International Communications in Heat and Mass Transfer 131 (2022) 105869

Contents lists available at ScienceDirect

International Communications in Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ichmt

Analytical solution of the convection-diffusion-reaction-source (CDRS) equation using Green's function technique

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ARTICLE INFO

Keywords:
Convection-diffusion-reaction-source (CDRS) equation
Green's function
Analytical modeling

ABSTRACT

Convection-diffusion-reaction-source (CDRS) equation has been used to model a variety of transport phenomena. While several numerical methods for solving the CDRS equation exist, there is a relative lack of analytical solutions for the CDRS problem for an arbitrary source term. This work presents a Green's function based analytical solution to a one-dimensional, transient CDRS equation with an independent source/sink that can be a general function of space and time. Results compare well with past work as well as an independent numerical simulation. The model presented here is simple, computationally fast, and does not suffer from stability problems commonly encountered in numerical solutions of the CDRS equation. Furthermore, the model is used to solve a representative CDRS problem. The model presented here may help analyze transport problems in various engineering applications, such as drug delivery, heat transfer in reacting systems, and air pollution dispersion. The analytical solution may also serve as a building block for solving more complicated problems such as transport in a multilayer body, as well as for verifying numerical simulation tools.

1. Introduction

Conservation equations involving diffusion, convection, and reaction, commonly known as CDR equations, have been used to model a variety of engineering problems, including drug delivery in drug-eluting stents [1], mass transfer through porous media [2,3], chemicals dispersion in reactors [4], trickle beds [5], contaminant transport, pollution, and environmental applications [6–8]. A large number of analytical solutions have been presented for CDR equations in single-layer and multi-layer bodies. However, there are relatively fewer available analytical solutions for a convection-diffusion-reaction equation involving an independent source or sink term, known as a CDRS equation. Past papers have suggested that an analytical solution of the CDRS equation is, in general, difficult to obtain [9,10].

Analytical solutions have been derived for special cases such as convection-diffusion equation with a constant source term to model contaminant transport in streams and rivers [7], or diffusion-source equation without the effect of convective transport [11]. A few studies have derived analytical solutions to CDRS problems with more general source terms. For example, a generalized integral transform technique (GITT) was used to develop an exact solution for a CDRS problem with a space-dependent source term and coefficients [12] and a general source term and constant boundary conditions [13]. A combination of Laplace transform with the GITT was used to obtain an analytical solution to the CDRS problem in a semi-infinite domain with a time-dependent boundary condition. However, the source term in this study was a product of a space-dependent and a time-dependent function [14]. Laplace transform was used to derive analytical solutions for the CDRS problem involving uniform varying pulse input point sources [3]. The eigenfunction expansion method was used to derive an analytical solution for the CDRS problem involving a general source term, time-dependent temperature boundary conditions, and spatially varying diffusivity and velocity [8]. Green's function method was used to obtain analytical solution of the infinite domain CDRS problem to study solute transport in groundwater [15]. A one-sided Laplace transform was used to derive an analytical solution to the general CDRS equation [9]. A transfer function analysis of generalized diffusion equations using Green's functions has been presented for infinite [16] and semi-infinite media [17]. Unlike the limited number of available analytical solutions, a significant amount of past literature is available on numerical and approximate analytical solutions of the CDRS equation. Early work by Codina [18] presented a comparison between a number of finite-element methods for solving the CDRS equation. A numerical solution

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https://doi.org/10.1016/j.icheatmasstransfer.2021.105869

Nomenclature

Bi	Biot number
h	convective heat transfer coefficient ($Wm^{-2}\ K^{-1}$)
k	thermal conductivity ($Wm^{-1}\ K^{-1}$)
L	length (m)
N	eigenvalue norm
Pe	Péclet number, the non-dimensional ratio of diffusion and convection terms
T	temperature (relative to ambient) (K)
T_0	initial temperature (K)
U	velocity (ms^{-1})
x	spatial coordinate (m)
s	source/sink term (Ks^{-1})
$\bar{s}$	non-dimensional source/sink
t	time (s)
α	diffusivity (m^2s^{-1})
β	generation/consumption coefficient (s^{-1})
$\bar{\beta}$	non-dimensional generation/consumption coefficient
τ	non-dimensional time
θ	non-dimensional temperature
θ_0	non-dimensional initial temperature
ξ	non-dimensional spatial coordinate
λ	non-dimensional eigenvalue

