

Numerical study on gas flow through a micro–nano porous medium based on finite difference schemes on quasi-uniform grids

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ABSTRACT

In this paper, the unsteady isothermal flow of a gas through a semi-infinite micro–nano porous medium described by a non-linear two-point boundary value problem on a semi-infinite interval has been considered. We solve this problem by a nonstandard finite difference method defined on quasi-uniform grids in order to derive a new numerical approximation. By introducing a stencil that is constructed in such a way that the boundary conditions at infinity are exactly assigned, the proposed method is effectively used to determine the numerical solution. In addition, a mesh refinement and the Richardson's extrapolation allow to improve the accuracy of the numerical solution and to define a posteriori estimator for the global error of the proposed numerical scheme. We determine the accurate initial slope $\frac{du}{dx}(0) = -1.1917906497194208$ calculated for $\alpha = 0.5$ with good capturing the essential behavior of $u(x)$. This clearly demonstrates that the numerical solutions presented in this paper result highly accurate and in excellent agreement with the existing solutions available in the literature.

1. Introduction

In the last decades, micro and nano flows in porous media are becoming a relevant research area due to their wide application to engineering and scientific problems. Many of this problems can be modeled by strongly nonlinear boundary value problems (BVPs) on unbounded domains. In general, the BVPs on an infinite domain arise in many fields, e.g. thermodynamics, astrophysics, chemical kinetics, mathematical physics, population models, thermal behavior, fluid mechanics and many other topics.

In order to solve such a class of problems, the classical approach is to replace the infinite domain by a truncated finite interval considering a sufficiently large finite value, the so-called truncated boundary, and then, on this new truncated boundary to impose a suitable boundaries condition. To obtain a satisfactory accuracy of the numerical solution, a truncated boundary has to be determined by trial and errors and this seems to be the weakest point of this classical approach. Moreover, the definition of the suitable boundary conditions is an open problem (see for example [1–4]) and in some cases, their choice is not unique [5–7] and strongly affects the solutions. This approach is used for solving mathematical models in several fields of the applied sciences.

In order to avoid the drawbacks of the truncated domain, it is possible construct quasi-uniform meshes [8,9] by using smooth, strictly monotonic functions. In this way, the whole infinite domain is taken into

account in the mapping where the grid-points are located at mid-point of each sub-interval, then the difficulty caused by numerical treatment of the last infinite sub-interval is avoided.

In this paper, we use a smooth, strictly monotonic function to construct a quasi-uniform map and then we develop on the original semi-infinite domain a second order non-standard finite difference scheme defined on quasi-uniform grid that allows to impose the given boundary conditions exactly. In particular, we propose a non standard finite difference method on quasi-uniform mesh for obtaining a numerical solution of unsteady flow of gas through a porous medium. The physical problem is modeled by a second order highly nonlinear ordinary differential equation defined on a semi-infinite domain and represents a guideline for several problems arising in the gas flow theory. Because of its strongly non linearity, this equation has been numerically investigated by several authors. Up to now, only numerical or approximate solutions have been found under suitable boundary conditions. By using a modified Adomian decomposition method [10,11] or He's homotopy/variational iteration method [12] incorrect numerical results were found. By using spectral methods or finite difference methods, more accurate solutions were determined. Only Parand and al. [13], recently, by a collocation method based on rational Jacobi functions, found a good approximate solution. Because of the considerable numerical disagreement, we propose the recently developed finite difference method in order to study the physical model

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and to derive a new more accurate numerical approximation. The proposed numerical method is firstly developed in [14] and successively adopted in [15] and [16], where, numerical results show the efficiency and the reliability of the proposed numerical method. The key advantage of the presented approach is that the given BVP is solved on a semi-infinite interval by introducing a stencil that is constructed in such a way that the boundary conditions at infinity are exactly assigned. Finally, via a mesh refinement, by using the Richardson’s extrapolation and a posteriori error estimator we improve the accuracy of the obtained numerical results showing that they are in excellent agreement with the solutions found in literature.

