized small parameter ϵ [14]. The fact that many problems do not contain any obvious choice of a small parameter has been the motivation for alternative approaches, often called non-perturbation methods. Examples of non-perturbation methods are the Adomian decomposition method [2], the Homotopy analysis method [11], the exponential-function method [25], integral equations [22]

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and Green's functions [3,23]. Other approaches related to Taylor series expansions have also been used [13,15,20,21]. These non-perturbation methods have been applied to solve both linear and nonlinear differential equations with a wide range of applications including models of chemical and biological processes.

The focus of this work is to construct a solution of Eq. (2) and demonstrate how certain previous studies are special cases of a more general solution outlined here. Our approach does not require any specialized solution techniques [1,2,11,18] nor does it necessarily involve evaluating transcendental functions [12]. We derive an exact analytical solution that, unlike previous studies [1,12,18], is valid for a general class of reactive transport problems with an arbitrary reaction term $R(C)$ and any value of the Péclet number P. Specific examples will be used to demonstrate the accuracy of the Maclaurin series solution. We conclude with a discussion about generalizations of the solution technique developed here and also discuss certain situations where it does not apply.

2. General solution

We assume that the solution of Eq. (2), $C(x)$, can be expanded in a Maclaurin series

$$C(x)=\sum_{k=0}^{\infty}\frac{C^{(k)}(0)x^k}{k!}=C(0)+C'(0)x+\frac{C''(0)x^2}{2!}+\frac{C'''(0)x^3}{3!}+\cdots \quad (3)$$

To determine the values of the derivatives at $x=0$ we rewrite Eq. (2) as $C''=PC'+R(C)$. Assuming that $R(C)$ is sufficiently differentiable we may then evaluate derivatives of $C(x)$ recursively giving

$$\begin{aligned}
C''(x) &= PC'(x)+R(C)\\
C'''(x) &= PC''(x)+R'(C)C'(x)\\
C^{iv}(x) &= PC'''(x)+R''(C)C'(x)^2+R'(C)C''(x)\\
C^{v}(x) &= PC^{iv}(x)+R'''(C)C'(x)^3+3R''(C)C'(x)C''(x)+R'(C)C'''(x)\\
&\vdots
\end{aligned} \quad (4)$$

where $R'(C)=dR(C)/dC$, $R''(C)=d^2R(C)/dC^2$, $R'''(C)=d^3R(C)/dC^3$, ...

We now evaluate $C''(0)$, $C'''(0)$, $C^{iv}(0)$, $C^{v}(0)$, ... by substituting $x=0$ into Eq. (4). Furthermore, we can impose the boundary condition $C'(0)=0$ to give

$$\begin{aligned}
C'(0) &= 0\\
C''(0) &= R(C_0)\\
C'''(0) &= PC''(0)\\
C^{iv}(0) &= PC'''(0)+R'(C_0)C''(0)\\
C^{v}(0) &= PC^{iv}(0)+R'(C_0)C'''(0)\\
&\vdots
\end{aligned} \quad (5)$$

where C_0 is the unknown value $C(0)$. These terms allow us to express the Maclaurin series solution (Eq. (3)) as

$$C(x)=\sum_{k=0}^{\infty}\frac{C^{(k)}(0)x^k}{k!}=C_0+\frac{R(C_0)x^2}{2!}+\frac{PR(C_0)x^3}{3!}+\frac{(P^2R(C_0)+R'(C_0)R(C_0))x^4}{4!}+\frac{PR(C_0)(P^2+2R'(C_0))x^5}{5!}+\cdots \quad (6)$$

The kth term in the Maclaurin series is

$$\frac{x^k}{k!}\left(\frac{\partial^{k-2}}{\partial x^{k-2}}\left[PC'(x)+R(C)\right]\right)\Big|_{x=0}, \qquad k\geq 2. \quad (7)$$

Applying the ratio test to this series shows that it is convergent provided the derivatives of $R(C)$ are bounded. This condition will be met for all standard reaction terms $R(C)$ (e.g. polynomial functions and rational functions such the Michaelis–Menten model [6,28]). Therefore the Maclaurin series is an exact solution that always converges under the assumptions stated here. Since the Maclaurin series is convergent it can be evaluated by truncating after a finite number of terms. We will now compare the solution approach outlined here with previous approaches.

