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Approximate analytical solutions for multispecies convection-dispersion transport equation with variable parameters

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Multispecies pollutant migration often occurs in polluted groundwater systems. Most of the multispecies problems that have been dealt in the literature assume constant transport parameters, primarily because analytical solutions for varying parameters become a challenge. The present study analytically solves a two-species convection-dispersion transport equation, considering spatially varying dispersion coefficient and seepage velocity, which corresponds to the steady migration in a steady flow domain. Indeed, the methodology can be adopted for other cases, such as the transient migration in a steady flow domain and transient migration in an unsteady flow domain, without any difficulty. Three kinds of homotopy-based methods, namely the homotopy perturbation method (HPM), homotopy analysis method (HAM), and optimal homotopy asymptotic method (OHAM), are used to derive approximate analytical solutions in the form of truncated series. In homotopy analysis method, the convergence-control parameter $\hbar$ plays a key role in the convergence of the series solution. It is observed that for a specific case of this parameter, namely $\hbar=-1$, the HAM-based solution recovers the HPM-based solution. For the verification of homotopy-based solutions, we utilize the MATLAB routine *pdepe*, which efficiently solves a class of parabolic PDEs (single/system). An excellent agreement is found between the derived analytical solutions and the numerical solutions for all three methods. Further, a quantitative assessment is carried out for the derived solutions. Also, convergence theorems are proposed for the series solutions obtained using HAM and OHAM.

KEYWORDS

pollutant transport, multispecies, homotopy, analytical solution, series solution

1 Introduction

Pollution is caused by a number of sources, such as agricultural fertilizers, erosion, industries, energy generation, waste disposal, hospital wastage, vehicular transport, nuclear waste, and domestic waste. A significant portion of pollution generated by these sources finds its way either directly or indirectly into ground water (Sposito et al., 1979; Domenico 1987; Bear 1988; Clement et al., 1998; Batu 2005). Often pollutants are different species, and their chemical characteristics are different. In general, pollutant transport in groundwater is modeled using the conservation of mass of water, flux law for flow of water, conservation of mass of pollutant, and flux law for pollutant transport. Depending on the type, a pollutant can be physical, chemical, or biological. A chemical pollutant can be conservative or non-conservative for which production and decay functions need to be specified. When these equations are combined, the resulting equation is the convection-dispersion equation. This equation is for a specific species. This paper discusses the case of two species pollutant transport.

There are several works done for the analysis of multispecies pollutant transport problems. These works adopted either analytical or numerical methods. The analytical solutions were obtained using Fourier transforms, Laplace transform, general integral transforms, decomposition methods, series solutions, etc. (Lunn et al., 1996; Van Genuchten 1985; Fujikawa and Fukui 1990; Sun and Clement 1999; Sun et al., 1999; Chamkha 2005; Slodička and Balážová, 2008; Slodička and Balážová, 2010; Natarajan and Kumar 2010; Chen et al., 2012; Simpson and Ellery 2014). Numerical methods basically adopted the finite difference method (Arnold et al., 2017; Natarajan and Kumar 2018). However, the afore-mentioned works used constant transport parameter—a consideration that makes it easier to deal it mathematically. In reality, it is necessary to model the system using variable parameters in order to fully understand the pollutant dispersion behaviour. There are a few works available for the variable transport parameters; however, some are for single species or restricted formulation. Chaudhary and Singh (2020) used the homotopy analysis method (HAM) for two-species convection-dispersion transport equation, considering spatial-temporal varying dispersion coefficient and seepage velocity. They used the standard HAM to deal with the system of PDEs governing the phenomenon. However, since the inception of HAM, there have been several modifications done. The most popular variants of the method are homotopy perturbation method (HPM) and optimal homotopy asymptotic method (OHAM). On the other hand, it is worth mentioning that the transport of heavy metals in groundwater and the interactions between them and the soil medium are key concepts in environmental engineering. Such transport processes are useful for studying the damage to the environment caused by the smelting of metallic materials, the seepage of landfill leachates, the use of pesticides and chemical fertilizers, the treatment of municipal wastewater, etc. Furthermore, the solid particles (bacteria, silicon powders, etc.) present in the soil interact with the transport mechanism of the heavy metals by accelerating the migration rate of those. Thus, in order to choose a suspended matter of particular for removing the heavy metals from soils, it is crucial to understand the coupling mechanism. In fact, because of the suspended particles adsorb the heavy metals, they show an influence on the migration process of the metals in soil under seepage conditions. There are several factors affecting the coupling mechanism of heavy metals and suspended particles, such as the size and concentration of the particles, seepage velocity, types of heavy metals, porous media, coupling mechanism (solid-solid, solid-liquid, gas-liquid, etc.). The detail discussion can be found in Bai et al. (2021a), Bai et al. (2021b).

The core idea of homotopy-based methods is based on the concept of homotopy from topology. It creates a continuous mapping that deforms continuously to obtain one function from another. Liao (1992) used this concept to develop an analytical method for the solution of non-linear problems in terms of a series solution. Since then, it has been used extensively in different areas of science and engineering (Liao, 2003; Liao, 2012). On the other hand, He (1999) presented an analytical methodology named HPM. Recently, Marinca and Herişanu (2008) extended the concept of HAM using an approximation method to derive the so-called OHAM. These methods have their own advantages/disadvantages in terms of their applicability. Therefore, the present work presents three kinds of approximate series solutions using HAM, HPM, and OHAM. This paper considers the case of spatially varying transport parameters. Indeed, the methodologies can be adopted for other cases such as the ones provided in Chaudhary and Singh (2020).

2 Brief overview of homotopy-based methods

Here, first we describe the homotopy-based methods in a general framework considering a system of PDEs. Before doing so, it is pertinent to mention that all these methods are based on the mathematical concept called 'homotopy' from topology (Liao 1992). Two objects (mathematical) are homotopic if one can be continuously deformed into the other. Mathematically, a homotopy $\mathcal{H}(t;q)$ between two functions $f(t)$; $g(t)$, where t is a dimension (space or time), is itself a continuous function, defined as $\mathcal{H}: T\times[0,1]\rightarrow U$ and satisfies $\mathcal{H}(t;q)=f(t)$ when $q=0$ and $\mathcal{H}(t;q)=g(t)$ when $q=1$, where T and U are the topological spaces. This shows that as q goes from 0 to 1, $\mathcal{H}(t;q)$ varies from $f(t)$ to $g(t)$. The functions $f(t)$ and $g(t)$ are called homotopic. For example, in 2D, a circle can be continuously deformed into an ellipse or a square; similarly, in 3D, a doughnut and a coffee cup are homotopic. Since algebraic or differential equations represent curves (or functions), the concept of homotopy can be employed for solving non-linear differential or algebraic equations. Using this concept, Liao (1992) proposed the so-called homotopy analysis method (HAM). Two other popular variants of this method are homotopy perturbation method (HPM) and optimal homotopy asymptotic method (OHAM). These three methods are employed in this paper.

2.1 Homotopy analysis method

Let a system of PDEs be written as:

$$\mathcal{N}_i(y_i(x,t))=0 \tag{1}$$

where $\mathcal{N}_i$ are the non-linear operators or the original operators of the system of equations; y_i are the unknown variables for say $i=1,2,\ldots,n$; x and t are the independent variables. Now, the zeroth-order deformation equation can be constructed as follows (Liao 2003):

$$(1-q)\mathcal{L}_i[\Phi_i(x,t;q)-y_{i,0}(x,t)]=q\hbar_i H_i(x,t)\mathcal{N}_i[\Phi_i(x,t;q)],\quad i=1,2,\ldots,n \tag{2}$$

subject to the initial and boundary conditions:

$$\mathcal{B}\left(\Phi_i,\frac{\partial\Phi_i}{\partial x},\frac{\partial\Phi_i}{\partial t}\right)=0,\quad I\left(\Phi_i,\frac{\partial\Phi_i}{\partial x},\frac{\partial\Phi_i}{\partial t}\right)=0 \tag{3}$$

where q is the embedding parameter, $\Phi_i(x,t;q)$ are the representations of solutions across q, $y_{i,0}(x,t)$ are the initial approximations, $\hbar_i$ are the auxiliary parameters, $H_i(x,t)$ are the auxiliary functions, and $\mathcal{L}_i$ and $\mathcal{N}_i$ are the linear and non-linear operators, respectively. Eq. 2 shows that as $q=0$, $\Phi_i(x,t;0)=y_{i,0}(x,t)$, and as $q=1$, $\Phi_i(x,t;1)=y_i(x,t)$. This means as q varies from 0 to 1, $\Phi_i(x,t;q)$ transforms from the initial approximation to the final solution. The higher-order terms can be calculated from the higher-order deformation equation given as follows (Liao 2003):

$$\mathcal{L}_i\left[y_{i,m}(x,t) - \chi_m y_{i,m-1}(x,t)\right] = \hbar_i H_i(x,t) R_{i,m}\left(\vec{y}_{i,m-1}\right),\ m = 1,2,3,... \tag{4}$$

where

$$\chi_m = \begin{cases} 0 \text{ when } m = 1, \\ 1 \text{ otherwise} \end{cases} \tag{5}$$

and

$$R_{i,m}\left(\vec{y}_{i,m-1}\right) = \frac{1}{(m-1)!} \left.\frac{\partial^{m-1}\mathcal{N}_i[\Phi_i(x,t;q)]}{\partial q^{m-1}}\right|_{q=0} \tag{6}$$

where $y_{i,m}$ for $m \geq 1$ are the higher-order terms. Eq. 4 is obtained by differentiating the zeroth-order deformation Eq. 2 in succession. Also, it is interesting to note from Eq. 4 that the original governing equations are transformed into an infinite system of linear equations, which are easier to solve. This idea is a central concept for all perturbation-based approaches. Now, the final solutions can be obtained as follows:

$$y_i(x,t) = y_{i,0}(x,t) + \sum_{m=1}^{\infty} y_{i,m}(x,t) \tag{7}$$

One can truncate the series Eq. 7 to obtain an approximate solution to a non-linear system. It can be seen that the method involves several operators and functions, which should be adequately chosen in order to have a convergent series. For that purpose, Liao (2003) proposed three generalized rules, namely *rule of solution expressions*, *rule of coefficient ergodicity*, and *rule of solution existence*. These rules will be discussed in a later section in relation to the problem under consideration.

2.2 Homotopy perturbation method

Here, we rewrite a system of PDEs as follows:

$$\mathcal{N}_i(y_i(x,t)) = f(x,t) \tag{8}$$

Now, we can construct a homotopy that satisfies (He 1999):

$$\begin{aligned}(1-q)[\mathcal{L}_i(\Phi_i(x,t;q)) - \mathcal{L}_i(y_{i,0}(x,t))] \\ + q[\mathcal{N}_i[\Phi_i(x,t;q)] - f(x,t)] = 0, \\ i = 1,2,\ldots,n\end{aligned} \tag{9}$$

where the symbols denote the same variables as mentioned in the previous section. Also, similar to HAM, Eq. 9 shows that at $q = 0$, $\Phi_i(x,t;0) = y_{i,0}(x,t)$, and at $q = 1$, $\Phi_i(x,t;1) = y_i(x,t)$. Let us now express $\Phi_i(x,t;q)$ as a series in terms of q as follows:

$$\Phi_i(x,t;q) = \Phi_{i,0} + q\Phi_{i,1} + q^2\Phi_{i,2} + q^3\Phi_{i,3} + q^4\Phi_{i,4} + ... \tag{10}$$

where $\Phi_{i,m}$ for $m \geq 1$ are the higher-order terms. As $q \to 1$, Eq. 10 produces the final solutions as:

$$y_i(x,t) = \lim_{q \longrightarrow 1} \Phi_i(x,t;q) = \sum_{k=0}^{\infty} \Phi_{i,k} \tag{11}$$

In this method, similar to the classical perturbation approach, one can substitute the series (10) in Eq. 9 and then equate the like powers of q to obtain the terms of the series $\Phi_{i,k}$. The difference between HAM and HPM is evident from the construction of the zeroth-order deformation equation. HAM contains an additional auxiliary function and auxiliary parameters, which help obtain a rapid convergence series (Liao, 2003; Liao, 2012). Interestingly, subject to the same set of linear and non-linear operators and unit auxiliary function, HPM solution is a subcase of HAM for $\hbar_i = -1$.

