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On the solution of a parabolic PDE involving a gas flow through a semi-infinite porous medium

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ABSTRACT

Taking as start point the parabolic partial differential equation with the respective initial and boundary conditions, the present research focuses onto the flow of a sample of waste-water derived from a standard/conventional dyeing process. In terms of a highly prioritized concern, meaning environment decontamination and protection, in order to remove the dyes from the waste waters, photocatalyses like ZnO or TiO_2 nanoparticles were formulated, due to their high surface energy which makes them extremely reactive and attractive. According to the basics of ideal fluid, the key point is the gas flow through an ideal porous pipe consisting of nanoparticles bound one to each other, forming a porous matrix/pipe. The modeling of the gas flow through a porous media is quite valuable because of its importance in investigating the gas-solid processes.

The present study is a valid contribution to the existing literature, by developing a nonstandard line method for the partial differential equation, in order to obtain a numerical solution of unsteady flow of gas through nano porous medium. Hence, the physical problem is modeled by a highly nonlinear ordinary differential equation detailed on a semi-finite domain and represents a guidance for several questions originating in the gas flow theory.

The findings of this study offered a facile approach to improve an attractive issue related to materials science/chemistry, like synthesis of ZnO or TiO_2 nanoparticles forming an ideal nano porous pipe with efficiency in industrial waste waters decontamination.

Preliminaries

Diffusion, which is the irregular movement of atoms and molecules, is a universal phenomenon of mass transfer occurring in all states of matter. It is of equal importance for the fundamental research and the technological applications as well. Many challenges in performing reliable observations of these phenomena in nano-porous materials have been found in the literature. The transport phenomena and the diffusion in micro-nano porous materials have attracted the attentions for a long period of time. Some of these problems are engineered by strongly nonlinear boundary value problems BVPs on unbounded domains. Generally speaking, the nonlinear boundary value problems on an infinite domain occur in numerous domains such as: thermodynamics, chemical kinetics, mathematical physics, thermal behavior, fluid mechanics and many other topics [1,2]. The conventional approach is the substitution of the infinite domain with a truncated finite interval considering a sufficiently large finite value, the so-called truncated boundary, with an adequate boundaries condition. Hence, the truncated boundary found applications in numerous areas of the applied sciences where the mathematical modeling is mandatory. The weakest point of this classical approach is to achieve a satisfactory accurate truncated boundary by the trial and errors. In fact, the concept of the adequate boundary conditions is an open problem and affect the outcomes [3–6]. Thus, by using the strictly monotonic functions [7,8] the entire infinite domain is considered in a mapping where the grid-points are located at a mid-point of each sub-interval. In this way, the difficulty caused by numerical treatment of the last infinite sub-interval is avoided. Riccardo proposed a method effectively which is

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used to determine the numerical solution for the boundary conditions that were exactly assigned at infinity [9]. Such an example originates from the survey of the unsteady flow of a gas through a semi-infinite porous medium when the medium be initially filled with the gas at a uniform pressure P_0. To date, abundant and meaningful research achievements have been made emphasizing the accuracy and stability of the approach, by transforming unsteady gas equation into a non-linear ordinary differential equation ODE which quite simplified the original problem [10].

In terms of a highly prioritized concern, meaning environment decontamination and protection, in order to remove the dyes from the waste waters, photocatalysts like ZnO or TiO_2 nanoparticles have been synthesized, due to their high surface energy which makes them extremely reactive and attractive [11]. Usually, these types of nanoparticles/systems undergo aggregation. Moreover, there are authors reporting the fluid flow through a porous medium as a completely interconnected network, formed by the constricted channel between each pore so that the fluid may flow [12].

According to the basics of an ideal fluid, the key point of this endeavor is an ideal porous pipe consisting of nanoparticles bound one to each other, forming a porous matrix.

Thus, this novel approach formulated a gas flow through a nano-porous medium. The modeling of the gas flow through a porous media is quite valuable because of its importance in investigating the gas–solid processes. Although a lot of applications of porous media have been found in several fields of applied sciences and engineering, up to our knowledge this kind of approach has not yet been advanced.