3. Particular cases

3.1. Case 1: $P=0$, $R(C)=\phi^2C$

This case involves diffusive transport with a linear reaction term. The reaction rate is proportional to C, with the constant of proportionality being ϕ^2. In the context of reactive transport in porous catalyst pellets [19], the parameter ϕ is called the Thiele modulus [12]. Under these conditions the Maclaurin series solution becomes

$$C(x)=C_0\sum_{k=0}^{\infty}\frac{(\phi x)^{2k}}{(2k)!}. \quad (8)$$

This particular Maclaurin series corresponds to $C(x)=C_0\cosh(\phi x)$ [4] which is an exact closed-form solution for this particular case [12]. Applying the boundary condition, $C(1)=1$, gives $C_0=1/\cosh(\phi)$.

3.2. Case 2: $P=0$, $R(C)=\phi^2C^n$

This case involves diffusive transport with nth order reaction. The reaction term encodes either linear ($n=1$) or nonlinear ($n\neq 1$) reaction processes. Under these conditions the series solution, truncated after the x^{10} term, is given by

$$\begin{aligned}
C(x)=C_0&+\frac{C_0^n(\phi x)^2}{2!}+\frac{C_0^{2n-1}n(\phi x)^4}{4!}+\frac{C_0^{3n-2}n(4n-3)(\phi x)^6}{6!}\\
&+\frac{C_0^{4n-3}n(34n^2-63n+30)(\phi x)^8}{8!}\\
&+\frac{C_0^{5n-4}n(496n^3-1554n^2+1689n-630)(\phi x)^{10}}{10!}.
\end{aligned} \quad (9)$$

We remark that this series solution exactly coincides with the series solution obtained by Sun et al. [18] and Abbasbandy [1] (Note that the series reported by Sun et al. [18] contained typographical errors that were identified by Magyari [12].). These previous studies determined this series solution using the Adomian decomposition method [18] and the homotopy analysis method [1]. The solution technique presented here is simpler than those adopted in these two previous studies since our approach does not rely on either of these specialized methods of analysis. Our approach also gives new insight into the series solution as we have obtained the general form of the series and demonstrated that the series is convergent provided that the derivatives of $R(C)$ are bounded. Neither of the previous studies by Sun et al. [18] or Abbasbandy [1] were able to prove that the series was convergent. Here the ratio test confirms that the series always converges and we do not need to choose any auxiliary parameters to control convergence [1].

To evaluate the Maclaurin series solution (Eq. (9)) we must determine $C(0)=C_0$. Before doing this, it is instructive to consider some properties of the solution of the general reactive transport problem given by Eq. (2). With $R(C)>0$, we can show that the solution of Eq. (2) gives $0<C_0<1$. This property is implied by the fact that Eq. (2) satisfies the maximum principle [16] meaning that the maximum value of the solution, $C(x)$, must occur at either $x=0$ or $x=1$. Since $C'(0)=0$, we know that $x=0$ is a stationary point. Furthermore, we know that $C''(0)=R(C_0)$. Therefore, for all cases with $R(C)>0$ (such as $R(C)=\phi C^n$), the minimum of the solution is $C(0)=C_0$ and the maximum of the solution is $C(1)=1$. This gives the result that $0<C_0<1$. To determine the value of C_0 we apply the boundary condition $C(1) = 1$ to Eq. (9) and obtain

$$1 = C_0 + \frac{C_0^n\phi^2}{2!} + \frac{C_0^{2n-1}n\phi^4}{4!} + \frac{C_0^{3n-2}n(4n-3)\phi^6}{6!} + \frac{C_0^{4n-3}n(34n^2-63n+30)\phi^8}{8!} + \frac{C_0^{5n-4}n(496n^3-1554n^2+1689n-630)\phi^{10}}{10!}. \quad (10)$$

This algebraic equation can be solved to find C_0 using any standard root finding technique [8]. This approach will give an approximate value of C_0 because we are dealing with a truncated series. The accuracy of this approximation can be increased to any arbitrary level simply by retaining additional terms in the truncated series [18].

