Numerical Study on Gas Flow through a Micro-Nano Porous Media

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The present research examines the unsteady isothermal flow of a gas through a semi-infinite micro-nano porous medium, a nonlinear boundary value problem on semi-infinite interval. This problem is solved by two different methods and compare their results with solution of other methods is compared. Also through the convergence of these methods, the accurate initial slope $y(x)$ with good capturing the essential behavior of $y(x)$ is obtained.

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1. Introduction

There are many problems in science and engineering arising in unbounded domains which can be modeled by singular and nonsingular boundary value problems. The application of these problems involves chemical kinetics, astrophysics, experimental and mathematical physics, nuclear charge in heavy atoms, thermal behavior of a spherical cloud of gas, thermodynamics, population models, fluid mechanics and many other topics. Several techniques including decomposition, variational iteration, finite difference, polynomial spline, homotopy analysis method, and shooting methods have been developed for solving such problems.

Gas–solid processes like adsorption, are used in the chemical industries to separate solutes from a fluid stream. Transport phenomena and diffusion in micro--nano porous materials have attracted the researchers' attention for a long time. The modeling of gas flow through a porous media is quite valuable because of its importance in investigating gas-solid processes. The flow of gas through a semi-infinite porous medium initially fills with gas at a uniform pressure $P_0 > 0$, at time $t = 0$, the pressure on the outflow face is suddenly reduced from P_0 to $P_1 \geq 0$ ($P_1 = 0$ in the case of diffusion into a vacuum) and thereafter, maintained at this lower pressure. The unsteady flow of gas in a porous medium is modeled by a nonlinear partial differential equation [1–3] as follows:

$$\nabla^2(P^2) = (2\Phi\mu/k)\frac{\partial P}{\partial t}, \tag{1}$$

where P is the pressure within porous medium, Φ is the porosity, μ is the viscosity, k is the permeability and t is the time.

In the one-dimensional medium extending from $z = 0$ to $z = \infty$, Eq. (1) reduces to

$$\frac{\partial}{\partial z}\left(P\frac{\partial P}{\partial z}\right) = (\Phi\mu/k)\frac{\partial P}{\partial t}, \tag{2}$$

with the boundary conditions

$P(z, 0) = P_0,\ 0 < z < \infty;$

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

Now, by using the new independent variable [4]:

$$x = \frac{z}{\sqrt{t}}\left(\frac{A}{4P_0}\right)^{1/2}, \tag{3}$$

and the dimension-free variable y, defined by

$$y(x) = \alpha^{-1}\left(1 - \frac{P^2(z)}{P_0^2}\right), \tag{4}$$

where $A = \Phi\mu/k$ and $\alpha = 1 - \frac{P_1^2}{P_0^2}$, a similarity solution is obtained. In terms of these variables, the problem takes the form (unsteady gas equation)

$$y''(x) + \frac{2x}{\sqrt{1 - \alpha y(x)}}y'(x) = 0,$$
$$x > 0, \quad 0 < \alpha < 1. \tag{5}$$

The typical boundary conditions imposed by the physical properties are

$$y(0) = 1, \quad \lim_{x\to\infty} y(x) = 0. \tag{6}$$

A substantial amount of numerical and analytical work has been invested so far on this model [1–3]. The major drawback of these methods is huge computational work. This problem (5) was handled by Kidder [2]. Also a perturbation technique is carried out to include terms of second order, and the convergence of the obtained expansion is guaranteed through physical properties of $y(x)$, and it is shown that the complexity of the calculations increases rapidly with increasing order of the terms. Wazwaz [5] proposed modified Adomian decomposition method, and $[M/M]$ Padé approximation method for this equation, in spite of the fact that M is the degree of polynomial in series solution.