2.3 Optimal homotopy asymptotic method

In order to obtain an accurate approximate solution with just a few terms of the series, Marinca and Herişanu (2008) proposed a variant of homotopy-based method, known as the optimal homotopy asymptotic method (OHAM), using asymptotic expansions of the functions and operators. We consider a non-linear system of PDEs as:

$$\mathcal{L}_i[y_i(x,t)] + \mathcal{N}_i[y_i(x,t)] + h_i(x,t) = 0, \quad i = 1,2,\ldots,n \tag{12}$$

subject to the initial and boundary conditions:

$$\mathcal{B}\left(y_i, \frac{\partial y_i}{\partial x}, \frac{\partial y_i}{\partial t}\right) = 0, \quad I\left(y_i, \frac{\partial y_i}{\partial x}, \frac{\partial y_i}{\partial t}\right) = 0 \tag{13}$$

where symbols denote the same variables as discussed in the previous section. Following HAM, one can construct a family of equations as follows:

$$\begin{aligned}(1-q)\left[\mathcal{L}_i\left(\Phi_i\left(x,t,C_{i,j};q\right)\right) + h_i(x,t)\right] = H_i\left(x,t,C_{i,j};q\right) \\ \times\left[\mathcal{L}_i\left(\Phi_i\left(x,t,C_{i,j};q\right)\right) + h_i(x,t) + \mathcal{N}_i\left(\Phi_i\left(x,t,C_{i,j};q\right)\right)\right]\end{aligned} \tag{14}$$

where symbols have their usual meaning and $C_{i,j}$ are the unknown parameters. The auxiliary functions are defined as:

$$H_i\left(x,t,C_{i,j};q\right) = 0 \text{ for } q = 0 \neq 0 \quad \text{for} \quad q \in (0,1] \tag{15}$$

It is easy to verify that when $q = 0$, $\Phi_i(x,t,C_{i,j};q) = y_{i,0}(x,t)$ and when $q = 1$, $\Phi_i(x,t,C_{i,j};q) = y_i(x,t)$, which is the same as HAM and HPM, i.e., as q goes from 0 to 1, we have the continuous deformation from the initial approximation to the final solution. Now, the initial approximations $y_{i,0}(x,t)$ can be found by solving the following set of equations, which is obtained after substituting $q = 0$ in Eq. 14:

$$\mathcal{L}_i(y_{i,0}(x,t)) + h_i(x,t) = 0 \tag{16}$$

subject to the boundary conditions:

$$\mathcal{B}\left(y_{i,0}, \frac{\partial y_{i,0}}{\partial x}, \frac{\partial y_{i,0}}{\partial t}\right) = 0, \quad I\left(y_{i,0}, \frac{\partial y_{i,0}}{\partial x}, \frac{\partial y_{i,0}}{\partial t}\right) = 0 \tag{17}$$

In OHAM, expanding the auxiliary function with respect to the embedding parameter is the key step. The auxiliary function $H_i(x,t,C_{i,j};q)$ can be expressed as follows:

$$\begin{aligned}H_i\left(x,t,C_{i,j};q\right) = qH_{i,1}\left(x,t,C_{i,j}\right) + q^2H_{i,2}\left(x,t,C_{i,j}\right) + q^3H_{i,3}\left(x,t,C_{i,j}\right) \\ + \ldots\end{aligned} \tag{18}$$

where $H_i(x,t,C_{i,j})$'s are the auxiliary functions that depend on the independent variables x and t and parameters $C_{i,j}$. It can be noted that the series Eq. 18 is in accordance with the property Eq. (15). Now, the solution of Eq. 12 can be assumed to be of the form:

$$\Phi_i\left(\mathrm{x},\mathrm{t},C_{i,j};q\right) = y_{i,0}(x,t) + \sum_{j=1}^{\infty} y_{i,j}\left(x,t,C_{i,j}\right)q^j \tag{19}$$

Substituting Eq. 19 into Eq. 14, and equating the like powers of q, the following equations are obtained [q^0 corresponds to Eqs. 16, 17:

$$\mathcal{L}_i\left(y_{i,1}\left(x,t,C_{i,j}\right)\right) = H_{i,1}\left(x,t,C_{i,j}\right)\mathcal{N}_{i,0}\left(y_{i,0}(x,t)\right) \tag{20}$$

subject to the initial and boundary conditions:

$$\mathcal{B}\left(y_{i,1},\frac{\partial y_{i,1}}{\partial x},\frac{\partial y_{i,1}}{\partial t}\right) = 0,\quad I\left(y_{i,1},\frac{\partial y_{i,1}}{\partial x},\frac{\partial y_{i,1}}{\partial t}\right) = 0 \tag{21}$$

For $k = 2, 3, 4, ...,$

$$\begin{aligned}\mathcal{L}_i\left[y_{i,k}\left(x,t,C_{i,j}\right) - y_{i,k-1}\left(x,t,C_{i,j}\right)\right] &= H_{i,k}\left(x,t,C_{i,j}\right)\mathcal{N}_{i,0}\left(y_{i,0}(x,t)\right)\\ &+\sum_{j=1}^{k-1} H_{i,j}\left(x,t,C_{i,j}\right)\left[\mathcal{L}_i\left[y_{i,k-j}\left(x,t,C_{i,j}\right)\right]\right.\\ &+\mathcal{N}_{i,k-j}\left[y_{i,0}(x,t), y_{i,1}\left(x,t,C_{i,j}\right),\ldots,\right.\\ &\left.\left. y_{i,k-j}\left(x,t,C_{i,j}\right)\right]\right]\end{aligned} \tag{22}$$

subject to the initial and boundary conditions:

$$\mathcal{B}\left(y_{i,k},\frac{\partial y_{i,k}}{\partial x},\frac{\partial y_{i,k}}{\partial t}\right) = 0,\quad I\left(y_{i,k},\frac{\partial y_{i,k}}{\partial x},\frac{\partial y_{i,k}}{\partial t}\right) = 0 \tag{23}$$

where the term $\mathcal{N}_{i,k-j}[y_{i,0}(x,t), y_{i,1}(x,t,C_{i,j}),\ldots,y_{i,k-j}(x,t,C_{i,j})]$ is the coefficient of q^m, which is obtained by expanding $\mathcal{N}_i(\Phi_i(\mathrm{x},\mathrm{t},C_{i,j};q))$ as follows:

$$\begin{aligned}\mathcal{N}_i\left(\Phi_i\left(\mathrm{x},\mathrm{t},C_{i,j};q\right)\right) &= \mathcal{N}_{i,0}\left(y_{i,0}(x,t)\right)\\ &+q\mathcal{N}_{i,1}\left(y_{i,0}(x,t), y_{i,1}\left(x,t,C_{i,j}\right)\right)\\ &+q^2\mathcal{N}_{i,2}\left(y_{i,0}(x,t), y_{i,1}\left(x,t,C_{i,j}\right), y_{i,2}\left(x,t,C_{i,j}\right)\right) + \ldots\end{aligned} \tag{24}$$

It can be observed from Eq. 22 that like HAM and HPM, OHAM also converts the original non-linear equation into an infinite set of linear sub-equations. Further, the method does not depend on the presence of a small parameter in the governing equation. The convergence of the series Eq. 19 depends on the choice of $H_{i,j}(x,t,C_{i,j})$, and there exist many ways to choose it. According to Marinca and Herişanu (2015), one can choose $H_{i,j}(x,t,C_{i,j})$ in such a way that the product $H_{i,j}(x,t,C_{i,j})[\mathcal{L}_i[y_{i,k-j}(x,t,C_{i,j})]+\mathcal{N}_{i,k-j}[y_{i,0}(x,t), y_{i,1}(x,t,C_{i,j}),\ldots,y_{i,k-j}(x,t,C_{i,j})]]$ of Eq. 22 is of the same form as that of $H_{i,j}(x,t,C_{i,j})$. The considered functions can be of any type, such as polynomial, exponential, trigonometric, etc. Now, based on the choice of auxiliary function, if the series Eq. 19 converges at $q = 1$, then

$$y_i\left(x,t,C_{i,j}\right) = y_{i,0}(x,t) + \sum_{j=1}^{\infty} y_{i,j}\left(x,t,C_{i,j}\right) \tag{25}$$

Finally, the approximate solution can be obtained by considering a finite number of terms of the series Eq. 25. The unknown parameters $C_{i,j}$ and the choice of auxiliary function will be discussed later in relation to the problem under consideration.

3 Governing equation and solution methodologies

In a one-dimensional flow field, the general form for a reactive transport system which describes the phenomenon of multi-species migration having spatially and temporally varying parameters can be modelled as follows (Chaudhary and Singh 2020):

$$r_i\frac{\partial C_i}{\partial t} = \frac{\partial}{\partial x}\left(D(x,t)\frac{\partial C_i}{\partial x} - v(x,t)C_i\right) + k_{i-1}C_{i-1} - k_iC_i,\ i = 1, 2, ..., n \tag{26}$$

Here, $k_0 = 0$ and n represents the number of species; x and t denote the spatial and temporal coordinates, respectively; r_i is the retardation factor for the i-th species; C_i is the concentration strength for the i-th species; k_i is the decay rate coefficient for the i-th species; and $D(x,t)$ and $v(x,t)$ are the dispersion coefficient and seepage velocity, respectively.

The present work considers two-species system (i.e., $i = 1, 2$) and includes the effect of spatially and temporally dependent transport parameters on pollutant migration. To that end, the model becomes (Chaudhary and Singh 2020):

$$r_1\frac{\partial C_1}{\partial t} = \frac{\partial}{\partial x}\left(D(x,t)\frac{\partial C_1}{\partial x} - v(x,t)C_1\right) - k_1C_1 \tag{27}$$

$$r_2\frac{\partial C_2}{\partial t} = \frac{\partial}{\partial x}\left(D(x,t)\frac{\partial C_2}{\partial x} - v(x,t)C_2\right) - k_2C_2 + k_1C_1 \tag{28}$$

where C_1 and C_2 represent the pollutant concentration level for parent and daughter species, respectively.

The initial and boundary conditions for the model can be given as follows:

$$C_1(x,0) = f_1(x),\ C_1(0,t) = f_1(0),\ \lim_{x\to\infty} C_1(x,t) = 0 \tag{29}$$

$$C_2(x,0) = f_2(x),\ C_2(0,t) = f_2(0),\ \lim_{x\to\infty} C_2(x,t) = 0 \tag{30}$$

where $f_1(x)$ and $f_2(x)$ are considered as (Simpson and Ellery 2014):

$$f_1(x) = a_1 x exp(-a_2 x),\ f_2(x) = 0 \tag{31}$$

Eqs 29, 30, 31 show that spatially dependent pollution exists initially for the parent species. However, for the daughter species, the initial concentration is zero.