2. Mathematical model

We consider the following nonlinear partial differential equation, derived by Muskat [17], that describes the unsteady flow of a gas through a semi-infinite porous medium [18,19]

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

where ∇^2 is the Laplace operator, P is the pressure within the porous medium, Φ the porosity, μ the viscosity, k the permeability, and t the time. In the one-dimensional medium, $z \in [0, \infty]$, Eq. (1) reduces to

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

with the boundary conditions

$$\begin{aligned} P(z, 0) &= P_0 & 0 < z < \infty, \\ P(0, t) &= P_1 & \text{with } P_1 < P_0, \quad 0 \leq t < \infty. \end{aligned}$$

We suppose that, at the initial time, the porous medium is initially filled with a gas at a uniform pressure $P_0 > 0$, then the pressure at the outflow face is suddenly reduced at the value P_1 with $0 \leq P_1 < P_0$ and is, thereafter, maintained at this lower value. Note that, $P_1 = 0$ is the case of diffusion into a vacuum. New variables were introduced by Kidder [20], by Davis [21] and in [22] to transform the nonlinear partial differential equation (2) to a nonlinear ordinary differential equation. In terms of the new independent variable x and of the dimensionless variable $u(x)$

$$\begin{aligned} x &= \frac{z}{\sqrt{t}} \left(\frac{A}{4P_0} \right)^{1/2}, \\ u(x) &= \alpha^{-1} \left(1 - \frac{P^2(z)}{P_0^2} \right), \end{aligned}$$

with $A = \Phi\mu/k$ characterizing the property of the medium, and $\alpha = 1 - P_1^2/P_0^2$, the one dimensional nonlinear partial differential equation (2) reduces to the nonlinear ordinary differential equation given by (unsteady gas equation)

$$\frac{d^2u}{dx^2} + \frac{2x}{\sqrt{1-au}} \frac{du}{dx} = 0, \tag{3}$$

with the following boundary conditions on the semi-infinite domain required by the physical problem

$$u(0) = 1, \quad \lim_{x \rightarrow \infty} u(x) = 0, \quad 0 \leq \alpha \leq 1. \tag{4}$$

The problem (3) was handled by Kidder in [20] and is also called Kidder equation. The biggest value of the parameter, $\alpha = 1$ is special because, recalling the boundary condition $u(0) = 1$, the factor $\sqrt{1-au(x)}$ in the differential equation is singular at the origin. In [20], Kidder calculated an approximate analytical solution $u(x; \alpha = 0)$ of the problem (3) for $\alpha = 0$ as follows

$$u(x; \alpha = 0) = 1 - \text{erf}(x) = \text{erfc}(x), \tag{5}$$

where $\text{erf}(x) = (2/\sqrt{\pi}) \int_0^x \exp(-y^2) dy$ is the usual error function and $\text{erfc}(x)$ is the complementary error function. This solution was used by

many researchers to obtain an approximate solution for $u(x; \alpha)$ over the whole range of parameter α .

The unsteady gas equation (3) has been analytically and numerically investigated by several authors. Agarval and O’Regan studied the existence of solutions [23], upper and lower solutions [22] of the considered problem. Countryman and Kannan [24] proved that the solution is enclosed by a pair of explicit analytic functions, obtained as solutions. Baxley [25] studied the problem via an initial value problem approach in combination with the shooting method. Wazwaz [10,11] applied a modified Adomian decomposition method, but his results are incorrect; his best prediction for $\alpha = 0.5$ is $u_x(0) = -1.025$ versus the true value of -1.1917 . Noor and Mohyud-Din used He’s homotopy/variational iteration method [12], but obtained the same incorrect slope numbers as Wazwaz. Parand et al. applied a pseudospectral method with a rational Chebyshev basis and also with a basis of modified generalized Laguerre functions [26,27]. Parand et al. also employed generalized Laguerre functions, but in a nodal or Lagrangian basis [28]. Rad and Parand applied the homotopy perturbation method for obtaining the analytical solution of the model [29] whose value is $u_x(0) = 1.188976708$ for $\alpha = 0.5$. Khan et al. used a Laplace decomposition method combined with Padé approximants [30]. They obtained the value $u_x(0) = 1.373178096$ for $\alpha = 0.5$. Rezaei et al. used a pseudospectral method with the orthogonal rational Legendre and sinc functions and they carried their computations to moderately large degree, but converged, to $u_x(0) = -1.18868$, for $\alpha = 0.5$, which is too small by 0.3%, [31]. Abbasbandy [32] solved the problem by using two different schemes, the implicit finite-difference Keller-box method and the shooting one, comparing calculated numerical results for different values of accuracy of the independent variable at the edge of the boundary layer obtaining $u_x(0) = 1.1917907719590468$ for $\alpha = 0.5$. Iacono and Boyd [33] used a rational Chebyshev pseudospectral method in order to compute the slope at the origin given by $u_x(0) = 1.191790649719421$ for $\alpha = 0.5$. Recently, Parand and al. [13], using a collocation method based on rational Jacobi functions, found a new approximate solution of initial slope $u_x(0) = -1.1917906497194217341228284$ for $\alpha = 0.5$.