Aslam Noor and Mohyud-Din [6] considered modified variational iteration method for this equation. Parand

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et al. [7] solved this problem by using pseudospectral method with rational Chebyshev and modified generalized Laguerre functions. Taghavi et al. [8] solved it by Lagrangian method based on modified generalized Laguerre functions. Khan et al. [9] used modified Laplace decomposition method (MLDM) coupled with Padé approximation technique to solve this equation. Mohyud–Din et al. [10] applied the coupling of He's polynomials to the correct functional of variational iteration method to solve the problem (5). This equation has been recently considered by Rezaei et al. [11] with the orthogonal rational Legendre and Sinc functions with using pseudospectral method.

In this paper most of the obtained results of $y'(0)$ are the same, because the researcher used Padé approximation methods with different functions. See Table I to compare obtained results. In this table, N is the degree of orthogonal polynomial used in the method and MGLFM, RCM, MGL, SINC and RLP are the abbreviation for modified generalized Laguerre function method, rational Chebyshev method, modified generalized Laguerre function method, pseudospectral method based on sinc function, and rational Legendre pseudospectral method, respectively. More results can be found for other values of α in the mentioned papers.

TABLE I

Values of $y'(0)$ for $\alpha = 0.5$.

Paper	Method	$y'(0)$
Wazwaz [5]	Padé$_{[2/2]}$	-1.373178096
	Padé$_{[3/3]}$	-1.025529704
Aslam Noor [6]	Padé$_{[2/2]}$	-1.373178096
	Padé$_{[3/3]}$	-1.025529704
Parand [7]	MGLFM ($N = 6$)	-1.36417503
	MGLFM ($N = 7$)	-1.38213483
	RCM ($N = 6$)	-1.10805718
	RCM ($N = 7$)	-1.26259357
Taghavi [8]	MGL ($N = 6$)	-1.37310852
	MGL ($N = 7$)	-1.37317352
Khan [9]	Padé$_{[2/2]}$	-1.373178096
	Padé$_{[3/3]}$	-1.025529704
Mohyud-Din [10]	Padé$_{[2/2]}$	-1.373178096
	Padé$_{[3/3]}$	-1.025529704
Rezaei [11]	SINC ($N = 6$)	-1.188228002
	SINC ($N = 8$)	-1.188625937
	SINC ($N = 16$)	-1.188689251
	SINC ($N = 32$)	-1.188692320
	RLP ($N = 6$)	-1.188610520
	RLP ($N = 8$)	-1.188650543
	RLP ($N = 16$)	-1.188677428
	RLP ($N = 32$)	-1.188687197

It will be shown that the obtained results by Rezaei et al. [11] are more accurate than others. The aim of this paper is to obtain more accurate results by using two different approaches which are implicit finite-difference scheme known as the Keller-box method [12, 13] and the shooting method [13].

2. Solution procedures

2.1. Finite-difference method

To solve the differential Eq. (5) which is subject to boundary conditions (6), the first Eq. (5) is converted into a system of two first-order equations, and the difference equations are then expressed by using central differences. For this purpose, the new dependent variable $w(x)$ is introduced, so that Eq. (5) can be written as

$$y'(x) = w(x), \tag{7}$$

$$w'(x) = \frac{-2xw(x)}{\sqrt{1-\alpha y(x)}}. \tag{8}$$

Now, by using the Taylor series expansion of $\frac{1}{\sqrt{(.)}}$, Eq. (8) is changed to

$$w'(x) = -2xw(x)\Big[1 + c_1\alpha y(x) + c_2\alpha^2 y(x)^2 + \ldots + c_m\alpha^m y(x)^m\Big], \tag{9}$$

where m is an arbitrary constant natural number and $c_1 = \frac{1}{2}$, $c_2 = \frac{3}{8}$, $c_3 = \frac{5}{16}$, and so on. Now, we consider the segment $x_{j-1}x_j$, which is defined as:

$$x_0 = 0, \quad x_j = x_{j-1} + h_j, \quad x_J = x_\infty, \tag{10}$$

where h_j is Δx-spacing and $j = 0, 1, \ldots, J$ is a sequence number that indicates the coordinate location. In the Keller-box method, the finite-difference approximations to the ordinary differential Eqs. (7) and (9) are written for the midpoint $x_{j-1/2}$ of the segment $x_{j-1}x_j$ for $j = 1, 2, \ldots, J$ as