to the CDRS equation based on an improved spectral Galerkin method was recently presented [10]. A Lattice Boltzmann method based numerical solution of the convection-diffusion equation with a general source term has been presented [19]. A semi-analytical solution for the CDRS equation to model solute transport in a multi-layer porous media using Laplace transform has been presented [20]. Boundary Element Method (BEM), which may be seen as a numerical version of the analytical Green's function technique, has been also implemented to solve one- and two-dimensional convection-diffusion (CD) equations [21–23] and two-dimensional CDR equations [24]. Compared to other numerical methods, BEM only requires discretization at the boundaries and not the entire domain, resulting in computational efficiency.

These numerical models typically require considerable computational time or memory due to a large set of ordinary differential equations (ODEs) resulting from spatial discretization. Further, numerical models may suffer from instability under certain conditions [25]. These challenges are exacerbated in problems involving multi-layer media. Analytical solutions, on the other hand, offer better accuracy and computational speed, and provide useful insights into the fundamental nature of the problem. Therefore, a simple closed-form analytical solution of the CDRS equation is desirable. Such a solution for a single-layer body may serve as the basis for the analysis of more complicated multi-layered geometries. It may also help verify the accuracy of numerical simulation codes.

This paper presents an analytical solution of the one-dimensional CDRS equation for a finite domain with an arbitrary initial condition, a general source/sink term, and general time-dependent boundary conditions using the Green's function method. Unlike most of the previous studies that assumed constant or specific types of source/sink terms, the closed-form solution presented here can be used for problems with any general time- and space-dependent source/sink term. Despite the infinite-series nature of the solution, it is shown that only a few eigenvalues are sufficient for an accurate solution, resulting in a computationally fast model, compared to numerical methods. The analytical solution compares well with results from a past study as well as numerical simulations. The theoretical model presented here expands the understanding of multi-phenomena transport processes. The model presented here may be helpful for analytical solutions of transport problems occurring in several practical applications such as drug delivery, heat transfer in reacting systems, dispersion of air pollution and porous media.

2. Problem statement and non-dimensionalization

Consider a one-dimensional transient problem governed by a convection-diffusion-reaction-source (CDRS) equation, such as shown in Fig. 1. While discussed here as a heat transfer problem, the treatment is equally applicable to other transport problems, such as species transport governed by diffusion, convection, and species generation/consumption.

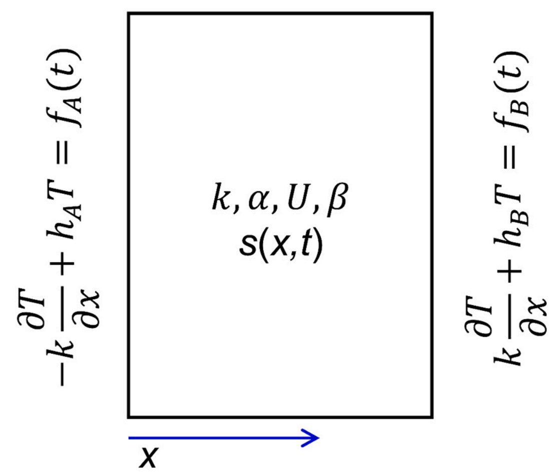

Fig. 1. Schematic of the single-layer problem with diffusion, convection, reaction and a general source term.

In the present problem, heat transfer occurs within this body due to diffusion as well as convection due to an imposed one-dimensional fluid flow. In addition, heat is generated or absorbed throughout the body at a rate proportional to the local temperature. Finally, an arbitrary source term that varies in both space and time is also imposed throughout the body. A general time-dependent boundary condition of the third kind is assumed at both boundaries. This can be reduced to boundary conditions of the first and second kinds by an appropriate choice of the convective heat transfer coefficient. Assuming temperature-independent properties, the governing energy conservation equation for this problem is

$$\frac{\partial T}{\partial t} = \alpha\frac{\partial^2 T}{\partial x^2} - U\frac{\partial T}{\partial x} + \beta T + s(x,t) \tag{1}$$