Based on the forms of $D(x,t)$ and $v(x,t)$, several scenarios can be considered. Here, we consider a specific case, specifically the steady migration phenomenon in the case of steady groundwater flow. It may be noted that the solution methodologies reported here can be adopted for other cases such as the transient migration in steady and unsteady flows (Chaudhary and Singh 2020). However, as our objective is to show the applicability of different homotopy-based methods by extending the work of Chaudhary and Singh (2020), we restrict our analysis for the case of steady migration in steady flow. To that end, we assume:

$$D(x,t) = D_0(\alpha_1 + \alpha_2 x)^2,\ v(x,t) = v_0(\alpha_1 + \alpha_2 x) \tag{32}$$

where D_0 and v_0 are the initial dispersion and velocity, respectively; α_1 and α_2 are the parameters, where α_2 is knows as the heterogeneity parameter. Eq. 32 shows that dispersion is directly proportional to the square of velocity (Batu 2005). For $\alpha_1 = 1$ and $\alpha_2 \to 0$, i.e., α_2 is very small, the system converts into a homogeneous one, where the effect of space on dispersion and seepage velocity is absent. As α_2 increases, the system becomes heterogeneous. It may be noted that the dispersion can be expressed differently but Eq. 32 is reasonable for purposes of this study.

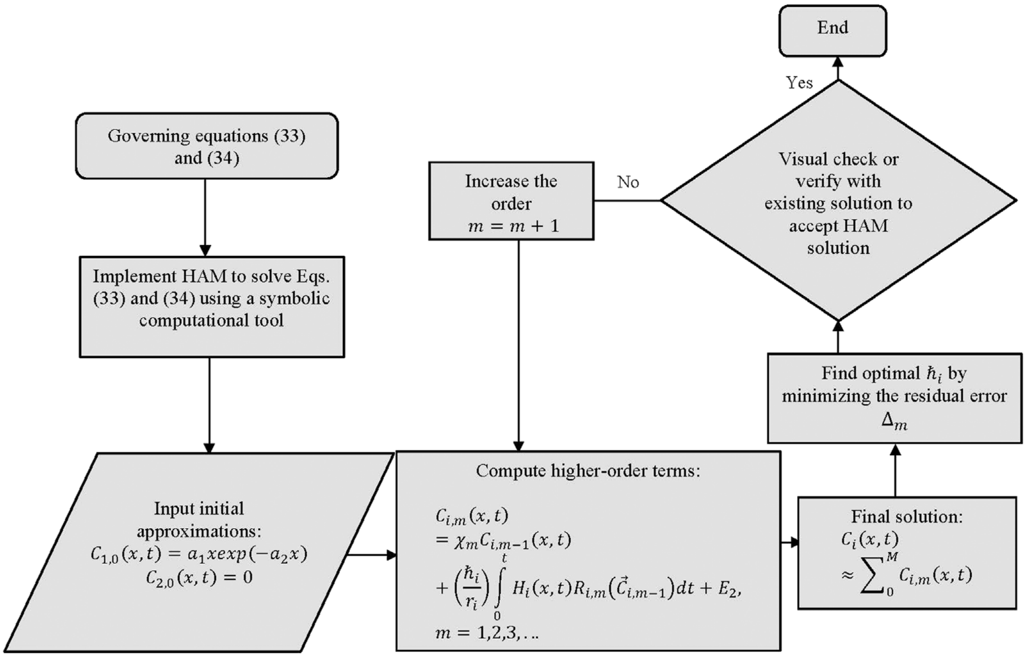

FIGURE 1
Flowchart for the HAM solution (45).

Further, seepage velocity given in Eq. 32 can also be expressed exponentially or in power form. However, for purposes of this study, Eq. 32 is reasonable, especially for homogeneous aquifers. Before applying the homotopy-based methods, for convenience, let us rewrite the governing Eqs 27, 28 in the following form:

$$r_1\frac{\partial C_1}{\partial t} = D\frac{\partial^2 C_1}{\partial x^2} + \left(\frac{\partial D}{\partial x} - v\right)\frac{\partial C_1}{\partial x} - \left(k_1 + \frac{\partial v}{\partial x}\right)C_1 \tag{33}$$

$$r_2\frac{\partial C_2}{\partial t} = D\frac{\partial^2 C_2}{\partial x^2} + \left(\frac{\partial D}{\partial x} - v\right)\frac{\partial C_2}{\partial x} - \left(k_2 + \frac{\partial v}{\partial x}\right)C_2 + k_1 C_1 \tag{34}$$

3.1 HAM-based solution

As discussed in Section 2.1, one can apply the HAM to the system of Eqs 33, 34 by constructing some operators and functions that are given below. The non-linear operators for the problem are selected as:

$$\mathcal{N}_1[\Phi_i(x,t;q)] = r_1\frac{\partial \Phi_1(x,t;q)}{\partial t} - D\frac{\partial^2\Phi_1(x,t;q)}{\partial x^2} - \left(\frac{\partial D}{\partial x} - v\right)\frac{\partial \Phi_1(x,t;q)}{\partial x} + \left(k_1 + \frac{\partial v}{\partial x}\right)\Phi_1(x,t;q) \tag{35}$$

$$\mathcal{N}_2[\Phi_i(x,t;q)] = r_2\frac{\partial \Phi_2(x,t;q)}{\partial t} - D\frac{\partial^2\Phi_2(x,t;q)}{\partial x^2} - \left(\frac{\partial D}{\partial x} - v\right)\frac{\partial \Phi_2(x,t;q)}{\partial x} + \left(k_2 + \frac{\partial v}{\partial x}\right)\Phi_2(x,t;q) - k_1\Phi_1(x,t;q) \tag{36}$$

The above equations are the original operators of the equations, which is always an easy and convenient consideration for the non-linear operators in the framework of HAM. Therefore, using Eqs 35, 36, terms $R_{i,m}$ can be calculated from Eq. 6 as follows:

$$R_{1,m}(\vec{C}_{i,m-1}) = r_1\frac{\partial C_{1,m-1}}{\partial t} - D\frac{\partial^2 C_{1,m-1}}{\partial x^2} - \left(\frac{\partial D}{\partial x} - v\right)\frac{\partial C_{1,m-1}}{\partial x} + \left(k_1 + \frac{\partial v}{\partial x}\right)C_{1,m-1} \tag{37}$$

$$R_{2,m}(\vec{C}_{i,m-1}) = r_2\frac{\partial C_{2,m-1}}{\partial t} - D\frac{\partial^2 C_{2,m-1}}{\partial x^2} - \left(\frac{\partial D}{\partial x} - v\right)\frac{\partial C_{2,m-1}}{\partial x} + \left(k_2 + \frac{\partial v}{\partial x}\right)C_{2,m-1} - k_1 C_{1,m-1} \tag{38}$$

Now, as discussed earlier, we need to follow three fundamental rules provided by Liao (2003) to have a convergent series solution. First, we consider the following set of base functions to represent the solutions $C_i(x,t)$ of the present problem:

$$\left\{x^m t^p\, exp(-nbx)\,\middle|\, m, n, p = 0, 1, 2, 3, ...\right\} \tag{39}$$

so that

$$C_i(x,t) = \sum_{p=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=1}^{\infty}\beta_{m,n,p}x^m t^p\, exp(-nbx) \tag{40}$$

where $\beta_{m,n,p}$ are the coefficients of the series. Eq. 40 provides the so-called *rule of solution expression*. Following the rule of solution expression, the linear operators and the initial approximations are chosen, respectively, as follows:

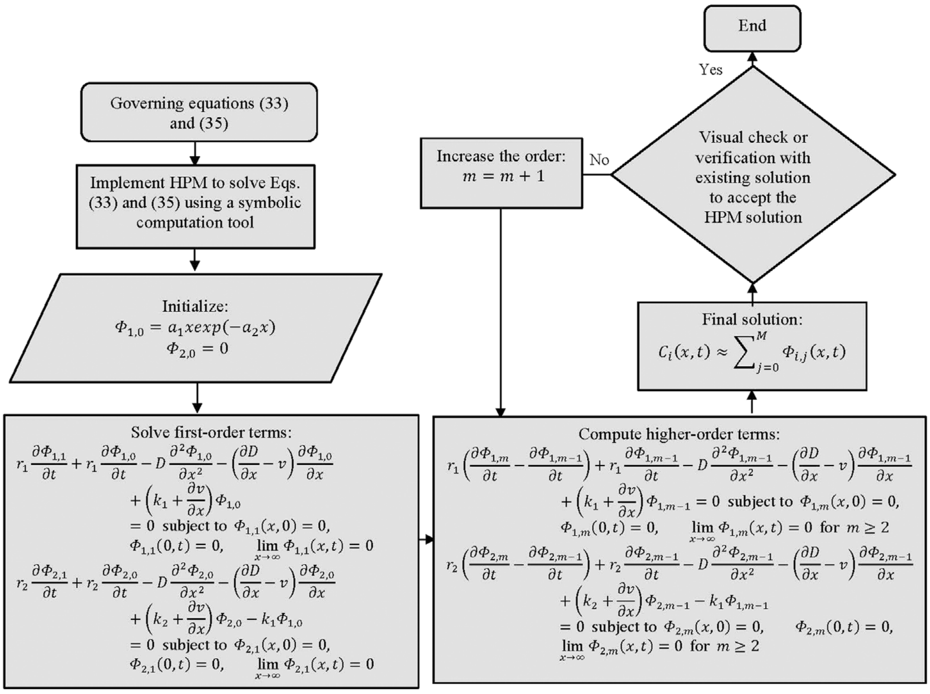

FIGURE 2
Flowchart for the HPM solution (55).

$$\mathcal{L}_i[\Phi_i(x,t;q)] = r_i \frac{\partial \Phi_i(x,t;q)}{\partial t} \quad \text{with the property} \quad \mathcal{L}_i[E_2] = 0 \tag{41}$$

$$C_{1,0}(x,t) = f_1(x) = a_1 x \exp(-a_2 x),\ C_{2,0}(x,t) = f_2(x) = 0 \tag{42}$$

where E_2 is an integral constant. It may be noted that the choice for Eq. 41 is not unique. Using Eq. 41, the higher-order terms can be obtained from Eq. 4 as follows:

$$C_{i,m}(x,t) = \chi_m C_{i,m-1}(x,t) + \left(\frac{\hbar_i}{r_i}\right)\int_0^t H_i(x,t) R_{i,m}\left(\vec{C}_{i,m-1}\right)dt + E_2,\ m = 1,2,3,\ldots \tag{43}$$

where $R_{i,m}$ are given by Eqs 37, 38, and constant E_2 can be determined from the initial condition for the higher-order deformation equations, which simply yields $E_2 = 0$ for all $m \geq 1$.

Now, the auxiliary functions $H_i(x,t)$ can be determined from the *rule of coefficient ergodicity*. Based on the rule of solution expression, the general form of $H_i(x,t)$ should be:

$$H_i(x,t) = x^{n_1} t^{n_3} \exp(-b n_2 x) \tag{44}$$

where n_1, n_2, and n_3 are the integers. However, for simplicity, we can take $H_i(x,t) = 1$ (Vajravelu and Van Gorder 2013). Finally, the approximate solutions can be obtained as follows:

$$C_i(x,t) \approx C_{i,0}(x,t) + \sum_{m=1}^{M} C_{i,m}(x,t) \tag{45}$$

For the convenience of readers, a flowchart containing the steps of the method is provided in Figure 1.