$$y_j - y_{j-1} - \frac{1}{2}h_j(w_j + w_{j-1}) = 0, \tag{11}$$

$$w_j - w_{j-1} + h_j x_{j-1/2}(w_j + w_{j-1}) \times\Big[1 + \frac{c_1\alpha}{2}(y_j + y_{j-1}) + \frac{c_2\alpha^2}{4}(y_j + y_{j-1})^2 \ldots + \frac{c_m\alpha^m}{2^m}(y_j + y_{j-1})^m\Big] = 0. \tag{12}$$

The transformed boundary layer thickness x_J is sufficiently large, so that it is beyond the edge of the boundary layer. The boundary conditions are

$$y_0 = 1, \quad y_J = 0. \tag{13}$$

Now by Newton's method, the nonlinear system is linearized (11), (12) and then, the obtained linearized difference equations can be solved by the block-elimination method as outlined by [3, 13], since the obtained system has block-tridiagonal structure. The obtained results for linear initial profile and stop criterion 10^{-8} on $y'(0)$ with $h_j = h$ and $x_\infty = hJ$ are shown in Table II. Table III shows the values of $y(x)$ by using perturbation technique [2], and Padé$_{[3/3]}$ [5] for $\alpha = 0.5$. Table IV shows that the initial slope $y'(0)$ increases with the increase of α.

TABLE II

Values of $y'(0)$ for $\alpha = 0.5$ for different x_∞.

M	J	h	$y'(0)$
6	30	1/10	−1.1938713177347504
	60	1/20	−1.1922883859473303
	90	1/30	−1.1919951287546457
	120	1/40	−1.1918924798983241
	150	1/50	−1.1918449665961557
	300	1/100	−1.1917816140076933
	600	1/200	−1.1917657755896378
	1200	1/400	−1.1917618159682022
8	1200	1/400	−1.1918059634783928
10		1/400	−1.1918126190284244
12		1/400	−1.1918137142588647
14		1/400	−1.1918139058828805
16		1/400	−1.1918139409674497
18		1/400	−1.1918139476201857
20		1/400	−1.191813948917348
20	2000	1/40	−1.1919230334799826
	5000	1/100	−1.1918118315451425
	10000	1/200	−1.1917959449569746
	50000	1/1000	−1.1917908612172277
30	2000	1/40	−1.1919230338118607
30	5000	1/100	−1.1918118318711821
30	10000	1/200	−1.1917959452821487
30	50000	1/1000	−1.1917908615421229

TABLE IV

Initial slopes $y'(0)$ for various values of α, for $M = 30$, $J = 50000$.

α	Padé$_{[2/2]}$	Padé$_{[3/3]}$	Present method
0.1	−3.556558821	−1.957208953	−1.139007356865483
0.2	−2.441894334	−1.786475516	−1.1504756481362894
0.3	−1.928338405	−1.478270843	−1.1629416335500269
0.4	−1.606856838	−1.231801809	−1.1766158581496988
0.5	−1.373178096	−1.025529704	−1.1917908615421229
0.6	−1.185519607	−0.8400346085	−1.2088944130728032
0.7	−1.021411309	−0.6612047893	−1.228598743345502
0.8	−0.8633400217	−0.4776697286	−1.2520835659442726
0.9	−0.6844600642	−0.2772628386	−1.281847782063427

2.2. Shooting method

The non-linear ordinary differential Eq. (5) together with the boundary conditions (6) are solved numerically using Nachtsheim–Swigert shooting iteration technique [14] (guessing the missing value) along with explicit Runge–Kutta initial value solver with stiffness detection capability by Mathematica Software.