3.3. Case 3: $P \neq 0$, $R(C) = \phi^2 C^n$

This case involves advective and diffusive transport with an nth order reaction term. This particular case highlights the general nature of our solution approach compared to that of Magyari [12] who was able to directly integrate the governing equation for the special case that $P = 0$ and $R(C) = \phi^2 C^n$. This direct integration approach, however, does not apply for the more general case where $P \neq 0$. Instead, we use this case to demonstrate that these generalizations are easily and accurately handed by the Maclaurin series solution. For this case, the Maclaurin series solution, truncated after the x^{10} term, is given by

$$\begin{aligned}C(x) = {} & C_0 + \frac{C_0^n\phi^2x^2}{2!} + \frac{PC_0^n\phi^2x^3}{3!} + \frac{[P^2\phi^2C_0^n + \phi^4nC_0^{2n-1}]x^4}{4!} + \frac{P\phi^2[P^2C_0^n + 2\phi^2nC_0^{2n-1}]x^5}{5!} \\ & + \frac{\phi^2[P^4C_0^n + 3P^2\phi^2nC_0^{2n-1} + \phi^4C_0^{3n-2}n(4n-3)]x^6}{6!} + \frac{P\phi^2[P^4C_0^n + 4P^2\phi^2nC_0^{2n-1} + \phi^4C_0^{3n-2}n(16n-13)]x^7}{7!} \\ & + \frac{\phi^2[P^6C_0^n + 5P^4\phi^2nC_0^{2n-1} + P^2\phi^4C_0^{3n-2}n(44n-38) + \phi^6C_0^{4n-3}n(34n^2-63n+30)]x^8}{8!} \\ & + \frac{P\phi^2[P^6C_0^n + 6P^4\phi^2nC_0^{2n-1} + P^2\phi^4C_0^{3n-2}n(104n-94) + \phi^6C_0^{4n-3}n(232n^2-468n+240)]x^9}{9!} \\ & + \frac{\phi^2[P^8C_0^n + 7P^6\phi^2nC_0^{2n-1} + P^4\phi^4C_0^{3n-2}n(228n-213) + P^2\phi^6C_0^{4n-3}n(1032n^2-2242n+1120) + \phi^8C_0^{5n-4}n(496n^3-1554n^2+1689n-630)]x^{10}}{10!}.\end{aligned} \quad (11)$$

3.4. Case 4: $P \neq 0$, $R(C) = AC/(B + C)$

This case involves advective and diffusive transport with the Michaelis–Menten reaction model that is routinely used to represent biochemical processes [6,9,28]. Here the half saturation concentration is given by B, and the characteristic reaction rate is given by A. For this case the terms in the Maclaurin series solution are more complicated than the previous terms for the power-law reaction term. Therefore we report the series truncated after the x^6 term, which is given by

$$\begin{aligned}C(x) = {} & C_0 + \frac{AC_0x^2}{2!(B+C_0)} + \frac{PAC_0x^3}{3!(B+C_0)} + \frac{AC_0(P^2B^2 + 2P^2BC_0 + P^2C_0^2 + AB)x^4}{4!(B+C_0)^3} + \frac{PAC_0(P^2B^2 + 2P^2BC_0 + P^2C_0^2 + 2AB)x^5}{5!(B+C_0)^3} \\ & + \frac{AC_0(P^4B^4 + 4P^4B^3C_0 + 6P^4B^2C_0^2 + 4P^4BC_0^3 + P^4C_0^4 + 3P^2AB^3 + 6P^2AB^2C_0 + 3P^2ABC_0^2 - 6A^2BC_0 + A^2B^2)x^6}{6!(B+C_0)^5}.\end{aligned} \quad (12)$$