In this paper, we present a new approximate solution of Eq. (3) obtained by a nonstandard finite difference scheme defined on quasi-uniform grids.

3. Numerical method

In this Section, we provide the details about the proposed finite difference method and its implementation in order to obtain the approximate solution of the given BVP (3).

In order to solve the problem (3) on the semi-infinite domain, first we construct a quasi-uniform map from a reference finite domain, then we develop on the original domain a non-standard finite difference scheme that allows to impose the given boundary conditions exactly. More details of the numerical method proposed for the class of BVPs can be found in [14]. Finite difference schemes and non-uniform grids were used in [34] for solving fractional partial differential equations.

There are several typical maps that relate infinite and finite domains to each other. Since it is well known that the solution of the unsteady isothermal flow of a gas through a porous medium decays exponentially as x goes to infinity, it is expected that good results are given by using of the following quasi-uniform map $x = x(\xi)$, [35,36]

$$x = -c \cdot \ln(1 - \xi), \tag{6}$$

where $\xi \in [0, 1]$, $x \in [0, \infty]$, and $c > 0$ is a control parameter which defines the grid point distribution in the original physical infinite domain. The use of the logarithmic map (6) is especially convenient because gives a slightly better resolution near to $x = 0$, where the solution has a transient behavior, with an increasing spatial resolution going toward infinity.

Fig. 1 shows the quasi-uniform mesh $x = x_n$, $n = 0, 1, \dots, N$ defined by (6) with $c = 5$ and $N = 20$.

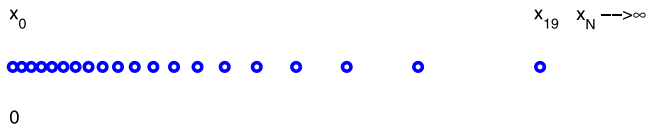


Fig. 1. Quasi-uniform mesh (6). We notice that the last mesh-point is $x_N = \infty$.

By (6), a family of uniform grids $\xi_n = n/N$ defined on finite interval $[0, 1]$ generates a one-parameter family of quasi-uniform grids $x_n = x(\xi_n)$ on the semi-infinite interval $[0, \infty]$. The BVP (3) is discretized by introducing a uniform grid ξ_n of $N + 1$ nodes in $[0, 1]$ such that $\xi_0 = 0$ and $\xi_{n+1} = \xi_n + h$ with $h = 1/N$. In this way, x_n is a quasi-uniform grid in $[0, \infty]$. The last interval in (6), namely $[x_{N-1}, x_N]$, is infinite but the point $x_{N-1/2}$ is finite, because the non integer nodes are defined by $x_{n+j} = x(\xi = \frac{n+j}{N})$, with $n \in \{0, 1, \dots, N - 1\}$ and $0 < j < 1$. This map allows to describe the infinite domain by a finite number of intervals. The last node of such grid is placed at infinity, $x_N = x(\xi_N) = \infty$, so right boundary conditions are taken into account correctly.

We approximate the values of the scalar variable $u(x)$ and its derivative at mid-points of the grid $x_{n+1/2}$, for $n = 0, \dots, N - 1$, using non-standard difference discretizations

$$u_{n+1/2} \approx \frac{x_{n+3/4} - x_{n+1/2}}{x_{n+3/4} - x_{n+1/4}} u_n + \frac{x_{n+1/2} - x_{n+1/4}}{x_{n+3/4} - x_{n+1/4}} u_{n+1}, \quad (7)$$

$$\frac{du}{dx} \Big|_{n+1/2} \approx \frac{u_{n+1} - u_n}{2(x_{n+3/4} - x_{n+1/4})}.$$

We emphasize that the key advantage of our non-standard finite difference formulation is to overcome the difficulty of the numerical treatment of the boundary conditions at the infinity. In fact, the formulae (7) use the value $u_N = u(\infty)$, but not $x_N = \infty$ and then, the boundary conditions at infinity are taken into account in a natural way.