Where T represents the temperature relative to ambient temperature. α and U represent thermal diffusivity and velocity, respectively. β is the source coefficient that models heat generation/absorption that is linearly dependent on the temperature field, such as in a first-order exothermic/endothermic chemical reaction. $s(x,t)$ is an arbitrary source term that represents a non-homogeneity in the governing equation. The associated boundary conditions are taken to be

$$-k\frac{\partial T}{\partial x} + h_A T = f_A(t) at\ x = 0 \tag{2}$$

$$k\frac{\partial T}{\partial x} + h_B T = f_B(t)\ at\ x = L \tag{3}$$

Note that Eqs. (2) and (3) can be transformed to the temperature and flux boundary conditions by choosing k, h, and f appropriately. Further, an arbitrary initial temperature distribution is assumed as follows:

$$T = T_0(x)\ at\ t = 0 \tag{4}$$

Eqs. (1)–(4) are non-dimensionalized using the non-dimensional parameters defined below:

$\theta = \frac{T}{T_{ref}}$, $\xi = \frac{x}{L}$, $\tau = \frac{\alpha_2 t}{L^2}$, $Pe = \frac{UL}{\alpha}$, $\overline{\beta} = \frac{\beta L^2}{\alpha}$, $\theta_0 = \frac{T_0}{T_{ref}}$, $Bi_A = \frac{h_A L}{k}$, $Bi_B = \frac{h_B L}{k}$, $\overline{s} = \frac{sL^2}{\alpha T_{ref}}$, $F_A = \frac{Lf_A}{kT_{ref}}$, $F_B = \frac{Lf_B}{kT_{ref}}$.

Here, Pe is the Péclet number that represents the ratio of diffusion and convection terms.

Based on this, the non-dimensional CDRS equations are

$$\frac{\partial\theta}{\partial\tau} = \frac{\partial^2\theta}{\partial\xi^2} - Pe\frac{\partial\theta}{\partial\xi} + \overline{\beta}\theta + \overline{s}(\xi,\tau) \tag{5}$$

$$-\frac{\partial\theta}{\partial\xi} + \mathrm{B}i_A\theta = F_A(\tau) at\ \xi = 0 \tag{6}$$

$$\frac{\partial\theta}{\partial\xi} + Bi_B\theta = F_B(\tau)\ at\ \xi = 1 \tag{7}$$

$$\theta = \theta_0\ (\xi)\ at\ \tau = 0 \tag{8}$$

The general solution to a non-dimensional transport equation using Green's function approach can be written as:

$$\psi(\xi\tau) = \int_{L'} G(\xi,\tau|\xi',\tau')_{\tau'=0}\psi_0(\xi')\xi'^p d\xi' + \int_{\tau=0}^{t}\int_{L'} G(\xi,\tau|\xi',\tau')g(\xi',\tau')\xi'^p d\xi' d\tau' + \sum_{i=1}^{N}\left\{\int_{\tau=0}^{t}\int [\xi'^p G(\xi,\tau|\xi',\tau')]_{\xi'=\xi_i} F_i(\tau')d\tau'\right\} \tag{9}$$

where L is the domain of the 1-D region, ψ is a general transport variable, $\theta(\xi,\tau)$ in this casee. ξ'^p is the Sturm–Liouville weight function, and $p = 0$, 1 or 2 represents slabs, cylinders or spheres respectively. $\psi_0(\xi')$, $g(\xi',\tau')$, and $F_i(\tau')$ are the non-homogeneities in the initial condition, source/sink, and the boundary conditions. Thus, the first, second, and third terms in Eq. (9) describes the contribution of the initial condition θ_0, source/sink $\overline{s}$, and the boundary conditions F_A and F_B, respectively. G is the Green's function that must be determined from the solution of the homogeneous CDRS equation. In the case of the first type boundary conditions, the third term on the right-hand side of Eq. (9) must be modified, as described in [26]. By defining a new variable $\varphi(\xi,\tau) = \theta(\xi,\tau)exp\left(-\frac{Pe\xi}{2}\right)$, the corresponding homogeneous problem can be written as follows:

$$\frac{\partial\varphi}{\partial\tau} = \frac{\partial^2\varphi}{\partial\xi^2} + \left(\overline{\beta} - \frac{Pe^2}{4}\right)\varphi \tag{10}$$

$$-\frac{\partial\varphi}{\partial\xi} + Bi_A^*\varphi = 0\ at\ \xi = 0 \tag{11}$$