4. Comparing series solutions and numerical solutions

To demonstrate the accuracy of the Maclaurin series solution, we generate numerical solutions of Eq. (2) and compare these with the Maclaurin series solutions. Spatial derivatives in Eq. (2) are replaced with a standard centered in space finite difference approximation on a uniform grid with spacing δx [8]. This gives a tridiagonal system of nonlinear algebraic equations. The nonlinear algebraic system is linearised using a Picard iteration technique [28]. The tridiagonal system of linear equations are solved using the Thomas algorithm [8] and iterations are performed until the maximum change in the value of the dependent variable across the grid falls below some small tolerance ϵ_1. For all results presented here we use a fine grid and a strict convergence tolerance by setting $\delta x = 1 \times 10^{-5}$ and $\epsilon_1 = 1 \times 10^{-8}$. We also generated results using a finer grid and an even stricter convergence tolerance which, for all problems considered in this work, gave results that were visually indistinguishable from the numerical results on the original fine grid. This grid-refinement procedure ensured that our numerical results are grid independent. To generate the corresponding Maclaurin series solutions we truncated all series after the x^{10} term and found the value of C_0 using the bisection algorithm with absolute convergence tolerance $\epsilon_2 = 1 \times 10^{-8}$ [8].

We compare a range of truncated Maclaurin series solutions for two common reaction models: (i) a power law reaction model given by $R(C) = \phi^2 C^n$ and (ii) the Michaelis–Menten biochemical reaction model $R(C) = AC/(B + C)$. Results in Fig. 1 give a wide range of solution profiles for various values of P, n, A and B, as indicated. We observe that, in all cases, the Maclaurin series solutions are indistinguishable from the grid-independent numerical solutions.

5. Convergence behaviour

Although we have evaluated the Maclaurin series solution by truncating after the x^{10} term (Fig. 1), it is possible to use other levels of truncation. Intuitively we expect that gradually varying solutions will be accurately predicted using a coarse truncation, while rapidly varying solution profiles will require more terms to obtain a sufficiently accurate result. For the results shown in Fig. 1, we simply chose to represent the Maclaurin series solutions using a uniformly truncated series that are truncated after the x^{10} term. To provide further insight into the convergence behaviour of the series