For the class of BVPs

$$\begin{aligned} \frac{du}{dx} &= \mathbf{f}(x, \mathbf{u}), \quad x \in [0, \infty), \\ \mathbf{g}(\mathbf{u}(0), \mathbf{u}(\infty)) &= \mathbf{0}, \end{aligned} \quad (8)$$

where $\mathbf{u}(x)$ is a d -dimensional vector with ${}^\ell u(x)$ for $\ell = 1, \dots, d$ as components, $\mathbf{f}: [0, \infty) \times \mathbb{R}^d \rightarrow \mathbb{R}^d$, and $\mathbf{g}: \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^d$, a non-standard finite difference scheme on a quasi-uniform grid can be defined by using the approximations given by (7) above, and it can be written as follows

$$\begin{aligned} \mathbf{U}_{n+1} - \mathbf{U}_n - a_{n+1/2} \mathbf{f}(x_{n+1/2}, b_{n+1/2} \mathbf{U}_{n+1} + c_{n+1/2} \mathbf{U}_n) &= \mathbf{0}, \\ \mathbf{g}(\mathbf{U}_0, \mathbf{U}_N) &= \mathbf{0}, \end{aligned} \quad (9)$$

for $n = 0, 1, \dots, N - 1$, where

$$\begin{aligned} a_{n+1/2} &= 2(x_{n+3/4} - x_{n+1/4}), \\ b_{n+1/2} &= \frac{x_{n+1/2} - x_{n+1/4}}{x_{n+3/4} - x_{n+1/4}}, \quad c_{n+1/2} = \frac{x_{n+3/4} - x_{n+1/2}}{x_{n+3/4} - x_{n+1/4}}. \end{aligned}$$

The finite difference formulation (9) has order of accuracy $O(N^{-2})$. Note that the discrete system (9) is a system of $d(N + 1)$ non linear equations in the $d(N + 1)$ unknowns $\mathbf{U} = (\mathbf{U}_0, \mathbf{U}_1, \dots, \mathbf{U}_N)^T$. For the solution of (9) we can apply the classical Newton's method along with the simple termination criterion

$$\frac{1}{d(N + 1)} \sum_{\ell=1}^d \sum_{n=0}^N |\Delta^\ell U_n| \leq \text{TOL}, \quad (10)$$

where $\Delta^\ell U_n$, for $n = 0, 1, \dots, N$ and $\ell = 1, 2, \dots, d$, is the difference between two successive iterate components, and TOL is a fixed tolerance.

4. Numerical results

In this Section, we present the numerical results obtained by solving the mathematical model (3) using the non-standard finite difference

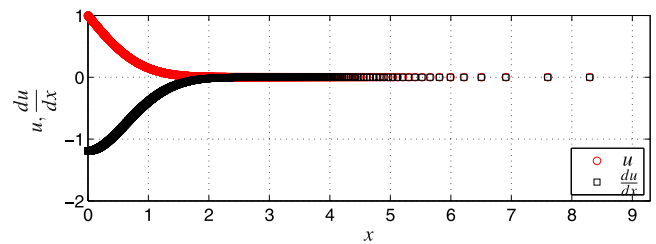


Fig. 2. Numerical solution for the problem (3) for $\alpha = 0.5$.

scheme (9) on the quasi-uniform grid defined by the logarithmic map (6) with control parameter $c = 1$. Now, let us rewrite the model (3) as a first order system as follows

$$\begin{aligned} \frac{d^1 u}{dx} &= {}^2 u, \quad x \in [0, \infty), \\ \frac{d^2 u}{dx} &= -\frac{2x}{\sqrt{1 - \alpha^1 u}} {}^2 u, \end{aligned} \quad (11)$$

with

$${}^1 u(0) = 1, \quad {}^1 u(\infty) = 0,$$

or, in an equivalent form,

$$\begin{aligned} \mathbf{u} &= ({}^1 u, {}^2 u)^T, \\ \mathbf{f}(x, \mathbf{u}) &= \left({}^2 u, -\frac{2x}{\sqrt{1 - \alpha^1 u}} {}^2 u \right)^T, \\ \mathbf{g}(\mathbf{u}(0), \mathbf{u}(\infty)) &= ({}^1 u(0) - 1, {}^1 u(\infty))^T, \end{aligned}$$

where $\mathbf{u}(x)$ is a two-dimensional vector with components ${}^\ell u(x)$ for $\ell = 1, 2$, and $\mathbf{f}: [0, \infty) \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ and $\mathbf{g}: \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^d$, with $d = 2$.