Specifically, the present research developed a nonstandard line method for the partial differential equation, in order to obtain a numerical solution of unsteady flow of gas through a nano-porous medium. Hence, the physical problem is modeled by a highly nonlinear ordinary differential equation detailed on a semi-infinite domain and represents a guidance and an application for several questions originating in the gas flow theory. In other terms, it was revealed a solution to this problem by the reduction to a boundary value problem for the ordinary differential equation. Having a strong non linearity, this equation has been numerically studied by numerous authors. Until now, only numerical or approximate solutions have been found under appropriate boundary conditions. By employing a converted Adomian decomposition method [13,14] or He's homotopy/variational iteration method [15], Riccardo found incorrect numerical results [16]. In different circumstances, using both spectral or finite difference methods, more precise and consistent outcomes were obtained. Recently Parand et al. [17], found a good approximate solution by using a method based on rational Jacobi functions.

The present study is a valid contribution to the existing literature, by developing a nonstandard line method for the partial differential equation, in order to obtain a numerical solution of unsteady flow of gas through a nano porous medium.

The findings of this study offered a facile approach to improve an attractive issue related to materials science/chemistry, like synthesis of ZnO or TiO_2 nanoparticles forming an ideal nano porous pipe with efficiency in industrial waste waters decontamination.

The mathematical model

The research originated from the survey of the unsteady flow of a gas through a semi-infinite porous medium when the medium be initially filled with the gas at a uniform pressure P_0. In order to obtain a numerical solution of unsteady flow of gas through a nano-porous medium, we focused onto the flow of a liquid sample of waste-water derived from a standard/conventional dyeing process. With a view to removing the dyes from the polluted water/waste water, ZnO nanoparticles were synthesized with the assistance of (monochloro-triazinyl-cyclodextrin) by using a sol–gel method [18]. Usually, these types of nanoparticles/systems undergo aggregation. But an ideal porous pipe consisting of nanoparticles bound one to each other, forming a porous matrix/medium was proposed, especially considering the fluid flow through a porous medium as a completely interconnected network, formed by the constricted channel between each pore so that the fluid may flow [12]. The characteristics of gas behavior depend on pressure. At the time

$t = 0$

the pressure at the outflow face is suddenly reduced from P_0 to P_1 and is thereafter maintained at this lower pressure. The unsteady isothermal flow of gas has been described by the nonlinear partial differential equation

$$\nabla^2(P^2) = 2A\frac{\partial P}{\partial t}. \tag{1}$$

These nano porous media consist of voids (empty spaces) that are naturally filled with the sample of dyed water as gas and are characterized by its porosity whose formula is:

$$A = \frac{\phi\mu}{k},$$

where ϕ is the porosity, μ is the viscosity and k is the permeability.

The permeability k of a porous medium is a property based on the pore size and the pore structure as well. The fact that the permeability may vary from one geometry to another geometry allows the real applicability of (1) quite restrictive. At the same time , the dimensional analysis reveals that the permeability is just a function of the porosity ε and the particle diameter d; meaning the pore geometry and the pore size. However, the known Carman–Kozeny relationship associates these quantities empirically with a dimensional correctness by the relation [19]

$$A = \frac{\varepsilon \times \mu}{k} = \frac{\varepsilon \times \mu \times 180(1-\varepsilon)^2}{d^2\varepsilon^3} = \frac{\mu \times 180(1-\varepsilon)^2}{d^2\varepsilon^2}.$$

This indeed turns out to yield:

$$A = \frac{180\mu(1-\varepsilon)^2}{d^2\varepsilon^2}.$$

Since we are referring to a wastewater model, we are considering the viscosity μ for the water. The values for the ε (P), according to the plot below and the particle diameter d are found in the table and in Fig. 1 as below. By substituting the values of the viscosity and the pore diameter, we obtain all the time, the values of A in the range of $(0;1)$. For instance, we choose two different values for porosity and pore diameter in order to determine A. Thus, for $\mu = 1Pa \times s, \varepsilon(P) = 55, d = 14$ nm, we have:

$$A = \frac{180 \times 1 \times (1-55)^2}{(14)^2 \times (55)^2} = 0.8852.$$

Another situation, where $\mu = 1\mathrm{Pa} \times \mathrm{s}$, $\varepsilon(P) = 20$, $d = 121$ nm we, for A, obtain:

$$A = \frac{180 \times 1 \times (1-20)^2}{(121)^2 \times (20)^2} = 0.01109555.$$

As a conclusive remark, according to the scientific reports [20], the real parameter A should be within the range $(0;1)$, $(0 < A < 1)$. This, indeed, gives the same results as the academic community claimed.

The pore diameters d (nm) are determined by the BET (Brunauer, Emmett and Teller) method. The BET specific surface areas (S_{BET} (m^2/g)) were obtained from the nitrogen adsorption experiments measured at −196 °C after degassing the samples below 10^{-3} Torr at 473 K for 2 h on NOVA2200e (Quantachrome Instruments, Boynton Beach, FL, USA).