3.2 HPM-based solution

In relation to the discussion in Section 2.2, for simplicity, we consider the linear operator as follows:

$$\mathcal{L}_i[\Phi_i(x,t;q)] = r_i \frac{\partial \Phi_i(x,t;q)}{\partial t},\ i = 1,2 \tag{46}$$

The non-linear operators are selected as Eqs 35, 36. In the framework of HPM also, the selection of these operators is not unique; indeed, one can choose any other forms to check for a better solution. Using these expressions in Eq. 9 and then substituting the series Eq. 10, we obtain the following systems of differential equations after equating the like powers of q:

$$r_1\left(\frac{\partial \Phi_{1,0}}{\partial t} - \frac{\partial C_{1,0}}{\partial t}\right) = 0 \text{ subject to } \Phi_{1,0}(x,0) = f_1(x),\ \Phi_{1,0}(0,t) = f_1(0),\ \lim_{x\to\infty} \Phi_{1,0}(x,t) = 0 \tag{47}$$

$$r_2\left(\frac{\partial \Phi_{2,0}}{\partial t} - \frac{\partial C_{2,0}}{\partial t}\right) = 0 \text{ subject to } \Phi_{2,0}(x,0) = f_2(x),\ \Phi_{2,0}(0,t) = f_2(0),\ \lim_{x\to\infty} \Phi_{2,0}(x,t) = 0 \tag{48}$$

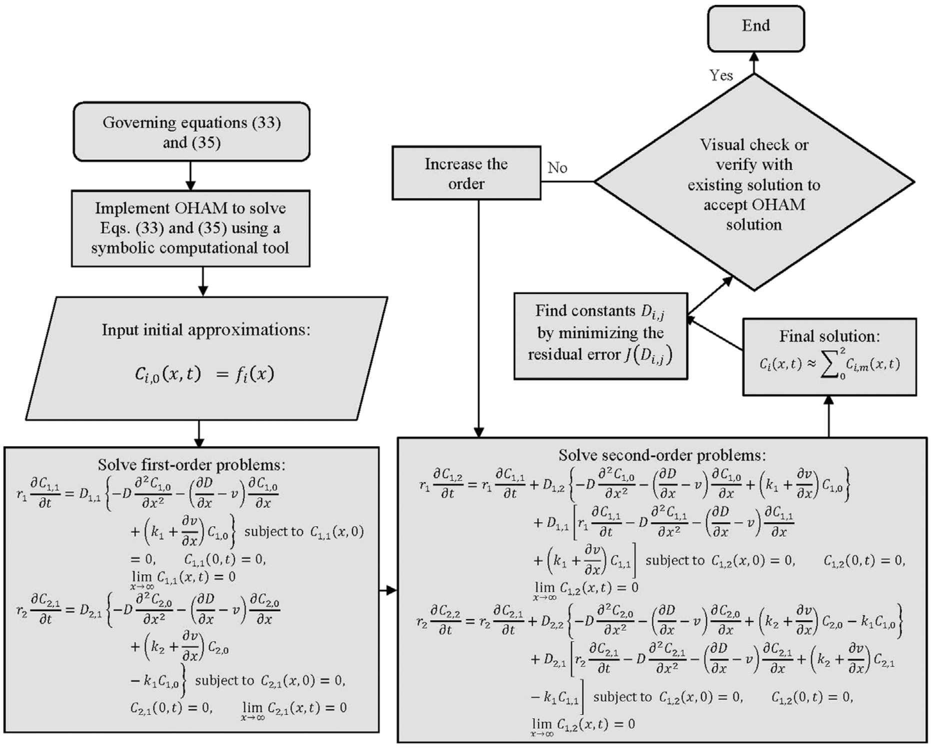

FIGURE 3
Flowchart for the OHAM solution (65).

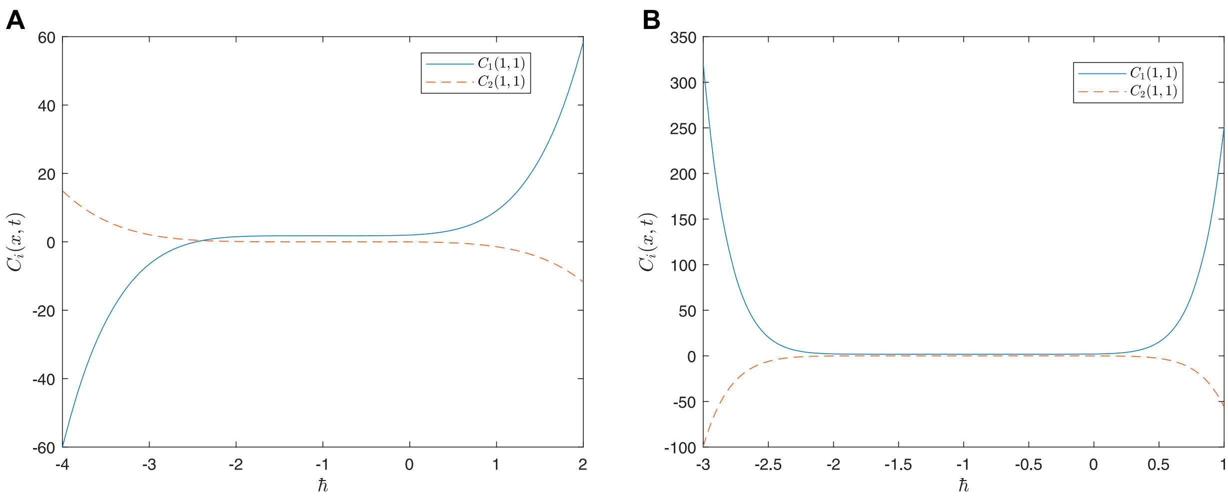

FIGURE 4
ħ– curves for $C_i(1,1)$ of the HAM solution: **(A)** 5th order approximation, and **(B)** 10th order approximation.

$$r_1\left(\frac{\partial \Phi_{1,1}}{\partial t}-\left(\frac{\partial \Phi_{1,0}}{\partial t}-\frac{\partial C_{1,0}}{\partial t}\right)\right)+r_1\frac{\partial \Phi_{1,0}}{\partial t}-D\frac{\partial^2 \Phi_{1,0}}{\partial x^2}-\left(\frac{\partial D}{\partial x}-v\right)\frac{\partial \Phi_{1,0}}{\partial x}+\left(k_1+\frac{\partial v}{\partial x}\right)\Phi_{1,0}=0 \text{ subject to } \Phi_{1,1}(x,0)=0,\ \Phi_{1,1}(0,t)=0,\ \lim_{x\to\infty}\Phi_{1,1}(x,t)=0 \quad (49)$$

$$r_2\left(\frac{\partial \Phi_{2,1}}{\partial t}-\left(\frac{\partial \Phi_{2,0}}{\partial t}-\frac{\partial C_{2,0}}{\partial t}\right)\right)+r_2\frac{\partial \Phi_{2,0}}{\partial t}-D\frac{\partial^2 \Phi_{2,0}}{\partial x^2}-\left(\frac{\partial D}{\partial x}-v\right)\frac{\partial \Phi_{2,0}}{\partial x}+\left(k_2+\frac{\partial v}{\partial x}\right)\Phi_{2,0}-k_1\Phi_{1,0}=0 \text{ subject to } \Phi_{2,1}(x,0)=0,\ \Phi_{2,1}(0,t)=0,\ \lim_{x\to\infty}\Phi_{2,1}(x,t)=0 \quad (50)$$

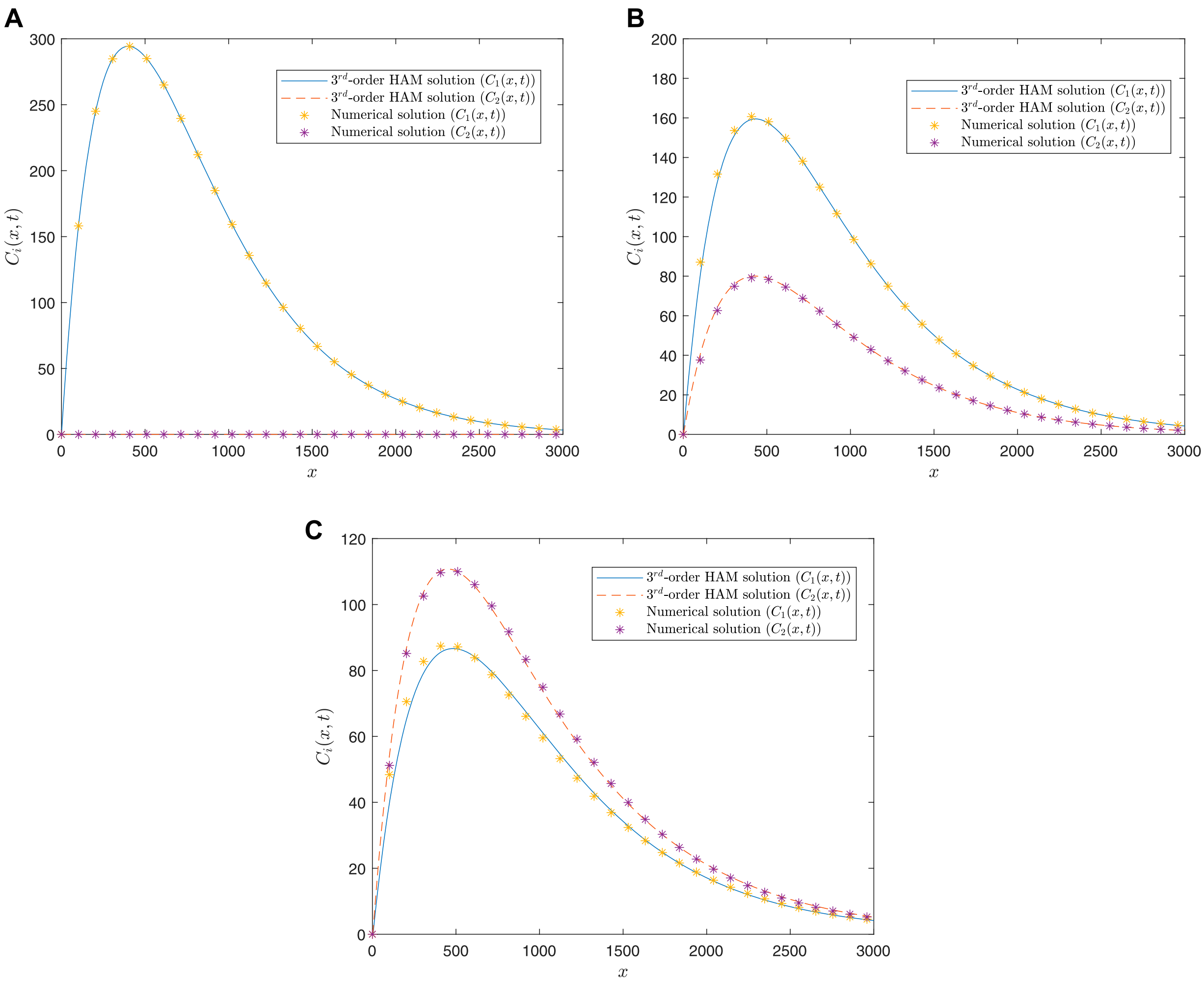

FIGURE 5
HAM-based pollutant concentrations versus distance for both species at: **(A)** $t = 0$ h, **(B)** $t = 20$ h, and **(C)** $t = 40$ h.