As we know, in a shooting method, the missing initial condition at the initial point of the interval is assumed by user, and the differential equation is solved numerically as an initial value problem to the terminal point. The accuracy of the assumed missing initial condition is then checked by comparing the calculated value of the dependent variable at the terminal point with its given value there. If a significant difference exists, then another value of the missing initial condition must be assumed and the process is repeated. This process is continued until the reasonable agreement between the calculated and the given condition at the terminal point is obtained within the specified degree of accuracy. For this type of iterative process, one naturally needs to a systematic way of finding each succeeding (assumed) value of the missing initial condition.

In this method the asymptotic boundary condition (6) is replaced by the condition that $y(x) = 0$ to a sufficient degree of accuracy at $x = x_\infty$, where x_∞ is the value of the independent variable at the edge of the boundary layer. The boundary-value problem is equivalent to the problem of finding a value of $y'(0)$ for which the boundary condition at the edge of the boundary layer is satisfied. With the notation $z = y'(0)$. It is observed that a small change Δz in z changes value of y by the amount

$$\frac{\partial y}{\partial z}\Delta z,$$

so, the necessary correction to the first approximation comes from the solution of the following linear equation:

$$y(x) + \frac{\partial y}{\partial z}\Delta z = 0, \tag{14}$$

at $x = x_\infty$. The solution of (14) for Δz can be obtained if we can evaluate $\frac{\partial y}{\partial z}$ at x_∞. So, we must use differentiation of (5). With notation

$$y_z = \frac{\partial y}{\partial z}, \quad y'_z = \frac{\partial y'}{\partial z}, \ldots,$$

and taking differentiation of (5) with respect to z, we have

$$y''_z(x) + \frac{2x}{\sqrt{1-\alpha y(x)}} y'_z(x) + y'(x) y_z(x) \times \frac{\alpha x}{\sqrt{[1-\alpha y(x)]^3}} = 0, \tag{15}$$

with initial conditions

$$y_z(0) = 0, \quad y'_z(0) = 1. \tag{16}$$

Given an arbitrary initial estimation of $z = y'(0)$, subsequent values of z can be computed by integrating Eqs. (5) and (15) and applying the Newton–Raphson method to obtain the corrections. For this reason, we need to the value of x_∞ for getting the integration. After this, we show the tentative values of x_∞ by x_{stop}. We can start our process by a small value for x_{stop}, and in each iteration try to find Δz and modify x_{stop}. For this, we use from the boundary condition (6) at infinity and its derivative. That is, Δz should be chosen so that both equations

$$y(x) + y_z(x)\Delta z = 0, \quad y'(x) + y'_z(x)\Delta z = 0, \tag{17}$$

TABLE III

Approximations of $y(x)$ for present methods in comparison with other method, for $\alpha = 0.5$, $M = 30$, $J = 50000$.

x	Kidder [2]	Padé$_{[3/3]}$ [5]	Rezaei [11]	Present method
0.1	0.8816588283	0.8979167028	0.8816297930	0.8813646572742952
0.2	0.7663076781	0.7985228199	0.7666243657	0.7658288222744776
0.3	0.6565379995	0.7041129703	0.6565307085	0.656000694626484
0.4	0.5544024032	0.6165037901	0.5545172476	0.5538989492480791
0.5	0.4613650295	0.5370533796	0.4628652574	0.4609427659504205
0.6	0.3783109315	0.4665625669	0.3814536078	0.37798158206878896
0.7	0.3055976546	0.4062426033	0.3095060359	0.3053523296040834
0.8	0.2431325473	0.3560801699	0.2466311657	0.24295437638061612
0.9	0.1904623681	0.3179966614	0.1927749120	0.19033421260699213
1.0	0.1587689826	0.2900255005	0.1478076673	0.14677328712194618

are satisfied at $x = x_{\rm stop}$. Now, we have two equations with one unknown Δz, and by least squares method we can find it. Let $\delta_1 = y(x_{\rm stop}) + y_z(x_{\rm stop})\Delta z$, $\delta_2 = y'(x_{\rm stop}) + y'_z(x_{\rm stop})\Delta z$, and the error $E = \delta_1^2 + \delta_2^2$. It can be found that E takes its minimum when Δz is obtained by doing least squares method on Eqs. (17). In Fig. 1, the error E is shown plotted as a function of z for various values of $x_{\rm stop}$.