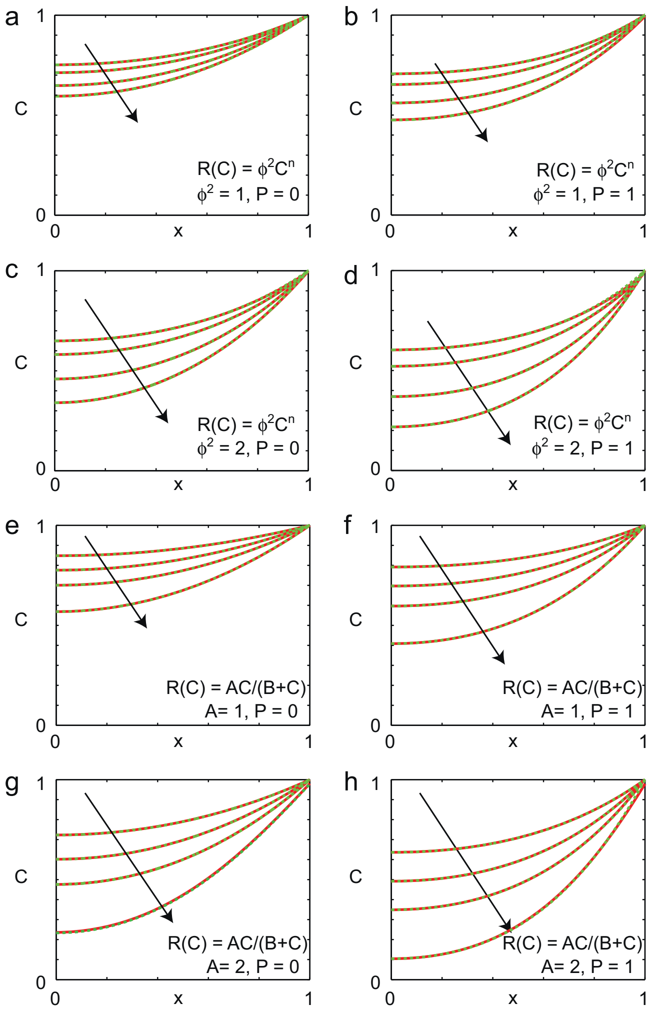

Fig. 1. Comparison of the Maclaurin series solution (solid red) and the fine-mesh numerical solution (dotted green) of Eq. (2) for $R(C) = \phi^2 C^n$ and $R(C) = AC/(B + C)$. Results in (a)–(d) are given for $R(C) = \phi^2 C^n$ with $P = 0$, 1 and $\phi^2 = 1$, 2. Each subfigure (a)–(d) contains four different solutions corresponding to different powers, $n = 0.50$, 1.00, 2.00, 3.00, with the direction of decreasing n indicated by the arrow. Results in (e)–(h) are given for $R(C) = AC/(B + C)$ with $P = 0$, 1 and $A = 1$, 2. Each subfigure (e)–(h) contains four different solutions corresponding to different half saturation values, $B = 0.10$, 0.50, 1.00, 2.00, with the direction of decreasing B indicated by the arrow. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of the article.)

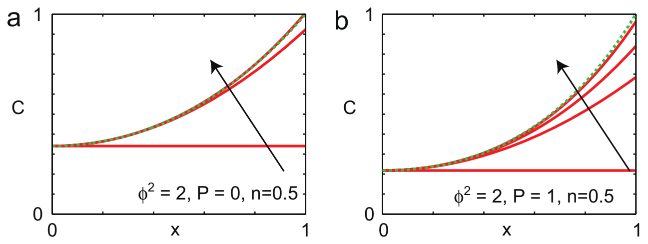

Fig. 2. Convergence behaviour of various truncated Maclaurin series solutions (solid red) and the fine-mesh numerical solution (dotted green) of Eq. (2) for $R(C) = \phi^2 C^n$. Profiles in (a) correspond to $P = 0$ and we note that the coefficients of odd powers of x in the Maclaurin series are identically zero and we plot the series solution truncated after one (constant), two (quadratic) and four (quartic) terms which show rapid convergence to the fine-mesh numerical solution. Profiles in (b) correspond to $P = 1$ and we plot the series solution truncated after one (constant), two (quadratic), three (cubic) and four (quartic) terms which also shows rapid convergence to the fine-mesh numerical solution. The arrow shows the direction of increasing truncation level. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of the article.)

we present further results in Fig. 2 illustrating rapid convergence of the series. Solution profiles in Fig. 2 show the effect of truncating the series after the first, second, third and fourth terms for two representative problems selected from Fig. 1. In both cases we observe that the truncated series retaining only the quartic term (truncated after the x^4 term) becomes indistinguishable from the numerical solution. This rapid convergence explains why retaining terms up to the x^{10} term for the results in Fig. 1 always gave very accurate results.

The rapid convergence behaviour illustrated in Fig. 2 is expected since we have proved that the Maclaurin series is always convergent using the ratio test. Although the ratio test proves that the series is convergent, it does not provide any indication about how many terms ought to be retained in the truncated series to obtain sufficiently accurate results [4,17]. It is, however, straightforward to determine how many terms are required for any particular application by systematically solving each problem iteratively and retaining an additional term in the series at each iteration. This iterative process will show how the truncated series solution converges to the desired result. This iterative process is particularly straightforward to implement if the truncated series are evaluated using a symbolic software package (e.g. Maple or Mathematica).

6. Alternative boundary conditions and limitations

As we mentioned in Section 1, the choice of boundary conditions, $C'(0) = 0$ and $C(1) = 1$, was made so that the new solution developed here applies to the previous problems considered by Abbasbandy [1], Magyari [12] and Sun et al. [18]. We will now show that the Maclaurin series can also be applied to problems with different boundary conditions.