$$r_1\left(\frac{\partial \Phi_{1,2}}{\partial t}-\frac{\partial \Phi_{1,1}}{\partial t}\right)+r_1\frac{\partial \Phi_{1,1}}{\partial t}-D\frac{\partial^2 \Phi_{1,1}}{\partial x^2}-\left(\frac{\partial D}{\partial x}-v\right)\frac{\partial \Phi_{1,1}}{\partial x}+\left(k_1+\frac{\partial v}{\partial x}\right)\Phi_{1,1}$$
$$= 0 \text{ subject to } \Phi_{1,2}(x,0)=0,\ \Phi_{1,2}(0,t)=0,\ \lim_{x\to\infty}\Phi_{1,2}(x,t)=0 \tag{51}$$

$$r_2\left(\frac{\partial \Phi_{2,2}}{\partial t}-\frac{\partial \Phi_{2,1}}{\partial t}\right)+r_2\frac{\partial \Phi_{2,1}}{\partial t}-D\frac{\partial^2 \Phi_{2,1}}{\partial x^2}-\left(\frac{\partial D}{\partial x}-v\right)\frac{\partial \Phi_{2,1}}{\partial x}+\left(k_2+\frac{\partial v}{\partial x}\right)\Phi_{2,1}$$
$$-k_1\Phi_{1,1}$$
$$= 0 \text{ subject to } \Phi_{2,2}(x,0)=0,\ \Phi_{2,2}(0,t)=0,\ \lim_{x\to\infty}\Phi_{2,2}(x,t)=0 \tag{52}$$

Proceeding in a like manner, one can arrive at the following recurrence relation:

$$r_1\left(\frac{\partial \Phi_{1,m}}{\partial t}-\frac{\partial \Phi_{1,m-1}}{\partial t}\right)+r_1\frac{\partial \Phi_{1,m-1}}{\partial t}-D\frac{\partial^2 \Phi_{1,m-1}}{\partial x^2}-\left(\frac{\partial D}{\partial x}-v\right)\frac{\partial \Phi_{1,m-1}}{\partial x}$$
$$+\left(k_1+\frac{\partial v}{\partial x}\right)\Phi_{1,m-1}$$
$$= 0 \text{ subject to } \Phi_{1,m}(x,0)=0,\ \Phi_{1,m}(0,t)=0,\ \lim_{x\to\infty}\Phi_{1,m}(x,t)$$
$$= 0 \text{ for } m\geq 2 \tag{53}$$

$$r_2\left(\frac{\partial \Phi_{2,m}}{\partial t}-\frac{\partial \Phi_{2,m-1}}{\partial t}\right)+r_2\frac{\partial \Phi_{2,m-1}}{\partial t}-D\frac{\partial^2 \Phi_{2,m-1}}{\partial x^2}-\left(\frac{\partial D}{\partial x}-v\right)\frac{\partial \Phi_{2,m-1}}{\partial x}$$
$$+\left(k_2+\frac{\partial v}{\partial x}\right)\Phi_{2,m-1}-k_1\Phi_{1,m-1}$$
$$= 0 \text{ subject to } \Phi_{2,m}(x,0)=0,\ \Phi_{2,m}(0,t)=0,\ \lim_{x\to\infty}\Phi_{2,m}(x,t)$$
$$= 0 \text{ for } m\geq 2 \tag{54}$$

The initial approximation can be chosen as $\Phi_{1,0} = f_1(x) = a_1 x exp(-a_2 x)$ and $\Phi_{2,0} = f_2(x) = 0$. Using this initial approximation, we can solve the equations iteratively using a symbolic software. Finally, the HPM-based solutions can be approximated as follows:

$$C_i(x,t) \approx \sum_{k=0}^{M}\Phi_{i,k} \tag{55}$$

A flowchart containing the steps of the method is given in Figure 2.

3.3 OHAM-based solution

In relation to the discussion given in Section 2.3, we choose the following operators:

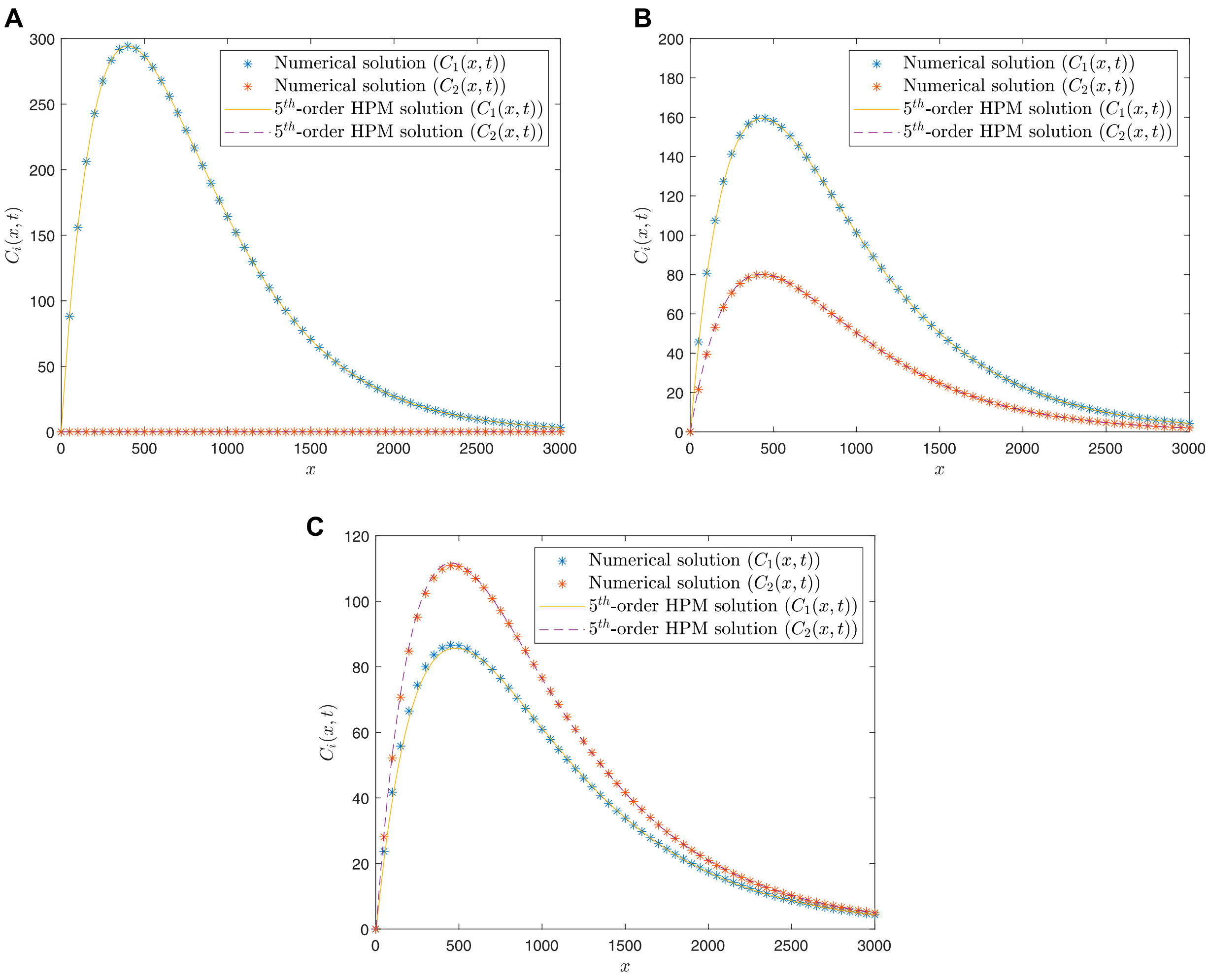

FIGURE 6
HPM-based pollutant concentrations versus distance for both species at: **(A)** t = 0 h, **(B)** t = 20 h, and **(C)** t = 40 h.

$$\mathcal{L}_i[C_i(x,t)] = r_i \frac{\partial C_i(x,t)}{\partial t} \tag{56}$$

$$\mathcal{N}_1[C_i(x,t)] = -D\frac{\partial^2 C_1(x,t)}{\partial x^2} - \left(\frac{\partial D}{\partial x} - v\right)\frac{\partial C_1(x,t)}{\partial x} + \left(k_1 + \frac{\partial v}{\partial x}\right)C_1(x,t) \tag{57}$$

$$\mathcal{N}_2[C_i(x,t)] = -D\frac{\partial^2 C_2(x,t)}{\partial x^2} - \left(\frac{\partial D}{\partial x} - v\right)\frac{\partial C_2(x,t)}{\partial x} + \left(k_2 + \frac{\partial v}{\partial x}\right)C_2(x,t) - k_1 C_1(x,t) \tag{58}$$

and

$$h_i(x,t) = 0 \tag{59}$$

With these considerations, we can solve the zeroth-order Eq. 16 to have the following solution:

$$C_{i,0}(x,t) = f_i(x) \tag{60}$$

Now to have the higher-order equations, we need the expressions $\mathcal{N}_{i,0}, \mathcal{N}_{i,1}, \mathcal{N}_{i,2}$, etc. as can be seen from Eq. 20. For that, one can use Eq. 24 in relation with Eqs 57, 58. Using this we have the first-order equations:

$$r_1\frac{\partial C_{1,1}}{\partial t} = H_{1,1}(x,t,D_{1,i})\left[-D\frac{\partial^2 C_{1,0}}{\partial x^2} - \left(\frac{\partial D}{\partial x} - v\right)\frac{\partial C_{1,0}}{\partial x} + \left(k_1 + \frac{\partial v}{\partial x}\right)C_{1,0}\right] \text{ subject to } C_{1,1}(x,0) = 0,\ C_{1,1}(0,t) = 0,\ \lim_{x\to\infty} C_{1,1}(x,t) = 0 \tag{61}$$

$$r_2\frac{\partial C_{2,1}}{\partial t} = H_{2,1}(x,t,D_{2,i}) \times\left[-D\frac{\partial^2 C_{2,0}}{\partial x^2} - \left(\frac{\partial D}{\partial x} - v\right)\frac{\partial C_{2,0}}{\partial x} + \left(k_2 + \frac{\partial v}{\partial x}\right)C_{2,0} - k_1 C_{1,0}\right] \text{ subject to } C_{2,1}(x,0) = 0,\ C_{2,1}(0,t) = 0,\ \lim_{x\to\infty} C_{2,1}(x,t) = 0 \tag{62}$$