The measurement of the pore size distribution was performed from the desorption branch of the isotherm using BJH (Barrett–Joyner–Halenda) method. The total pore volume (TPV, cm^3/g) was calculated as the amount of the nitrogen adsorbed at a relative pressure of approximately 0.99 [21].

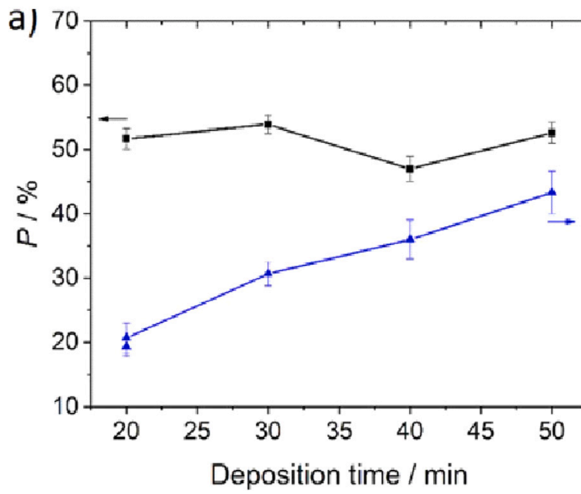

Fig. 1. Deposition time/min.

Annealing $T/^0$C	S_{bet} (m^2/g)	*Pore volume* (cm^3/g)	*Average pore width* (nm)	BJH pore diameter	d_{BET} (nm)
ZnO precursor	76.32	0.2425	17.20	14.89	14
265	14.25	0.0825	31.4	39.04	43
365	11.79	0.1124	33.36	34.96	45.8
475	14.15	0.0495	23.6	37.16	60.52
500	7.67	0.016	17.6	23.57	121.4

In the one-dimensional case, the extended medium from $x = 0$ to $x = \infty$ suggests to have:

$$\frac{\partial}{\partial x}\left(P\frac{\partial P}{\partial x}\right) = A\frac{\partial P}{\partial t}. \tag{2}$$

with boundary conditions imposed as:

$$P(x,0) = P_0,\ \ 0 < x < \infty, \tag{3}$$

$$P(0,t) = P_1\ (< P_0),\ \ 0 \le t < \infty.$$

To acquire alike solution, Waltman [22] have introduced the new independent variable:

$$z = \frac{x}{\sqrt{t}}\left(\frac{A}{4P_0}\right)^{\frac{1}{2}},$$

where as the dimension-free dependent variable u is given by:

$$u(z) = A^{-1}\left(1 - \frac{P^2(z)}{P_0^2}\right),$$

where A is the real parameter defined as:

$$A = 1 - \frac{P_1^2}{P_0^2}. \tag{4}$$

In terms of the dependent and independent variables, the problems would take the following equation form:

$$u''(z) + \frac{2z}{\sqrt{1 - Au(z)}}u'(z) = 0. \tag{5}$$

The typical boundary conditions imposed by the physical properties are:

$$u(0) = 1, u(\infty) = 0, \tag{6}$$

$$A = 0.8852, A = 0.01109555, \tag{7}$$

where $0 < A < 1$ is the real parameter given by (4). Obviously, we should expect u to be a member of the interval $J = [0,1]$, in such case we would have:

$$L_1(z) = 2z \le \frac{2z}{[1 - Au(z)]^{\frac{1}{2}}} \le 2(1 - A)^{-1/2}z = L_2(z).$$

The solution u should respect the physical requirements:

$$0 \le u(z) \le 1. \tag{8}$$

By using Theorem 7.1 and 7.5, Bailey [22] proved that the ordinary differential equation (5) is the second order differential equation given as

$$u''(z) + 2zu'(z) = 0. \tag{9}$$

Main results

Analytical solution

By using the idea which is due to Shampine [23], the ordinary differential equation (9) is approximately given as:

$$\frac{u''(z)}{u'(z)} = -2z.$$

By integrating with respect to z, the previous differential equation reduces to give:

$$\ln u'(z) = -z^2 + \beta.$$

Or, in a brief notation, it can consequently be formulated as:

$$u'(z) \sim \beta e^{-z^2}.$$

Therefore, by integrating and imposing boundary conditions at infinity, the above equation, indeed, reveals

$$u(z) = \beta\int_0^z e^{-t^2}dt + \gamma, u(\infty) = 0.$$

Hence, the condition $u(\infty) = 0$, imposed on the above integral equation, leads to have

$$\beta\int_0^\infty e^{-t^2}dt + \gamma = 0.$$

But, by virtue of the known computation of the improper integral

$$\int_0^\infty e^{-t^2}dt = \frac{\sqrt{\pi}}{2},$$

we directly reach a value of γ given by

$$\gamma = -\beta\frac{\sqrt{\pi}}{2}.$$

Hence, our result can be read as

$$u(z) \sim \beta\int_z^\infty e^{-t^2}dt \sim \frac{-\beta\sqrt{\pi}}{2}\,\mathrm{erf}\,c\ u(z).$$