Instead of imposing a Dirichlet boundary condition $C(1) = 1$, it might be more appropriate to apply a Robin-type boundary condition to represent a known flux, $J(x)$, at $x = 1$. To achieve this we recall that the flux associated with the governing nondimensional equation (Eq. (2)) can be written as,

$$J(x) = -C'(x) + PC(x) \tag{13}$$

To impose a Robin-type boundary condition at $x = 1$, assume that we have already generated the solution described previously in Section 2 for $C'(0) = 0$. We then express the Robin-type boundary condition (Eq. (13)) in terms of the Maclaurin series solution

$$J(x) = -\sum_{k=1}^{\infty} \frac{C^{(k)}(0)x^{k-1}}{(k-1)!} + P\sum_{k=0}^{\infty} \frac{C^{(k)}(0)x^k}{k!}. \tag{14}$$

To impose a known flux, $J(1)$, we substitute $x = 1$ and the specified value of $J(1)$ into Eq. (14). The resulting expression is truncated at some desired level to give an algebraic relationship between the imposed flux, $J(1)$, and the unknown value of $C(0) = C_0$. The solution of this algebraic relationship gives us the value of C_0.

To demonstrate the application of the Robin-type boundary condition we solve Eq. (2) with $R(C) = \phi^2 C^n$, and apply the boundary conditions $C'(0) = 0$ with a specified value of $J(1)$ and show the solution profiles in Fig. 3. The solution profiles in Fig. 3 were obtained by truncating the series solution after the x^{10} term, and we observe that the series solutions are indistinguishable from the fine-mesh numerical solutions in all cases. We note that changing the boundary condition at $x = 1$ means that the solution no longer satisfies $C(1) = 1$. We observe that larger values of the inward flux J lead to profiles with larger values of $C(1)$ which is intuitively reasonable.

Considering the application of alternative boundary conditions allows us to make some general concluding remarks about further applications of the series solution. As a starting point we assumed that the solution of Eq. (2) could be expanded in a Maclaurin series

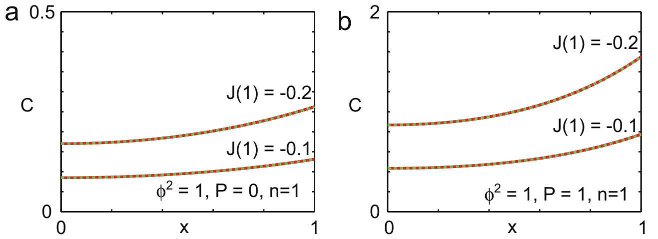

Fig. 3. Comparing Maclaurin series solutions (solid red) and the fine-mesh numerical solution (dotted green) of Eq. (2) with $C'(0)=0$ and $J=-C'(1)+PC(1)$ for $R(C)=\phi^2C^n$. Profiles in (a) and (b) correspond to $P=0$ and $P=1$, respectively. In both cases solutions are given for $J(1)=-0.1$ and $J(1)=-0.2$ as indicated. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of the article.)

about $x=0$. Provided that there is some flux-type boundary condition imposed at $x=0$ (either a Robin or a Neumann condition), we can always use this boundary condition together with the governing differential equation to recursively construct all the terms in the Maclaurin series solution. It is also straightforward to develop a similar series solution by considering a flux-type boundary condition imposed at the other boundary $x=1$. In this case, we can assume that the solution could be written as a power series about the point $x=1$ and use the flux-type boundary condition at $x=1$, together with the governing differential equation, to recursively evaluate all the terms in the power series solution. We note, however, that if a power series solution is developed about the point $x=1$ instead of the point $x=0$, then the solution will be a Taylor series rather than a Maclaurin series [4]. The key element of the series solution strategy is the application of a flux-type boundary condition and the limitations of this approach become clear if we consider problems without any flux-type boundary condition. For example, if we consider solving Eq. (2) with two Dirichlet boundary conditions, $C(0)=C_a$ and $C(1)=C_b$, then the series solution does not apply. This is because these boundary conditions give us no expression for the first derivative of the solution $C'(0)$ (for a Maclaurin series solution) or $C'(1)$ (for a Taylor series solution).