The auxiliary functions can be chosen in many ways. Here, we select $H_{1,1}(x,t,D_{1,i}) = D_{1,1}$ and $H_{2,1}(x,t,D_{2,i}) = D_{2,1}$. Putting $k = 2$ in Eq. 22 and then using the expansion of $\mathcal{N}$, we have the following second-order equation:

$$r_1\frac{\partial C_{1,2}}{\partial t} = r_1\frac{\partial C_{1,1}}{\partial t} + D_{1,2}\left[-D\frac{\partial^2 C_{1,0}}{\partial x^2} - \left(\frac{\partial D}{\partial x} - v\right)\frac{\partial C_{1,0}}{\partial x} + \left(k_1 + \frac{\partial v}{\partial x}\right)C_{1,0}\right] + D_{1,1}\left[r_1\frac{\partial C_{1,1}}{\partial t} - D\frac{\partial^2 C_{1,1}}{\partial x^2} - \left(\frac{\partial D}{\partial x} - v\right)\frac{\partial C_{1,1}}{\partial x} + \left(k_1 + \frac{\partial v}{\partial x}\right)C_{1,1}\right] \text{ subject to } C_{1,2}(x,0) = 0,\ C_{1,2}(0,t) = 0,\ \lim_{x\to\infty} C_{1,2}(x,t) = 0 \tag{63}$$

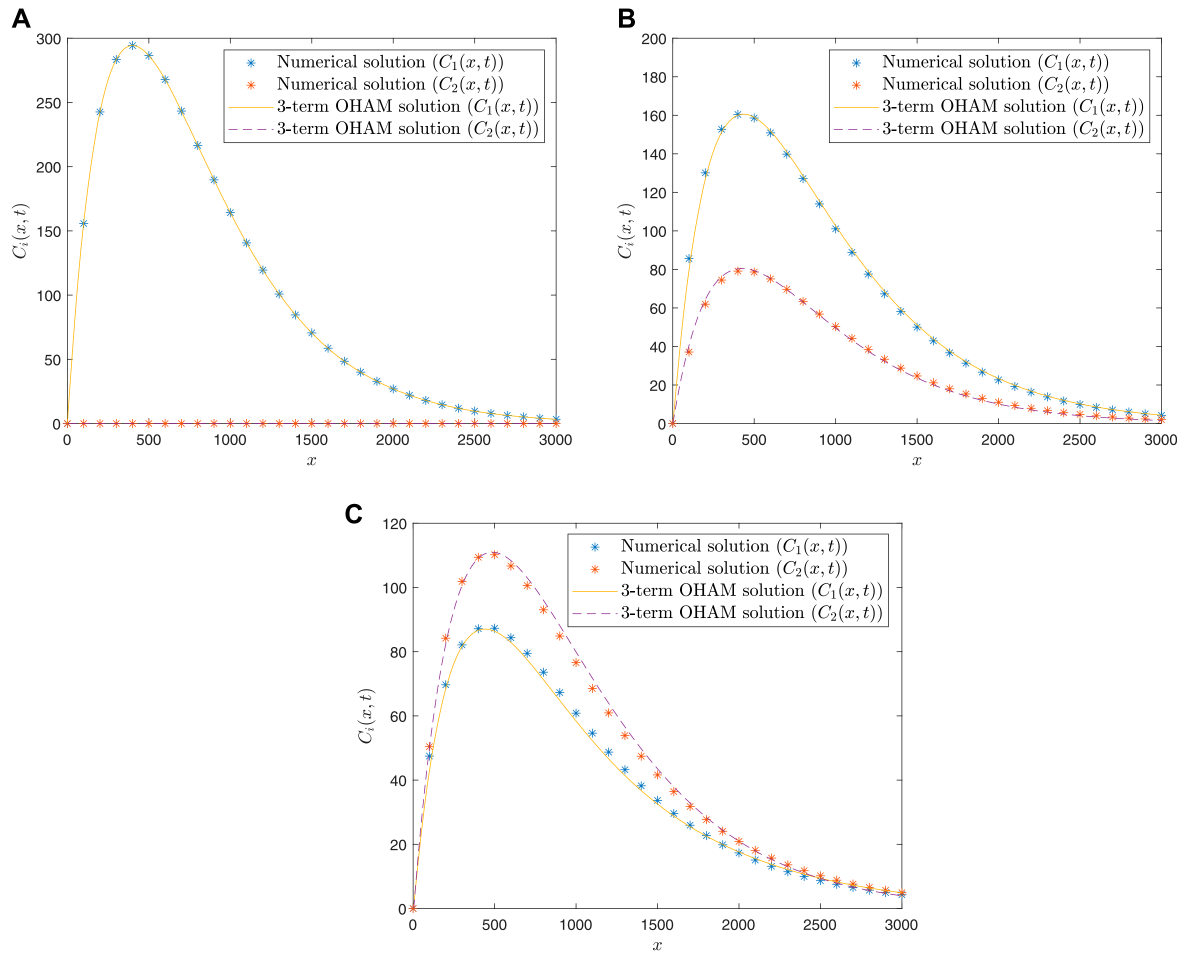

FIGURE 7
OHAM-based pollutant concentrations versus distance for both species at: **(A)** t = 0 h, **(B)** t = 20 h, and **(C)** t = 40 h.

$$r_2\frac{\partial C_{2,2}}{\partial t} = r_2\frac{\partial C_{2,1}}{\partial t} + D_{2,2}\left[-D\frac{\partial^2 C_{2,0}}{\partial x^2} - \left(\frac{\partial D}{\partial x} - v\right)\frac{\partial C_{2,0}}{\partial x} + \left(k_2 + \frac{\partial v}{\partial x}\right)C_{2,0} - k_1 C_{1,0}\right]$$
$$+D_{2,1}\left[r_2\frac{\partial C_{2,1}}{\partial t} - D\frac{\partial^2 C_{2,1}}{\partial x^2} - \left(\frac{\partial D}{\partial x} - v\right)\frac{\partial C_{2,1}}{\partial x} + \left(k_2 + \frac{\partial v}{\partial x}\right)C_{2,1} - k_1 C_{1,1}\right]$$
$$\text{subject to } C_{1,2}(x,0) = 0,\ C_{1,2}(0,t) = 0,\ \lim_{x\to\infty} C_{1,2}(x,t) = 0 \quad (64)$$

Here, we choose $H_{1,2}(x,t,D_{2,i}) = D_{1,2}$ and $H_{2,2}(x,t,D_{2,i}) = D_{2,2}$. The terms of the series can be computed using the equations developed here. One can compute these terms without any difficulty using a symbolic computation software, such as MATLAB. Further, following Eq. 22, the higher-order terms can be computed in a similar manner. However, our aim is to produce an accurate solution with just two-three terms of OHAM-based series. Therefore, we restrict our calculation up to $k = 2$. Finally, the approximate solution can be found as:

$$C_i(x,t) \approx C_{i,0}(x,t) + C_{i,1}(x,t,D_{i,i}) + C_{1,2}(x,t,D_{i,i}) \quad (65)$$

where the terms are given by Eqs. 60, 61, 62, 63, 64. A flowchart containing the steps of the method is provided in Figure 3.

In Section 2, we discussed the homotopy-based methods from a general framework of system of PDEs. Indeed, the methodologies are equally applicable to single equations, integral equations, etc. Then, in Section 3, the methodologies were applied to a system of equations describing two-species pollutant transport. It can be seen from the application of these methods that they are different from the construction of different functions, operators, and parameters, and therefore may have advantages or disadvantages while dealing with a particular problem. From a theoretical perspective, the convergence theorems for HAM- and OHAM-based solutions are provided in Appendix A.

4 Results and discussion

First, we discuss the expressions and the values of parameters needed for the assessment of the developed solutions. Then, the numerical convergence of the HAM-based analytical solution is established for a specific test case, and then the solution is validated over a numerical solution. Finally, the HPM- and OHAM-based analytical solutions are validated by comparing them with the numerical solution.

TABLE 1 Comparison between HAM-, HPM-, and OHAM-based approximations and numerical solution for the selected case for $t = 0$ h: (a) $C_1(x,t)$ and (b) $C_2(x,t)$. (a) Species, $C_1(x,t)$ (b) Species, $C_2(x,t)$

x (cm)	$t = 0$ h			
	Numerical solution	3rd order HAM-based approximation	5th order HPM-based approximation	Three-term OHAM-based approximation
0	0	0.0000	0.0000	0.0000
250	267.6307	267.6299	267.6299	267.6299
500	286.5048	286.5039	286.5039	286.5040
750	230.0325	230.0318	230.0318	230.0319
1000	164.1700	164.1696	164.1696	164.1696
1250	109.8423	109.8421	109.8421	109.8421
1500	70.5532	70.5531	70.5531	70.5531
1750	44.0585	44.0585	44.0585	44.0585
2000	26.9518	26.9518	26.9518	26.9518
2250	16.2295	16.2295	16.2295	16.2295
2500	9.6523	9.6523	9.6523	9.6523
2750	5.6831	5.6831	5.6831	5.6831
3000	3.3185	3.3185	3.3185	3.3185
x (cm)	$t = 0$ h			
	Numerical solution	3rd order HAM-based approximation	5th order HPM-based approximation	Three-term OHAM-based approximation
0	0	0	0	0
250	0	0.0005	0.0005	0.0005
500	0	0.0006	0.0006	0.0005
750	0	0.0005	0.0005	0.0004
1000	0	0.0003	0.0003	0.0003
1250	0	0.0002	0.0002	0.0002
1500	0	0.0001	0.0001	0.0001
1750	0	0	0	0
2000	0	0	0	0
2250	0	0	0	0
2500	0	0	0	0
2750	0	0	0	0
3000	0	0	0	0

4.1 Selection of expressions and parameters

For the assessment of solutions, it can be seen that the dispersion coefficient $D(x,t)$ and seepage velocity $v_0(x,t)$ are taken as given by Eq. 2. Using these equations, we have:

$$\frac{\partial D}{\partial x} = 2\alpha_2 D_0 (\alpha_1 + \alpha_2 x), \ \frac{\partial v}{\partial x} = \alpha_2 v_0 \tag{66}$$

For the validation of solutions, space and time domains are considered as $0 \le x(\text{cm}) \le 3000$ and $0 \le t(\text{hr}) \le 40$. The required parameters are chosen as (Simpson and Ellery 2014; Chaudhary and Singh 2020): $a_1 = 2$, $a_2 = 0.0025$, $k_1 = 0.05$ (/hr), $k_2 = 0.01$ (/hr), $v_0 = 0.2$ (cm/hr), and $D_0 = 0.5$ (cm^2/hr). Also, the other parameters are considered as $r_1 = 2$, $r_2 = 2.5$, $\alpha_1 = 1$, and $\alpha_2 = 0.05$ (/cm).