$$\frac{\partial\varphi}{\partial\xi} + Bi_B^*\varphi = 0\ at\ \xi = 1 \tag{12}$$

$$\varphi = \theta_0(\xi)exp\left(-\frac{Pe\xi}{2}\right) = \varphi_0\ (\xi)\ at\ \tau = 0 \tag{13}$$

where $Bi_A^* = Bi_A - \frac{Pe}{2}$ and $Bi_B^* = Bi_B + \frac{Pe}{2}$. Using separation of variables, the solution to the above equations can be written to be of the following form:

$$\varphi(\xi,\tau) = \sum_{n=1}^{\infty} A_n\left[cos(\omega_n\xi) + \frac{Bi_A^*}{\omega_n}sin(\omega_n\xi)\right]exp\left(-\lambda_n^2\tau\right) \tag{14}$$

where $\omega_n = \sqrt{\lambda_n^2 + \overline{\beta} - \frac{Pe^2}{4}}$. The eigenvalues and coefficients in the spatial term need to be chosen to satisfy the boundary conditions, whereas coefficients A_n need to be chosen in order to account for the initial condition. Substituting Eq. (13) into the boundary conditions given by Eq. (12) results in the following eigenequation:

$$\omega_n\left[-sin(\omega_n) + \frac{Bi_A^*}{\omega_n}cos(\omega_n)\right] + Bi_B^*\left[cos(\omega_n) + \frac{Bi_A^*}{\omega_n}sin(\omega_n)\right] = 0 \tag{15}$$

Applying the initial condition on Eq. (14) results in the following expression for A_n:

$$A_n = \frac{1}{N_n}\int_0^1 \phi_0(\xi')\left[cos(\omega_n\xi') + \frac{Bi_A^*}{\omega_n}sin(\omega_n\xi')\right]d\xi' \tag{16}$$

where the norm N_n is given by

$$N_n = \int_0^1 \left[cos(\omega_n\xi) + \frac{Bi_A^*}{\omega_n}sin(\omega_n\xi)\right]^2 d\xi \tag{17}$$

The final expression for $\varphi(\xi,\tau)$ can be written as:

$$\varphi(\xi,\tau) = \sum_{n=1}^{\infty}\int_0^1 \frac{1}{N_n}exp\left(-\lambda_n^2\tau\right)\left[\left(cos(\omega_n\xi) + \frac{Bi_A^*}{\omega_n}sin(\omega_n\xi)\right)\left(cos(\omega_n\xi') + \frac{Bi_A^*}{\omega_n}sin(\omega_n\xi')\right)\right]\phi_0(\xi')d\xi' \tag{18}$$

Comparing Eq. (18) with Eq. (9) results in the following Green's function calculated for $\tau' = 0$:

$$G(\xi,\tau|\xi',\tau')_{\tau'=0} = \sum_{n=1}^{\infty}\frac{1}{N_n}exp\left(-\lambda_n^2\tau\right)\left[\left(cos(\omega_n\xi) + \frac{Bi_A^*}{\omega_n}sin(\omega_n\xi)\right)\left(cos(\omega_n\xi') + \frac{Bi_A^*}{\omega_n}sin(\omega_n\xi')\right)\right] \tag{19}$$

The general expression of the Green's function is obtained by replacing τ with $\tau - \tau'$in Eq. (19) as follows:

$$G(\xi,\tau|\xi',\tau') = \sum_{n=1}^{\infty}\frac{1}{N_n}exp\left(-\lambda_n^2(\tau-\tau')\right)\left[\left(cos(\omega_n\xi) + \frac{Bi_A^*}{\omega_n}sin(\omega_n\xi)\right)\left(cos(\omega_n\xi') + \frac{Bi_A^*}{\omega_n}sin(\omega_n\xi')\right)\right] \tag{20}$$

Finally, the complete solution for φ is obtained by substituting Eq. (20) into the general form of the solution given by Eq. (9). The temperature field is then obtained by using $\theta(\xi,\tau) = \varphi(\xi,\tau)exp\left(\frac{Pe\xi}{2}\right)$.