From a physical points of view, it is well known that the solution of the unsteady isothermal flow of a gas through a porous medium decays exponentially at infinity. Then, we choose as first guess for the Newton's iteration, and for the whole range of α , the following initial data

$${}^1 u(x) = \exp(\lambda x), \quad {}^2 u(x) = \lambda \exp(\lambda x),$$

with $\lambda = -2$, so that the iterative method converges within a fixed precision in a small number of iterations. Moreover, for all tests we consider a fixed tolerance $\text{TOL} = 10^{-12}$ and $N = 2000$.

Fig. 2 shows the numerical solution obtained for $\alpha = 0.5$. The recovered value of the first order derivative of the solution at the origin is $\frac{du}{dx}(0) = -1.191790644594857$, obtained in 4 iterations.

Table 1 shows the comparison of the numerical results for the model (11) for increasing values of α . For our method, the termination criterion (10) is verified in 4 iterations, for the whole range of α . We choose to report only the numerical results recently obtained by Parand and al. in [13] because are more accurate than the others results found in the literature. On the left, we report the results obtained by using the finite difference scheme on quasi-uniform grid with first guess given by (12) and $N = 2000$. On the right, the numerical values computed by the method based on rational Jacobi functions by Parand and al. The numerical results are in agreement up to six or seven decimal places, except the last value obtained for $\alpha = 1$.

Note that Parand et al. did not report the numerical solutions for the parameter values $\alpha = 0$ and $\alpha = 1$. The parameter value $\alpha = 1$ is special because, recalling the boundary condition $u(0) = 1$, the factor $\sqrt{1 - \alpha u(x)}$ in the differential equation is singular at the origin. It is important to note that, in order to construct the numerical method (9), we approximate the values of the scalar variable $u(x)$ and of its first order derivative with the finite difference formulae (7) at the mid-points of the grid, $x_{n+1/2}$ for $n = 0, 1, \dots, N - 1$, by using the non-integer nodes, so that, for $n = 0$, we have

$$\sqrt{1 - \alpha u(x)} \approx \sqrt{1 - \alpha (c_{1/2} u_0 + b_{1/2} u_1)} \neq 0.$$

Table 1
Comparison of the values of $\frac{du}{dx}$ at point $x = 0$ for increasing values of α .

α	Quasi-uniform grid	Rational Jacobi function [32]
0.0	-1.128379137175471	
0.1	-1.139007180276811	-1.1390072061783004873998771
0.2	-1.150475464757216	-1.1504754862162862032929541
0.3	-1.162941442801447	-1.1629414582959125684491997
0.4	-1.176615655957026	-1.1766156666833352029373331
0.5	-1.191790644594857	-1.1917906497194217341228284
0.6	-1.208894181745888	-1.2088941745409140190494022
0.7	-1.228598484558365	-1.2285984736959215491454848
0.8	-1.252083822445984	-1.2520837901439178944596684
0.9	-1.281881374379111	-1.2818813222033575541260553
1.0	-1.328230894324459	

Table 2
Maximum norm error for different values of α and $N = 2000$.

α	$E_\infty(N)$	α	$E_\infty(N)$
0.1	3.3408E-03	0.6	2.3003E-02
0.2	8.4401E-03	0.7	2.7790E-02
0.3	1.0531E-02	0.8	3.3027E-02
0.4	1.4428E-02	0.9	3.8878E-02
0.5	1.8570E-02	1.0	4.5714E-02

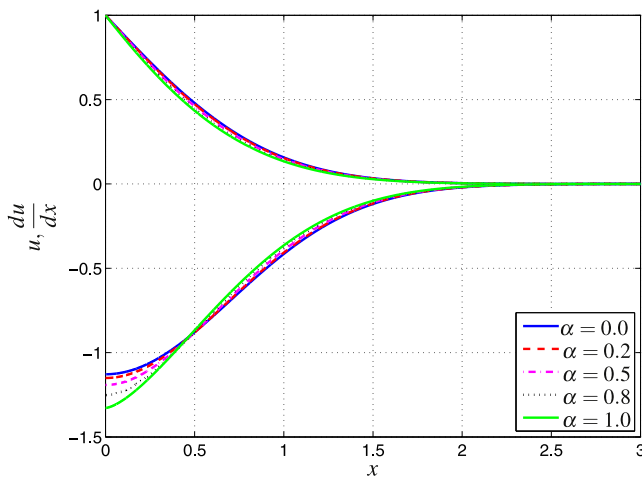


Fig. 3. Zoom of the numerical solutions for the BVP (3) for increasing values of α with $N = 2000$ and a fixed tolerance $TOL = 10^{-12}$.