4.2 Numerical convergence and validation of the HAM solution

There are two ways to handle the convergence of HAM: one is based on the $\hbar-$ curves, and the other is by finding the squared

TABLE 2 Comparison between HAM-, HPM-, and OHAM-based approximations and numerical solution for the selected case for $t = 20$ hr: (a) $C_1(x,t)$ and (b) $C_2(x,t)$. (a) Species, $C_1(x,t)$ (b) Species, $C_2(x,t)$

x (cm)	t = 20 h			
	Numerical solution	3rd order HAM-based approximation	5th order HPM-based approximation	Three-term OHAM-based approximation
0	0	0	−1.6183	0
250	140.4908	140.6578	140.4567	141.3510
500	157.6763	157.7893	157.6617	158.9841
750	133.5315	133.5544	133.5323	134.9613
1000	101.2569	101.2147	101.2632	102.6167
1250	72.5128	72.4397	72.5181	73.7020
1500	50.2082	50.1308	50.2103	51.1863
1750	34.0330	33.9673	34.0324	34.7970
2000	22.7495	22.7023	22.7475	23.3180
2250	15.0663	15.0383	15.0643	15.4687
2500	9.9165	9.9046	9.9151	10.1857
2750	6.5007	6.5008	6.5003	6.6685
3000	4.2511	4.2586	4.2513	4.3454
x (cm)	t = 20 h			
	Numerical solution	3rd order HAM-based approximation	5th order HPM-based approximation	Three-term OHAM-based approximation
0	0	0	−0.7254	0
250	70.9251	70.7487	70.9525	71.4407
500	79.2222	79.1049	79.2369	79.3371
750	66.7362	66.7144	66.7373	66.3508
1000	50.3063	50.3567	50.3017	49.5507
1250	35.7906	35.8784	35.7860	34.8341
1500	24.6059	24.7026	24.6035	23.5909
1750	16.5518	16.6392	16.5517	15.5772
2000	10.9746	11.0433	10.9759	10.0988
2250	7.2061	7.2536	7.2077	6.4560
2500	4.7005	4.7284	4.7018	4.0814
2750	3.0527	3.0646	3.0534	2.5566
3000	1.9770	1.9771	1.9771	1.5890

residual error (Liao 2012). It can be noted that for the system of equations considered here, we have chosen $\hbar_1 = \hbar_2 = \hbar$. One can indeed choose two different auxiliary parameters; however, it is better to first consider a common $\hbar$ to see the accuracy of solutions, as this assumption simplifies the problem. Here, we calculate the so-called $\hbar$ − curves to find a suitable choice for the auxiliary parameter $\hbar$, which determines the convergence of the HAM-based series solution. In this regard, for a particular order of approximation, we plot the approximate solution $C_i(x,t)$ (or its derivatives) at some point within the domain. The flatness of the ħ− curve determines a suitable choice for the auxiliary parameter ħ. In Figure 4, we plot the ħ− curves for 5th and 10th order HAM-based approximations for the value $C_i(1,1)$. From the exact solution, those quantities can be calculated, and it is observed from the figures that the curves exhibit the flat nature for a specific range of ħ. Any choice of ħ within this range determines an optimal value for which the series solutions converge (Abbasbandy et al., 2011).

TABLE 3 Comparison between HAM-, HPM-, and OHAM-based approximations and numerical solution for the selected case for $t = 40$ h: (a) $C_1(x,t)$ and (b) $C_2(x,t)$. (a) Species, $C_1(x,t)$ (b) Species, $C_2(x,t)$

x (cm)	t = 40 h			
	Numerical solution	3rd order HAM-based approximation	5th order HPM-based approximation	Three-term OHAM-based approximation
0	0	0	−1.8523	0
250	73.5227	72.6647	72.2756	76.3031
500	86.1393	86.6023	85.6178	86.3587
750	76.4081	77.7250	76.5445	74.4875
1000	60.9565	62.3186	61.3086	58.3735
1250	46.1183	47.0389	46.3814	43.9499
1500	33.8653	34.2290	33.9435	32.5570
1750	24.4288	24.3471	24.3591	23.9755
2000	17.4318	17.0942	17.2960	17.6135
2250	12.3584	11.9382	12.2277	12.9082
2500	8.7296	8.3447	8.6433	9.4223
2750	6.1556	5.8654	6.1230	6.8376
3000	4.3387	4.1579	4.3498	4.9247
x (cm)	t = 40 h			
	Numerical solution	3rd order HAM-based approximation	5th order HPM-based approximation	Three-term OHAM-based approximation
0	0	−1.7574	−1.8424	−2.4474
250	95.3208	96.0586	96.4530	92.9257
500	110.6372	110.1981	111.1681	110.9119
750	97.1614	95.9354	97.1046	99.6570
1000	76.6791	75.3736	76.3932	79.9126
1250	57.3454	56.4095	57.0978	60.1912
1500	41.5970	41.1632	41.4886	43.5274
1750	29.6238	29.6214	29.6432	30.5633
2000	20.8592	21.1365	20.9503	20.9755
2250	14.5865	14.9910	14.6929	14.1301
2500	10.1591	10.5758	10.2443	9.3708
2750	7.0611	7.4205	7.1103	6.1314
3000	4.9045	5.1760	4.9188	3.9647

Here, we test the performance of the HAM-based analytical solutions for the present problem by comparing them with a numerical solution. The numerical solution is obtained using an efficient MATLAB tool, namely 'pdepe'. This MATLAB routine uses the method of lines by discretizing a parabolic PDE (single or system) in one space direction (Skeel and Berzins 1990). For the parameters described in the previous section, the pollutant concentrations are computed using pdepde for $t = 0$, 20, and 40 h. On the other hand, HAM solutions are computed for each of the cases. The auxiliary parameter $\hbar$ is chosen as −0.87. Figure 5 depicts the pollutant concentration values for the selected cases. It can be seen from the figure that the 3rd order HAM solution agrees very well with the numerical solution.

4.3 Validation of HPM-based solution

The HPM-based analytical solutions for the selected test case are validated over the numerical solution obtained using *pdepe* of MATLAB. It is seen that the five-term HPM series produces accurate results over the selected domain.

Figure 6 compares the numerical solutions and the HPM-based approximations.

4.4 Validation of OHAM-based solution

For the assessment of the OHAM-based analytical solution, one needs to calculate the constants $D_{i,j}$'s. For that purpose, we calculate the residual as follows:

$$R_i(x,t,D_{i,j}) = \mathcal{L}_i\left[C_{i,OHAM}(x,t,D_{i,j})\right] + \mathcal{N}_i\left[C_{i,OHAM}(x,t,D_{i,j})\right] + h_i(x,t), j = 1,2,\ldots,s \tag{67}$$

where $C_{i,OHAM}(x,t,D_{i,j})$ is the approximate solution. When $R_i(x,t,D_{i,j}) = 0$, $C_{i,OHAM}(x,t,D_{i,j})$ becomes the exact solution to the problem. One of the ways to obtain the optimal $D_{i,j}$'s, for which the solution converges, is the minimization of squared residual error, i.e.,

$$J(D_{i,j}) = \int_{(x,t)\epsilon D}\sum_{i=1}^{2} R_i^2(x,t,D_{i,j})dxdt, \quad j = 1,2,...,s \tag{68}$$

where D is the domain of the problem. The minimization of Eq. 68 leads to a system of algebraic equations as follows:

$$\frac{\partial J}{\partial D_{1,1}} = \frac{\partial J}{\partial D_{1,2}} = \ldots = \frac{\partial J}{\partial D_{1,s}} = 0 \tag{69}$$

Solving this system, one can obtain the optimal values of the parameters. We obtain the optimal values using the MATLAB routine *fminsearch*, which minimizes an unconstrained multivariate function. Three-term OHAM solution is computed and compared in Figure 7 with the numerical solution obtained using pdepe to see the effectiveness of the proposed approach. It can be seen that the OHAM-based approximation agrees well with the numerical solution for all cases.

4.5 Comparison between different solutions

This work develops three kinds of analytical solutions for two-species pollutant transport equation using the homotopy-based methods. In this section, we validated the performances of different solutions. It is shown that all of them agree well with the corresponding numerical solutions to the non-linear problem. However, the methods have their own advantages or disadvantages. Specifically, the HAM provides a great freedom in choosing linear, non-linear operators, and auxiliary functions subject to the choice of base functions. Further, the convergence-control parameter present in HAM greatly enhances the radius of convergence of the series and monitors the rate of convergence. On the other hand, the OHAM solution is an improved version of homotopy-based method with the aim of obtaining an accurate approximation with just two-three terms of the series. For a quantitative assessment, the performances of different solutions are compared numerically in Tables 1, 2, 3.

5 Concluding remarks

Here, we derive the HAM-, HPM-, and OHAM-based analytical solutions for two-species transport equations with spatially varying dispersion coefficient and seepage velocity. The same equations were studied analytically using HAM by Chaudhary and Singh (2020). A numerical solution is also developed using the MATLAB routine *pdepe*. The proposed methods produce accurate solutions for all the cases. This work shows the potential of HAM, HPM, and OHAM in the context of obtaining a series solution for a system of parabolic PDEs. The theoretical as well as numerical convergence of the series solutions are provided.

Data availability statement

The original contributions presented in the study are included in the article/supplementary material, further inquiries can be directed to the corresponding author.

Author contributions

MK: conceptualization, methodology, writing—original draft. VS: conceptualization, supervision, writing—review and editing, project administration.

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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Appendix A. Convergence theorems

The convergence of the HAM- and OHAM-based solutions are proved theoretically using the following theorems.

A.1 Convergene Theorem of HAM-Based Solution.

The convergence theorem for the HAM-based solutions given by Eq. 45 can be proved using the following theorems.

Theorem A.1: If the homotopy series $\sum_{m=0}^{\infty} C_{i,m}(x,t)$, $\sum_{m=0}^{\infty} \frac{\partial C_{i,m}(x,t)}{\partial t}$, $\sum_{m=0}^{\infty} \frac{\partial C_{i,m}(x,t)}{\partial x}$, and $\sum_{m=0}^{\infty} \frac{\partial^2 C_{i,m}(x,t)}{\partial x^2}$ converge, then $R_{i,m}(\vec{C}_{i,m-1})$ given by Eqs. 37, 38 satisfies the relation $\sum_{m=1}^{\infty} R_{i,m}(\vec{C}_{i,m-1}) = 0$.

Proof: The auxiliary linear operators was defined as follows:

$$\mathcal{L}_i[C_i] = r_i \frac{\partial C_i}{\partial t} \tag{A1}$$

According to Eq. 4, we obtain:

$$\mathcal{L}_i[C_{i,1}] = \hbar R_{i,1}\left(\overrightarrow{C_{i,0}}\right) \tag{A2}$$

$$\mathcal{L}_i[C_{i,2} - C_{i,1}] = \hbar R_{i,2}\left(\overrightarrow{C_{i,1}}\right) \tag{A3}$$

$$\mathcal{L}[C_{i,3} - C_{i,2}] = \hbar R_{i,3}\left(\overrightarrow{C_{i,2}}\right) \tag{A4}$$

$$\mathcal{L}_i[C_{i,m} - C_{i,m-1}] = \hbar R_{i,m}\left(\overrightarrow{C_{i,m-1}}\right) \tag{A5}$$

Adding all the above terms, we get:

$$\mathcal{L}_i[C_{i,m}] = \hbar \sum_{k=1}^{m} R_{i,k}\left(\overrightarrow{C_{i,k-1}}\right) \tag{A6}$$

As the series $\sum_{m=0}^{\infty} C_{i,m}(x,t)$, $\sum_{m=0}^{\infty} \frac{\partial C_{i,m}(x,t)}{\partial t}$, $\sum_{m=0}^{\infty} \frac{\partial C_{i,m}(x,t)}{\partial x}$, *and* $\sum_{m=0}^{\infty} \frac{\partial^2 C_{i,m}(x,t)}{\partial x^2}$ are convergent, $\lim_{m \to \infty} C_{i,m}(x,t) = 0$ and $\lim_{m \to \infty} C_{i,m}{}'(x,t) = 0$. Now, recalling the above summand and taking the limit, the required result follows as

$$\hbar \sum_{k=1}^{\infty} R_{i,k}\left(\overrightarrow{C_{i,k-1}}\right) = \hbar \lim_{m \to \infty} \sum_{k=1}^{m} R_{i,k}\left(\overrightarrow{C_{i,k-1}}\right) = \lim_{m \to \infty} \mathcal{L}[C_{i,m}] = r_i \lim_{m \to \infty} C_{i,m}{}'(x,t) = 0 \tag{A7}$$

Theorem A.2: If $\hbar$ is so properly chosen that the series $\sum_{m=0}^{\infty} C_{i,m}(x,t)$, $\sum_{m=0}^{\infty} \frac{\partial C_{i,m}(x,t)}{\partial t}$, $\sum_{m=0}^{\infty} \frac{\partial C_{i,m}(x,t)}{\partial x}$, and $\sum_{m=0}^{\infty} \frac{\partial^2 C_{i,m}(x,t)}{\partial x^2}$ converge absolutely to $C_i(x,t)$, $\frac{\partial C_i(x,t)}{\partial t}$, $\frac{\partial C_i(x,t)}{\partial x}$, and $\frac{\partial^2 C_i(x,t)}{\partial x^2}$, respectively, then the homotopy series $\sum_{m=0}^{\infty} C_{i,m}(x,t)$ satisfies the original governing Eqs 33, 34.