This completes an analytical solution of the CDRS problem with an arbitrary source term. This solution is relatively straightforward and does not require computationally-intensive inverse Laplace transform. Note that the solution has been derived for a general boundary condition of the third kind. The boundary condition reduces to that of the first or second kind by setting the associated Biot number to infinity or zero, respectively. Finally, note that if both boundary conditions are adiabatic, i.e., $Bi_A = Bi_B = 0$, then the $\lambda = 0$ eigenvalue must be included [26].

3. Results and discussion

Since the analytical solution presented in the previous section contains an infinite eigenvalue-based series, the accuracy of results and the required computational time both depend on the number of eigenvalues

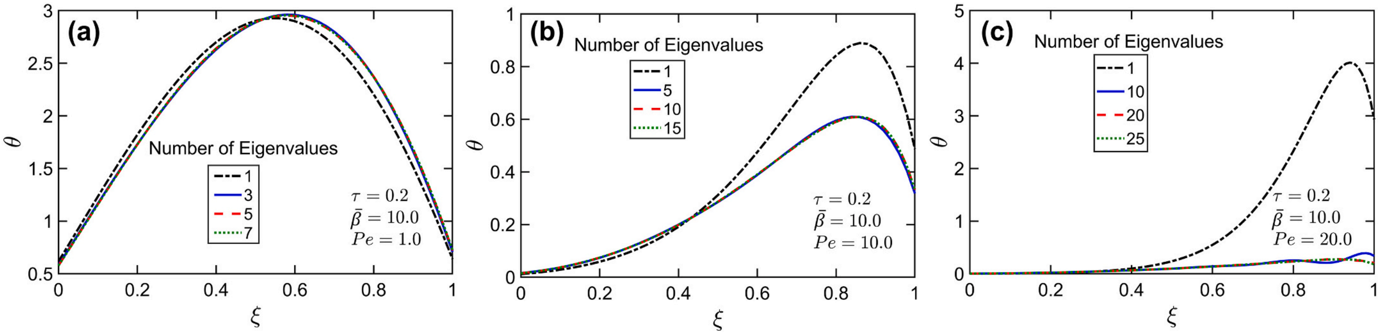

Fig. 2. Effect of the number of eigenvalues on the accuracy of the solution: Spatial variation in temperature θ at $\tau = 0.2$ for $\bar{s} = 60sin(\xi\tau)$, $Bi_A = 10$, $Bi_B = 15$, $Pe = 1$, and $\bar{\beta} = 10$ for: (a) $Pe = 1$, (b) $Pe = 10$, and (c) $Pe = 20$.

considered in the solution. In order to examine the effect of the number of eigenvalues, the non-dimensional temperature is plotted as a function of space for different numbers of eigenvalues in Fig. 2. A case with convective boundary conditions at both ends – $Bi_A = 10$ and $Bi_B = 15$ – is considered as an example. The values of α and $\bar{\beta}$ are taken to be 1 and 10. Three different values of $Pe = 1$, 10, and 20 are considered for this problem. Further, a periodic source term $\bar{s} = +60sin(\xi\tau)$ is considered in this case. Fig. 2(a), (b), and (c) show the temperature distribution as a function of space for $Pe = 1$, 10, and 20, respectively. Fig. 2 shows that the temperature distribution changes as the number of eigenvalues increases and converges to the final distribution for all the *Pe* values. As shown, the number of eigenvalues required for convergence increases as the Péclet number increases. However, even for a very large $Pe = 20$, the number of eigenvalues needed is still reasonably small. In general, for any given problem, it is important to independently determine the minimum number of eigenvalues needed for convergence, since this may depend on the values of specific parameters, as shown in Fig. 2. For this particular problem, 7, 15, and 25 eigenvalues are sufficient for convergence for $Pe = 1$, 10, and 20, respectively, resulting in a total computation time of around 0.4 s, 2.0 s, and 3.3 s, respectively, compared to 4.1 s for a discretization-based numerical technique.

A comparison against previous work [10] is carried out in order to validate the analytical solution developed in the present study. Zhong et al. presented a numerical solution to the transient CDRS equations subject to an independent source/sink term based on an improved spectral Galerkin method [10]. Note that this past work was carried out in the context of mass transfer, and results were presented with dimensional units [10]. Fig. 3 presents a comparison of the analytical model with the past work. Specifically, concentration is plotted as a function of space at three different locations in Fig. 3(a) and as a function of time at three specific locations in Fig. 3(b). The parameters used for comparison are $\alpha = 1$, $\beta = 1$, $U = 1$, $Pe = \pi$, and $s = e^{-0.5x}\sin(5x)$, consistent with the ones used by Zhong et al. [10]. Results show very good agreement between the present analytical model and the past work.