Then, we do not have any difficulty in solving the model that is singular at $x = 0$. The found value of the first order derivative of the solution at the origin is $\frac{du}{dx}(0) = -1.328230894324459$, for $\alpha = 1$, obtained in 4 iterations with $N = 2000$ and a fixed tolerance $TOL = 10^{-12}$.

As said before, the solution $u(x; \alpha = 0)$ can be considered an acceptable approximation to $u(x; \alpha)$, over the whole range of parameter α . Then, we use this value for evaluating the error of the numerical solution. We define the maximum norm error

$$E_\infty(N) = \max_{0 \leq n \leq N} |u_n - U_n|,$$

where $u_n = u(x_n; \alpha = 0)$, for $n = 0, \dots, N$, is the analytical solution given by (5) and $U_n \approx u(x_n; \alpha)$ is the approximate of the solution computed by the proposed numerical method for increasing values of α . In Table 2 we report the maximum norm error for $\alpha = 0.1, \dots, 1$. Note that the smaller value of the error $E_\infty(N)$ is found for $\alpha = 0.1$ and this value increases as $\alpha \rightarrow 1$.

We notice that the numerical approximations of solution $u(x; \alpha)$ appear as a small perturbation of $u(x; \alpha = 0)$, and moreover, the recovered values of the first derivative of the solution at initial point, $\frac{du}{dx}(0; \alpha)$, tend to $\frac{du}{dx}(0; \alpha = 0)$ for the parameter values decreasing. See Fig. 3.

5. Richardson’s extrapolation and error estimator

In the previous Section, we have presented the obtained numerical results pointing out that they are in agreement up to six or seven decimal places respect to numerical solution found recently in literature. In this Section, we show how improve the accuracy of the computed solution by the Richardson’s extrapolation [38].

The main aim of the Richardson’s extrapolation is to determine a more accurate solution through subsequent refinements of the computational domain. On the spatial domain of the problem, we build a quasi-uniform grid with a mesh-points number equal to N_0 and proceed with subsequent grid refinements. We denote with g , for $g = 0, 1, \dots, G$, the quasi uniform grids constructed with the corresponding number of mesh points N_g for $i = 0, 1, \dots, G$. The grid $g = 0$ is the grid built with the smallest number of mesh points N_0 . The grid $g = G$ is the grid built with the largest number of mesh points N_G . The number of mesh points N_{g+1} is chosen such that $N_{g+1} = rN_g$ with refinement factor $r = 2$. It is important to note that the grids g and $g + 1$ are constructed in such a way that all points of the mesh g coincide with the odd mesh points of the grid $g + 1$. On each grid, the numerical solution U_g , $g = 0, 1, \dots, G$ is computed using the non-standard finite difference method. In order to reduce the calculations, we adopt a continuation strategy, in fact we use the final solution obtained on the grid g as initial guess for calculating the solution on the grid $g + 1$. where the new grid values are approximated by linear interpolations. Now, we define the level of the Richardson’s extrapolation by the index k and, the two numerical solutions related to the grids g and $g + 1$ at the extrapolated level k by $U_{g,k}$ and $U_{g+1,k}$. Then, we use the following formula to calculate a more accurate approximation at the level $k + 1$

$$U_{g+1,k+1} = U_{g+1,k} + \frac{U_{g+1,k} - U_{g,k}}{2^{pk} - 1} \quad k = 0, 1, \dots, G - 1. \tag{12}$$

Note that, with $G + 1$ nested grids, we can apply Eq. (12) G times by executing G Richardson’s extrapolations. For $k = 0$, $U_{g+1,0}$ and $U_{g,0}$ represent the solutions on the grids g and $g + 1$ obtained by the non-standard finite difference method and without any extrapolation. The case $k = 1$ is the classical single Richardson’s extrapolation. $U_{g,k}$ and $U_{g+1,k}$ represent the extrapolated value at the extrapolation level k that have a leading order of accuracy equal to p_k , $U_{g+1,k+1}$ represents the extrapolated value at the extrapolation level $k + 1$, with order of accuracy equal to p_{k+1} . The Table 3 shows the values of the first order derivative of the numerical solution at point $x = 0$ for $\alpha = 0.5$, obtained by the Richardson’s extrapolation with $N_0 = 1000$, $N_1 = 2000$, $N_2 = 4000$ and $N_3 = 8000$ grid points and $G = 3$. The last extrapolated value (not reported in the table) is

$${}^2U_{3,3} = -1.1917906497194208,$$

and can be considered as our benchmark value for $\frac{du}{dx}(0)$. The extrapolated value is in agreement up to 14 decimal places respect to numerical solution reported in Table 1.