Proof: Theorem A.1 shows that if $\sum_{m=0}^{\infty} C_{i,m}(x,t)$, $\sum_{m=0}^{\infty} \frac{\partial C_{i,m}(x,t)}{\partial t}$, $\sum_{m=0}^{\infty} \frac{\partial C_{i,m}(x,t)}{\partial x}$, and $\sum_{m=0}^{\infty} \frac{\partial^2 C_{i,m}(x,t)}{\partial x^2}$ converge then $\sum_{m=1}^{\infty} R_{i,m}(\vec{C}_{i,m-1}) = 0$.

Therefore, using the expressions Eqs 37, 38, and simplifying further lead to:

$$r_1 \sum_{m=0}^{\infty} \frac{\partial C_{1,m}}{\partial t} - D \sum_{m=0}^{\infty} \frac{\partial^2 C_{1,m-1}}{\partial x^2} - \left(\frac{\partial D}{\partial x} - v\right) \sum_{m=0}^{\infty} \frac{\partial C_{1,m-1}}{\partial x} + \left(k_1 + \frac{\partial v}{\partial x}\right) \sum_{m=0}^{\infty} C_{1,m-1} = 0 \tag{A8}$$

$$r_2 \sum_{m=0}^{\infty} \frac{\partial C_{2,m-1}}{\partial t} - D \sum_{m=0}^{\infty} \frac{\partial^2 C_{2,m-1}}{\partial x^2} - \left(\frac{\partial D}{\partial x} - v\right) \sum_{m=0}^{\infty} \frac{\partial C_{2,m-1}}{\partial x} + \left(k_2 + \frac{\partial v}{\partial x}\right) \sum_{m=0}^{\infty} C_{2,m-1} - k_1 \sum_{m=0}^{\infty} C_{1,m-1} = 0 \tag{A9}$$

which is basically the original governing Eqs 33, 34. Furthermore, subject to the initial and boundary conditions $C_{i,0}(x,0) = f_i(x)$, $C_{i,0}(0,t) = f_i(0)$, $\lim_{x \to \infty} C_{i,0}(x,t) = 0$, and the conditions for the higher-order deformation equation $C_{i,m}(x,0) = 0 C_{i,m}(0,t) = 0$ $\lim_{x \to \infty} C_{i,m}(x,t) = 0$, for $m \geq 1$, we easily obtain $\sum_{m=0}^{\infty} C_{i,m}(x,0) = f_i(x)$, $\sum_{m=0}^{\infty} C_{i,m}(0,t) = f_i(0)$, and $\lim_{x \to \infty} \sum_{m=0}^{\infty} C_{i,m}(x,t) = 0$. Hence, the convergence result follows.

A.2 Convergence Theorem of OHAM-Based Solution.

Theorem A.3: If the series $C_{i,0}(x,t) + \sum_{j=1}^{\infty} C_{i,j}(x,t,D_{i,i})$, $i = 1, 2, ..., s$ converges, where $C_{i,j}(x,t,D_{i,i})$ are governed by Eqs 60, 61, 62, 63, 64, then Eq. 65 is a solution of the original Eqs 33, 34.

Proof: Based on the choice of the auxiliary function, suppose that the series Eq. 65 is convergent. Then, we get:

$$\lim_{j \to \infty} C_{i,j}(x,t,D_{i,i}) = 0, \quad i = 1, 2, ..., s \tag{A10}$$

One can write:

$$\begin{aligned} C_{i,j}(x,t,D_{i,i}) &= C_{i,0}(x,t,D_{i,i}) + [C_{i,1}(x,t,D_{i,i}) - C_{i,0}(x,t,D_{i,i})] \\ &\quad + [C_{i,2}(x,t,D_{i,i}) - C_{i,1}(x,t,D_{i,i})] + ... \\ &\quad + [C_{i,j}(x,t,D_{i,i}) - C_{i,j-1}(x,t,D_{i,i})] \\ &= C_{i,0}(x,t,D_{i,i}) \\ &\quad + \sum_{k=1}^{j} [C_{i,k}(x,t,D_{i,i}) - C_{i,k-1}(x,t,D_{i,i})], \ i \\ &= 1, 2, ..., s \end{aligned} \tag{A11}$$

Using Eq. A11, one can obtain from Eq. A10:

$$0 = \lim_{j \to \infty} C_{i,j}(x,t,D_{i,i}) = C_{i,0}(x,t,D_{i,i}) + \sum_{k=1}^{\infty} [C_{i,k}(x,t,D_{i,i}) - C_{i,k-1}(x,t,D_{i,i})], \ i = 1, 2, ..., s \tag{A12}$$

Eq. A12 can be rearranged as:

$$\begin{aligned} & C_{i,0}(x,t,D_{i,i}) + h_i(x,t) - h_i(x,t) + [C_{i,1}(x,t,D_{i,i}) - C_{i,0}(x,t,D_{i,i})] \\ & + \sum_{k=2}^{\infty} [C_{i,k}(x,t,D_{i,i}) - C_{i,k-1}(x,t,D_{i,i})], \ i \\ & = 1, 2, ..., s \end{aligned} \tag{A13}$$

Using the property of the linear operator, i.e., $\mathcal{L}[A_1(x,t) + A_2(x,t)] = \mathcal{L}[A_1(x,t)] + \mathcal{L}[A_2(x,t)]$ and $\mathcal{L}(0) = 0$, we have:

$$\begin{aligned} 0 &= \mathcal{L}_i(0) \\ &= \mathcal{L}_i[C_{i,0}(x,t,D_{i,i})] + h_i(x,t) + \mathcal{L}_i[C_{i,1}(x,t,D_{i,i})] - (\mathcal{L}_i[C_{i,0}(x,t,D_{i,i})] + h_i(x,t)) \\ &\quad + \sum_{k=2}^{\infty} (\mathcal{L}_i[C_{i,k}(x,t,D_{i,i})] - \mathcal{L}_i[C_{i,k-1}(x,t,D_{i,i})]) \\ &= H_{i,1}(x,t,D_{i,i}) N_{i,0}[C_{i,0}(x,t,D_{i,i})] \\ &\quad + \sum_{k=2}^{\infty} \left(H_{i,k}(x,t,D_{i,i}) N_{i,0}[C_{i,0}(x,t,D_{i,i})] + \sum_{l=1}^{k-1} H_{i,l}(x,t,D_{i,i}) [\mathcal{L}_i[C_{i,k-l}(x,t,D_{i,i})] \right. \\ &\quad \left. + N_{i,k-l}[C_{i,0}(x,t,D_{i,i}), C_{i,1}(x,t,D_{i,i}), ..., C_{i,k-l}(x,t,D_{i,i})]] \right) \\ &= \left[\sum_{k=1}^{\infty} H_{i,k}(x,t,D_{i,i})\right] N_{i,0}[C_{i,0}(x,t,D_{i,i})] + \sum_{k=2}^{\infty} \sum_{l=1}^{k-1} H_{i,l}(x,t,D_{i,i}) \\ &\quad \times [\mathcal{L}_i[C_{i,k-l}(x,t,D_{i,i})] + N_{i,k-l}[C_{i,0}(x,t,D_{i,i}), C_{i,1}(x,t,D_{i,i}), ..., C_{i,k-l}(x,t,D_{i,i})]] \\ &= H_i(x,t,D_{i,i}) N_{i,0}[C_{i,0}(x,t,D_{i,i})] \\ &\quad + \sum_{k=2}^{\infty} \sum_{l=1}^{k-1} H_{i,l}(x,t,D_{i,i}) \times [\mathcal{L}_i[C_{i,k-l}(x,t,D_{i,i})] + N_{i,k-l}[C_{i,0}(x,t,D_{i,i}), \\ &\quad C_{i,1}(x,t,D_{i,i}), ..., C_{i,k-l}(x,t,D_{i,i})]] = H_i(x,t,D_{i,i}) N_{i,0}[C_{i,0}(x,t,D_{i,i})] \\ &\quad + \sum_{k=1}^{\infty} H_{i,k}(x,t,D_{i,i}) \sum_{p=1}^{\infty} \left[\mathcal{L}_i\left[C_{i,p}(x,t,D_{i,i})\right] + N_{i,p}[C_{i,0}(x,t,D_{i,i}), \right. \\ &\quad C_{i,1}(x,t,D_{i,i}), ..., C_{i,p}(x,t,D_{i,i})]] = H_i(x,t,D_{i,i}) N_{i,0}[C_{i,0}(x,t,D_{i,i})] \\ &\quad + H_i(x,t,D_{i,i}) \\ &\quad \times \left[\mathcal{L}_i\left(\sum_{p=1}^{\infty} C_{i,p}(x,t,D_{i,i})\right) + \sum_{p=1}^{\infty} N_{i,p}[C_{i,0}(x,t,D_{i,i}), C_{i,1}(x,t,D_{i,i}), ..., C_{i,p}(x,t,D_{i,i})]\right] \\ &= H_i(x,t,D_{i,i}) N_{i,0}[C_{i,0}(x,t,D_{i,i})] \\ &\quad + H_i(x,t,D_{i,i}) \times [\mathcal{L}_i(C_i(x,t,D_{i,i})) - \mathcal{L}_i(C_{i,0}(x,t,D_{i,i})) + N_i(C_i(x,t,D_{i,i})) - N_i(C_{i,0}(x,t,D_{i,i}))] \\ &= H_i(x,t,D_{i,i}) N_{i,0}[C_{i,0}(x,t,D_{i,i})] + H_i(x,t,D_{i,i}) \\ &\quad \times [\mathcal{L}_i(C_i(x,t,D_{i,i})) - [\mathcal{L}_i(C_{i,0}(x,t,D_{i,i})) + h_i(x,t)] + h_i(x,t) \\ &\quad + N_i(C_i(x,t,D_{i,i})) - N_i(C_{i,0}(x,t,D_{i,i}))] = H_i(x,t,D_{i,i}) [\mathcal{L}_i(C_i(x,t,D_{i,i})) + h_i(x,t) \\ &\quad + N_i(C_i(x,t,D_{i,i}))], \ i = 1, 2, ..., s \end{aligned} \tag{A14}$$

Now, since $H_i(x,t,D_{i,i}) \neq 0$, from Eq. A14 we have

$$\mathcal{L}_i(C_i(x,t,D_{i,i})) + h_i(x,t) + N_i(C_i(x,t,D_{i,i})) = 0, \ i = 1, 2, ..., s \tag{A15}$$

which shows that $C_i(x,t,D_{i,i})$ is the exact solution of Eqs 33, 34.