Bender [20] shows that the asymptotic representation of the complementary error function is approximately given as:

$$\mathrm{erf}\,c\ u(z) \sim \frac{e^{-z^2}}{z\sqrt{\pi}}.$$

Therefore, we obtain:

$$u(z) \sim -\beta\frac{1}{2}\frac{e^{-z^2}}{z}.$$

Now, to solve the ordinary differential equation (9) with the conditions (6) we may proceed by treating β as the unknown parameter, to have:

$$u'(z) = \beta e^{-z^2}.$$

Therefore, instead of having $u(z) = 0$, the solution will be easily obtained as follows:

$$u(z) = -\frac{\beta}{2z}e^{-z^2}.$$

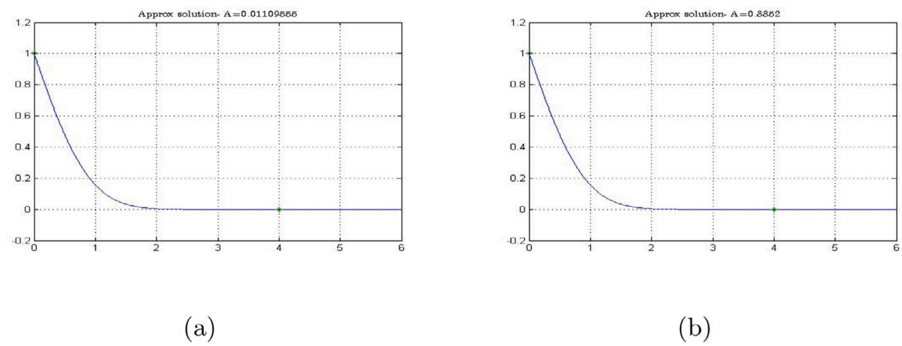

Fig. 2. BVP for ODE.

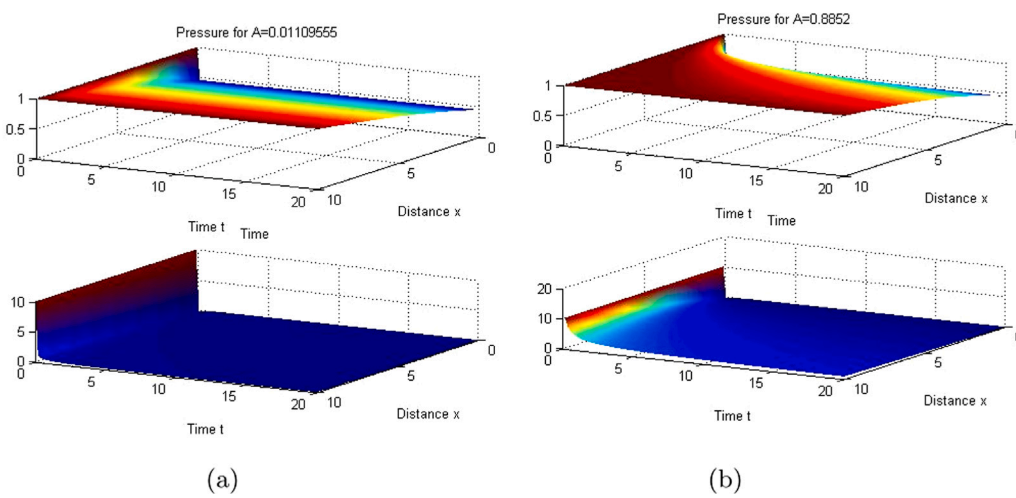

Fig. 3. Line method.