By extending these arguments we can show that the series solution technique does not apply to the transient analogue of Eq. (2) given by

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2} - P\frac{\partial C}{\partial x} - R(C). \tag{15}$$

To develop a series solution of Eq. (15) we could begin by expanding the solution in a series about the point $(x, t)=(x_0, t_0)$

$$\begin{aligned} C(x,t) &= C(x_0,t_0) + (x-x_0)\left.\frac{\partial C}{\partial x}\right|_{x=x_0,t=t_0} + (t-t_0)\left.\frac{\partial C}{\partial t}\right|_{x=x_0,t=t_0} \\ &\quad + \frac{1}{2!}\left[(x-x_0)^2\left.\frac{\partial^2 C}{\partial x^2}\right|_{x=x_0,t=t_0} + (t-t_0)^2\left.\frac{\partial^2 C}{\partial t^2}\right|_{x=x_0,t=t_0}\right. \\ &\quad \left. + 2(x-x_0)(t-t_0)\left.\frac{\partial^2 C}{\partial t \partial x}\right|_{x=x_0,t=t_0}\right] + \cdots \end{aligned} \tag{16}$$

To use this series we must obtain expressions for all of the derivative terms that appear in the series. We note that standard boundary and initial conditions applied to Eq. (15) give insufficient information to evaluate the required derivative expressions. Similar considerations also restrict the application of the series solution technique to particular cases of multidimensional or multispecies reactive transport problems. The applicability of the series solution technique always depends on whether the boundary conditions can be combined with the governing equation to evaluate the necessary coefficients in the series solutions. Just like the one-dimensional model of steady reactive transport considered here (Eq. (2)), the series solution approach will be valid for certain generalizations and invalid for others. The application of the approach can be assessed on a case-by-case basis. These limitations do not lessen the significance of the one-dimensional solutions presented here as these solutions give us new insight into a general class of reactive transport problems where other solution approaches do not apply.

7. Conclusion

We have derived a simple analytical solution of a general model of reactive transport with many applications in chemical and environmental engineering. Our solution takes the form of a convergent Maclaurin series and is presented in a general format so that it can be applied for any general reaction term $R(C)$ and any value of the Péclet number P.

We show that our Maclaurin series solution relaxes to previously reported solutions obtained for particular cases of the general reactive transport model with $P=0$ and $R(C)=\phi^2C^n$ [1,18]. Unlike these previously reported solutions based on the Adomian decomposition method and the homotopy analysis method, our approach avoids any specialized mathematical techniques. Furthermore, we are able to formulate the general term in the Maclaurin series and show that the series is convergent. Neither Sun [18] or Abbasbandy [1] proved that their series solutions were convergent.

Our approach also extends the work of Magyari [12] who developed a closed-form solution for the special case where $P=0$ and $R(C)=\phi^2C^n$, showing that the solution could be written in terms of Gauss' hypergeometric function. We show that Magyari's solution is a particular case of the Maclaurin series solution and we note that Magyari's approach does not generalize when $P \neq 0$.

The accuracy of the Maclaurin series solution is demonstrated by comparing the series solution with numerical computations for a range of problems. We explicitly compared the series and numerical solutions for models with variable P and $R(C)=\phi^2C^n$ and found that truncating the series after the x^{10} term was sufficient to provide series solutions that were visually indistinguishable from the numerical solution. We also compared the Maclaurin series solution with numerical solutions for a Michaelis–Menten reaction model with $R(C)=AC/(B+C)$ [6,28]. This additional test case also led to Maclaurin series solutions that were visually indistinguishable from the numerical solutions thereby demonstrating the accuracy and versatility of the approach described here.

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