In Table 4, we report the extrapolated values with $N_0 = 1000$, $N_1 = 2000$, $N_2 = 4000$ and $N_3 = 8000$ grid points and $G = 3$, for $\alpha = 0$. The last extrapolated value (not reported in the table) is

$${}^2U_{3,3} = -1.1283791670955117,$$

and can be considered as our benchmark value for $\frac{du}{dx}(0)$. This value can be compared with the value of the first order derivative at the origin of the erfc function

$$\frac{du}{dx}(0) = -1.128379167095513.$$

5.1. A posteriori error estimate

In the investigation of the solutions of the differential equations by the numerical methods, the study of the global error represents an important tool of evaluation of the efficiency of the same method and

Table 3
Extrapolated values at point $x = 0$ for $\frac{du}{dx}(0)$ with $\alpha = 0.5$.

N_g	${}^2U_{g,0}$	${}^2U_{g,1}$	${}^2U_{g,2}$
1000	-1.191790629222544		
2000	-1.191790644594857	-1.1917906497189612	
4000	-1.191790648438259	-1.1917906497193931	-1.1917906497194219
8000	-1.191790649399129	-1.1917906497194191	-1.1917906497194208

Table 4
Extrapolated values at origin $x = 0$ for $\frac{du}{dx}(0)$ with $\alpha = 0$.

N_g	$U_{g,0}$	$U_{g,1}$	$U_{g,2}$
1000	-1.128379047416873		
2000	-1.128379137175471	-1.1283791670950036	
4000	-1.128379159615479	-1.1283791670954819	-1.1283791670955137
8000	-1.128379165225502	-1.1283791670955097	-1.1283791670955117

the accuracy of the solution. In this Section, we describe a simple and efficient a posteriori estimate of the global error, recently proposed in [15]. The proposed global error estimate allows to solve the given problem with a suitable accuracy requiring that the error satisfies a suitable condition.

We define the global error e by the following

$$e = u - U, \tag{13}$$

that is the difference between the exact analytical solution u and the numerical approximation U . Here, we consider the (13) in the simple scalar case, and it can be applied component-wise at the given model. It is well known that, when the numerical error is caused prevalently by the discretization error and in the case of smooth enough solutions the discretization error can be decomposed into a sum of powers of the inverse of N , [37]

$$e = u - U = C_0 \left(\frac{1}{N}\right)^{p_0} + C_1 \left(\frac{1}{N}\right)^{p_1} + C_2 \left(\frac{1}{N}\right)^{p_2} + \dots, \tag{14}$$

where C_k , for $k = 0, 1, 2, \dots$, are coefficients that depend on u and its derivatives, but are independent on N , and p_k , for $k = 0, 1, 2, \dots$, are the true orders of the error. The values of p_k are usually positive integers such that $p_0 < p_1 < p_2 < \dots$. The value of p_0 is called the asymptotic order or the order of accuracy of the method or of the numerical solution U .

We get an estimate of the global error by using Eq. (12)

$$E_{g+1,k} = \frac{U_{g+1,k} - U_{g,k}}{2^{p_k} - 1}, \quad \text{for } g, k = 0, 1, 2, \dots, G - 1. \tag{15}$$

It is important to note that $E_{g+1,k}$ gives the estimate of the global error without knowledge of the exact solution, and, moreover, represents the error estimate for the more accurate numerical solution $U_{g+1,k}$ but only on the grid points of N_g . The (15) allows to solve the given problem with a prefixed tolerance ϵ requiring that the obtained estimate satisfies the following condition

$$\|E_{g+1,k}\|_{\infty} \leq \epsilon, \tag{16}$$

where the number ϵ , with $0 < \epsilon \ll 1$, is chosen according to the desired level of accuracy. Then, if the inequality (16) holds true, the numerical solution computed on the grid defined by N_{g+1} is accepted, otherwise we have to double the mesh points and repeat the computation.