The accuracy of the analytical solution presented here is further established through a comparison with a numerical simulation. The numerical simulation is carried out using an implicit finite difference method. Non-dimensional governing equations (Eqs. (5)–(8)) are discretized using a central difference scheme into 1000 spatial nodes and 1000 time steps. Comparison is carried out for two different cases. In the first case shown in Fig. 4(a), a constant initial condition of $\theta = 1$ and isothermal boundary conditions at the two ends, $\theta = 0$, are considered. The values of α and $\bar{\beta}$ are taken to be 1 and 10, respectively. The non-dimensional source term is taken to be $\bar{s} = 10\xi\tau$. Fig. 4(a) shows excellent agreement between the temperature profile predicted by the analytical solution and the numerical simulation for different values of *Pe* ranging from $Pe = 0$ to $Pe = 20$. These curves clearly show the impact of increasing *Pe*. As *Pe* increases, the impact of convection relative to diffusion increases, which is the reason why the curves in Fig. 4(a) shift somewhat towards the right, and the peaks go down, due to increased heat removal by convection. For further comparison, a case with a different source function is considered. Boundary conditions and values of other parameters α, β, θ_0 and *Pe* are taken to be the same as those in Fig. 4(a). A sinusoidal source term $\bar{s} = 60sin(\xi\tau)$ is considered. Results plotted in Fig. 4(b) show, similar to Fig. 4(a), excellent agreement between the analytical solution and the numerical simulation. Good agreement with the numerical simulation provides further confidence in the correctness of the analytical derivation presented here.

To demonstrate the capability of the present model, a more sophisticated source/sink function is considered next. The model is used to solve the CDRS equation subject to a source/sink term that combines sinusoidal variation in space with exponential reduction in time. A constant initial condition of $\theta = 0$ and convective boundary conditions at the two with $Bi_A = 0.5$ and $Bi_B = 0.25$ are considered. The values of α, $\bar{\beta}$, and *Pe* are taken to be 1, 2, and 1, respectively. Fig. 5(a) and (b) present plots of non-dimensional temperature as a function of non-dimensional space at $\tau = 1$ for two different sources – $\bar{s} = e^{-\tau}sin(2\pi x)$ and $\bar{s} = e^{-\tau}sin$

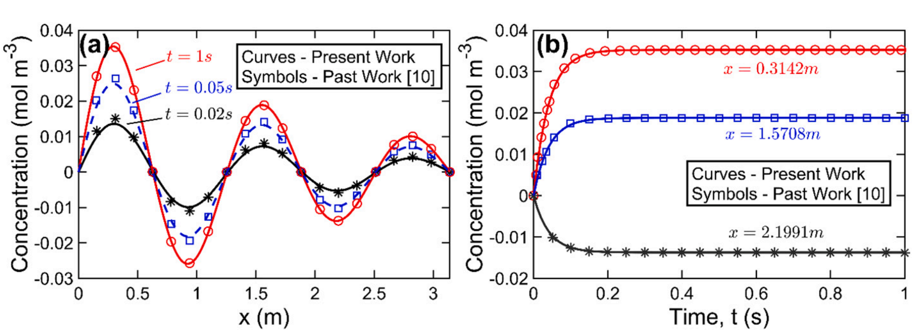

Fig. 3. Comparison of present analytical model against past numerical work [10]: (a) Concentration as a function of space at three different times, and (b) Concentration as a function of time at three different locations.