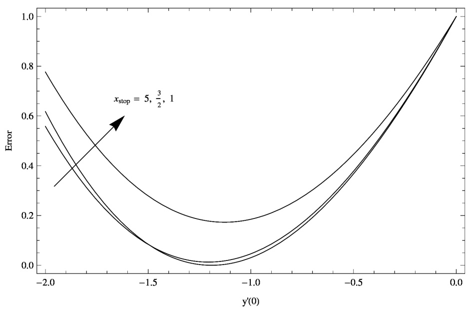

Fig. 1. Error as function of $y'(0)$ for different values of $x_{\rm stop}$.

Let $E_{\min}$ is the minimum of E with respect to z. Now, in next step we want to decrease the value of $E_{\min}$. At first, we start with a small value for $x_{\rm stop}$, say $x_{\rm stop} = 1$. A step size of $\Delta x = 0.01$ was selected to be satisfactory for a convergence criterion of 10^{-8} in all cases (as last subsection). The value of $x_{\rm stop}$ was found to each iteration loop by the statement $x_{\rm stop} = x_{\rm stop} + \Delta x$.

The maximum value of $x_{\rm stop}$ to each value of α determined when the value of Δz (the variation of the unknown boundary conditions at $x = 0$) does not change to successful loop with error less than 10^{-8}. See Fig. 2 for residual error of Eq. (5) obtained by this approach. Table V shows that the initial slope $y'(0)$ increases with the increase of α which obtained by this method. Figure 3 shows the obtained $y(x)$ for different values of α.

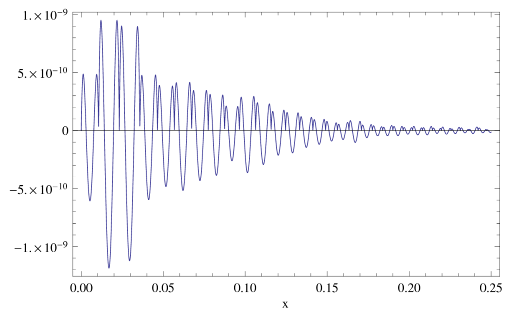

Fig. 2. Residual error of (5) for $\alpha = 0.5$.

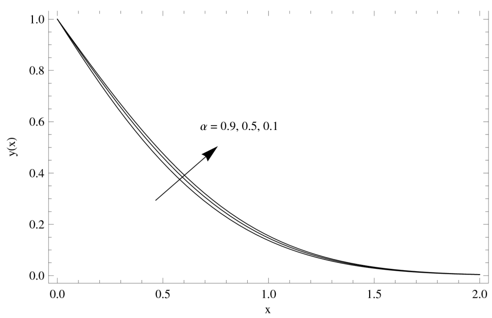

Fig. 3. Approximation of $y(x)$ for different values of α.

3. Concluding remarks

In this paper, two mentioned powerful and efficient methods are implicit finite-difference Keller-box method and shooting method to solve differential equation of gas flow through a micro-nano porous media. This model is quite valuable in order to its importance in investigating gas–solid processes. By comparison to other previous researcher's numerical solutions, the obtained results in these two methods have provided acceptable approach for nonlinear unsteady gas equation. Consequently we determine the accurate initial slope $y'(0) \approx -1.191791$

TABLE V

Initial slopes $y'(0)$ for various values of α.

α	x_{stop}	Present method
0.1	3.76	−1.1390073222058392
0.2	3.75	−1.1504756086298318
0.3	3.75	−1.1629415776840015
0.4	3.75	−1.176615782984229
0.5	3.74	−1.1917907719590468
0.6	3.74	−1.2088942932466626
0.7	3.73	−1.2285985979448646
0.8	3.73	−1.2520839101594896
0.9	3.72	−1.2818814468001043

for $\alpha = 0.5$ with good capturing the essential behavior of $y(x)$.

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