For showing how the global error estimate (15) allows to solve the given problem with a suitable accuracy, by way of example, we start with $N_0 = 125$ and $N_1 = 250$ by setting the tolerance $\epsilon = 5 \times 10^{-8}$ and repeat the computation by doubling the number of spatial grid-intervals. The proposed algorithm stops when $N_6 = 8000$, that is when the required accuracy is achieved (16). In Fig. 4, we report the computation related to the error estimator $E_{g+1,k}$, for $g = 5, k = 0$.

The order errors p_k that appear in the (15) are found according to the following formula

$$p_k = \frac{\log(|U_{g,k} - u|) - \log(|U_{g+1,k} - u|)}{\log(2)}, \tag{17}$$

Table 5
Orders p_k of the solution $u(x)$ for increasing values of N .

N_g	p_0
125	
250	2.001282207078140
500	2.001278914059869
1000	2.004204030790349
2000	2.017040547706095
4000	2.070403606498473
8000	2.321931644040558
16000	

Table 6
Orders p_k of the first derivative of the solution for increasing values of N .

N_g	p_0
125	
250	2.001031623573736
500	2.000938146390995
1000	2.004282976598188
2000	2.017083514045066
4000	2.070386378299823
8000	2.321928878317238
16000	

where u is the exact solution, or, if the exact solution is unknown, as in this case, a reference solution computed with a suitable large value of N , evaluated at the same grid-points of the numerical solution. Adopting the formula (17), where we replace u by the numerical solution obtained for $N_7 = 16,000$, we find the values of the orders reported in the following tables. Note that, in this way, the line related at $N_7 = 16,000$ cannot be evaluated, then, in order to obtain the results reported in Fig. 4, we choose $p_0 = 2.321931644040558$ for the solution and $p_0 = 2.321925134936687$ for its first derivative, that are the values found with the solutions computed with $N_5 = 4000$ and $N_6 = 8000$. In addition, by the results reported in Tables 5 and 6, we can conclude that $p_0 \approx 2$ represents the true order of the proposed finite difference method.

6. Concluding remarks

The main aim of this paper is to find an accurate solution for the unsteady flow of gas through a semi-infinite porous medium. We propose a non standard finite difference method on a quasi-uniform grid for solving the given problem and report a new numerical approximation of the solution. We solve the given BVP on a semi-infinite interval without imposing artificial boundary conditions on the truncated boundary because we introduce a stencil that is built in such a way that the boundary conditions at infinity are exactly assigned. In addition, the presented method allows to obtain the numerical solution also for $\alpha = 1$. Comparisons with some recently proposed results are carried out to validate the accuracy of the obtained numerical results, and to show the efficiency and the reliability of the proposed numerical method.

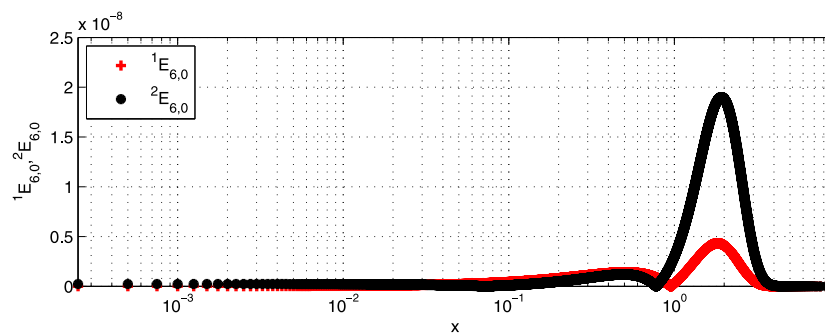


Fig. 4. A posteriori error estimate for the field variable and its first order derivative for (11) with $\alpha = 0.5$, $N_5 = 4000$ and $N_6 = 8000$. ${}^1E_{6,0}$ and ${}^2E_{6,0}$ are the error estimates provided by Eq. (15) of the solution and of the first order derivative, respectively.

Moreover, we improve the accuracy of the numerical results by the Richardson's extrapolation that allows to define an error estimator also if the exact solution is unknown. The numerical solutions presented in this paper result highly accurate and in excellent agreement with the existing solutions available in the literature. The value of initial slope $\frac{du}{dx}(0)$ calculated for $\alpha = 0.5$ is -1.1917906497194208 accurate up to the 14 decimal places.

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Declaration of absence of conflict of interest

The authors declare the absence of any conflict of interest.

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