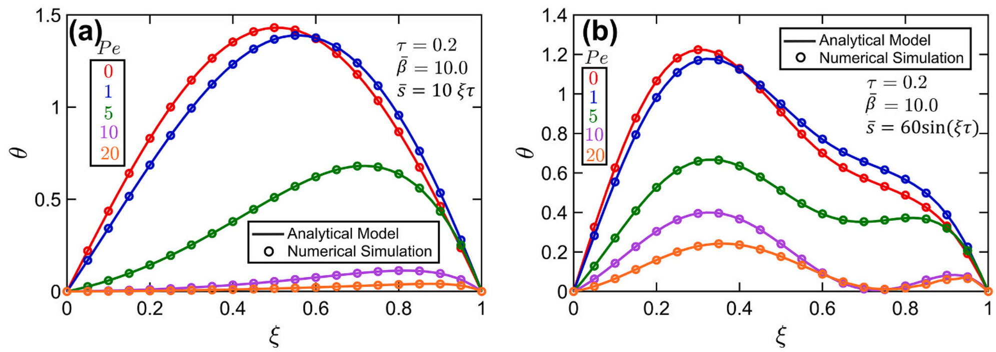

Fig. 4. Comparison of the analytical model against numerical simulations: Spatial variation in temperature θ at $\tau = 0.2$ for multiple values of Péclet number for (a) $\overline{s} = 10\xi\tau$ and $\overline{\beta} = 10$, and (b) $\overline{s} = 60sin(\xi\tau)$ and $\overline{\beta} = 10$.

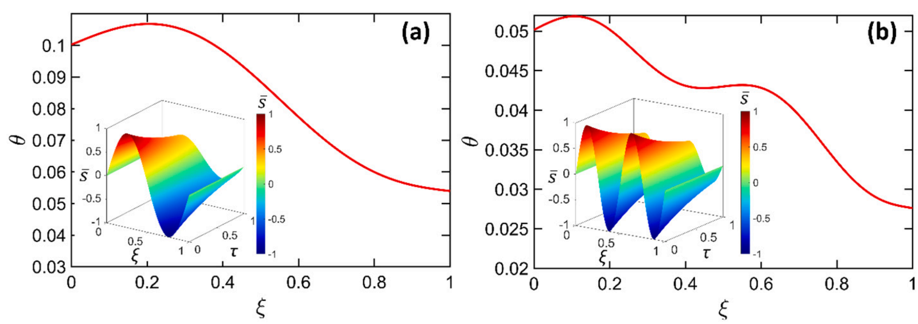

Fig. 5. Non-dimensional temperature θ as a function of ξ at $\tau = 1$ for (a) $\overline{s} = e^{-\tau}sin(2\pi x)$, and (b) $\overline{s} = e^{-\tau}sin(4\pi x)$. Insets show the source contour as a function of ξ and τ. Parameter values are $Bi_A = 0.5$, $Bi_B = 0.25$, $Pe = 1$, and $\overline{\beta} = 2$.

$(4\pi x)$ – respectively. The source/sink function is also shown in the inset. As shown in Fig. 5(a) inset, the source/sink starts from zero, becomes positive (heat generation), changes sign and becomes negative (heat consumption) at $\xi = 0.5$, and finally reaches zero at $\xi = 1$. Fig. 5(a) shows that the temperature profile captures the periodic nature of the source function, resulting in maximum temperature in the first half of the body due to heat generation and relatively lower temperatures in the second half of the body due to heat consumption. In a more complicated scenario, Fig. 5(b) shows multiple peaks and troughs in the computed temperature profile that are consistent with the underlying source/sink function. In both cases, in addition to the spatial variation, there is a gradual reduction in temperature over time due to the exponentially decaying nature of the heat generation term. These figures demonstrate the capability of the analytical model to model physical phenomena governed by CDRS equations involving arbitrary independent source/sink term.

4. Conclusions

This work presents a Green's function based analytical solution to a transient one-dimensional CDRS equation with any arbitrary source/sink term. The analytical solution accounts for arbitrary initial condition, source-sink term, and general time-dependent boundary conditions. The resulting analytical solution presented here is exact, computationally fast, and compares well with past work and an independent numerical simulation. Solution of a specific CDRS problem presented in the previous section demonstrates the capability of the analytical model. In general, the model is capable of solving problems with arbitrary source/sink term without the need for computationally intensive steps such as inverse Laplace transform. In addition to improving the understanding of multi-phenomena transport processes, this work may also help solve practically relevant transport problems in a variety of applications.

Declaration of Competing Interest

None.

Acknowledgments

Mohammad Parhizi acknowledges the Purdue Polytechnic Institute Post-Doctoral Fellowship Program for financial support on this project. This material is partly based upon work supported by CAREER Award No. CBET-1554183 from the National Science Foundation.

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