Numerical solution

Reduction to a BVP for ODE

In the following analysis we propose to solve the problem (9)+(6) with the embedded methods: B-splines functions and Runge Kutta methods [24–33] for further discussion. By making a free use of the substitution:

$$u(z) = y(z) \cdot f(z) \text{ where } f(z) = e^{-\frac{z^2}{2}},$$

the ordinary differential equation (9) reveals that:

$$u'(z) = y'(z)e^{-\frac{z^2}{2}} - ze^{-\frac{z^2}{2}} y(z). \tag{10}$$

and

$$u''(z) = y''(z)e^{-\frac{z^2}{2}} - zy'(z)e^{-\frac{z^2}{2}} - e^{-\frac{z^2}{2}} y(z) + z^2 e^{-\frac{z^2}{2}} y(z) - zy'(z)e^{-\frac{z^2}{2}}. \tag{11}$$

Hence, by multiplying (10) by $2z$ and adding (11), the ordinary differential equation (9) becomes:

$$y''(z) - (z^2+1)y(z) = 0, \tag{12}$$

whereas the boundary conditions which can be equipped with this equation are:

$$y(0) = 1 \text{ and } y(\infty) = 0. \tag{13}$$

However, we split the interval $[0, \infty)$ into two areas, namely, the asymptotically and the transient areas $[4, \delta)$ and $[0, 4]$, respectively. Therefore, we derive the approximation solutions of the aforementioned problem (12)+(13) as follows:

(a) on $[0, 4]$ with the B-splines functions of order $k+1$;

(b) on $[4, \delta)$ with the Runge–Kutta $k-$stages by MATLAB solver ODE45 [34]. The convergence of this embedded method is therefore given by [35, 4], whereas the results are depicted in Fig. 2.

Line method (MOL)

Here, we recall the given partial differential equation ((2))+(3) that describes this process and postulate a solution in the form:

$$P(x,t) = u(x) \cdot f(t),$$

where $f(t) = e^{-\frac{t^2}{2}}$ and $u(x)$ is the solution of the boundary value problem (12)+(13).

We propose to solve the problem (2) with the conditions (3) using the MOL method [36] and the MATLAB 2013b solver PDEPE [34]. For $A = 0.0110955$ and $A = 0.8852$, we obtain the following results depicted in Fig. 3

By aid of the tic-toc of the Matlab we have achieved the time 0.733778 s for the boundary value problem method and for the MOL method we have achieved the time 0.845321 s. On top of that, the problem (12) associated with the boundary conditions (13) has been adequately set on an infinite interval. Therefore, the experimentation which was very necessary to verify the sufficiently large δ has been specified.

Conclusion and perspective research

The theory of porous media plays an essential role in various fields of applied sciences and engineering. Taking this into account, we studied the flow of a liquid sample of waste-water derived from a standard/conventional dyeing process in nano-porous medium, consisting of ZnO nanoparticles bound one to each other, forming a porous matrix/medium. In order to obtain a numerical solution of unsteady flow of the liquid through the nano-porous medium, a well-configured nonstandard line method for the partial differential equation was considered. By the reduction to a boundary value problem for the ordinary differential equation, a solution to this problem was revealed.

The main attributes and outcomes of the research are summarized as follows:

- the time of 0.733778 s was achieved for the boundary value problem method;
- for the MOL method we have achieved the time 0.845321 s;
- the problem (12) associated with the boundary conditions (13) has been adequately set on an infinite interval;
- the experimentation which was very necessary to verify the sufficiently large δ has been specified.

Thus, this study is responsible for modeling the gas flow through a nano-porous media which is very relevant in investigating the gas–solid processes. Therefore, the physical problem is modeled by a highly nonlinear ordinary differential equation detailed on a semi-infinite domain and represents a guidance and an application for several questions originating in the gas flow theory.

Starting from the results achieved by this research, in perspective, we have in mind the following aspects: The mathematical modeling of catalytic photo-degradation of air contaminants; transforming unsteady gas equation into a nonlinear ordinary differential equation which quite simplified the original problem.

Availability of data and material

Please contact the authors for data requests.

CRediT authorship contribution statement

Daniel N. Pop: Conceptualisation, Methodology, Software, Formal analysis, Investigation, Writing - original draft, Validation. **N. Vrinceanu:** Conceptualisation, Methodology, Software, Investigation, Supervision, Writing - original draft, Validation. **S. Al-Omari:** Conceptualisation, Methodology, Software, Formal analysis, Supervision, Writing - original draft, Validation. **N. Ouerfelli:** Conceptualisation, Software, Supervision, Resources, Validation. **D. Baleanu:** Conceptualisation, Software, Formal analysis, Supervision, Validation. **K.S. Nisar:** Conceptualisation, Software, Formal analysis.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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