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Pore-scale modelling of fluid flow in porous media using the projection method for incompressible Navier-Stokes equations in irregular domains

This paper presents the results of numerical simulation of incompressible viscous flow in porous media, which comprise periodically arranged cylinders. This simulation is based on the numerical solution of the incompressible Navier-Stokes equations in irregular domains using the projection method on staggered grids, where the irregular boundary is represented by its level-set function at the pore-scale level. The main problem in numerical calculation of fluid flow through porous media occurs when the value of the porosity is close to 1 or is close to the threshold value since it is necessary to take a very fine numerical mesh, which requires additional computing power and increases the calculation time. There are exact analytical solutions for simple types of porous media which consist of periodically arranged cylinders. In this paper, the permeabilities of these porous media were numerically calculated and compared with the previous works based on the numerical solution of the Lattice-Boltzmann equation in irregular domains, when the fluid flow obeys Darcy's law. The comparison of numerical and theoretical values of porosity shows that this method is sufficiently accurate for porosity values φ=0.2–0.8.

Keywords: Navier-Stokes equations, numerical simulation, projection method, fibrous porous medium, permeability, porosity, grid, irregular boundary, fluid flow, geometry of pore space.

Introduction

Many of the environmental and industrial problems are related to the fluid flow in porous media. Therefore, understanding the processes that take place inside a porous medium plays a key role in science and technology.

Rabbani and Babaei [1] used pore network modeling (PNM) with a Lattice Boltzmann Method (LBM) to benefit from the strengths of both approaches. They calculated permeabilities of all throats using the LBM and substituted in the pore network model. Solving the LBM for every throat leads to an accurate representation of flow, but the algorithm is computationally expensive. LBM is used to model the steady-state incompressible fluid flow through different throat images and an Artificial Neural Network (ANN) is trained to mimic the trend of throat's permeabilities based on cross–sectional images [1].

The disadvantage of the PNM is that it cannot be applied to an inaccurate geometry. The main limitation of direct methods is the high computational cost [2], which could be a major obstacle in the case of large-sized and high-resolution volumetric images of porous material. As a solution to this size and time limitation, domain decomposition and parallel computation have been comprehensively hired to increase the models' efficiency and scalability. As another solution to deal with computational limitations, machine learning can be employed to mimic the behavior of complex solid/fluid systems. The main idea is to save the computational sources by solving a series of typical problems and extend the results to all similar cases.

With the development of high-performance computing and micro-CT technologies which allows to construct detailed geometrical description of material microstructure, it is possible to use numerical experiments for direct evaluation of material properties. In geophysical applications, such techniques are called digital rock physics and are meant to accompany and supply conventional laboratory measurements for evaluation of transport properties of rock core samples [3].

To distinguish porous media from each other, it is necessary to determine the geometry of pore space, due to microscopic pore sizes and a large number of pores per unit volume of porous medium. It is a difficult task. In most cases, statistical methods are used to determine the geometry of pore space [4, 5]. The main problem of the investigation of porous media properties is the problem of finding a relation between macroscopic parameters (e.g., permeability, elastic constants, electric or thermal conductivity) and the pore space geometry of porous media (the microstructure of porous media). For example, when the fluid flows through porous media at a low Reynolds number and it obeys Darcy's law [6]:

$$\vec{U} = \frac{K}{\mu}\nabla(p + \rho g z) \tag{1}$$

where $\vec{U}$ is the flow rate, K is the permeability of porous medium, μ is the fluid viscosity, p is the pressure in the porous medium and ρgz is the hydrostatic pressure. The main problem in this case is finding a relation between the permeability and geometrical parameters of porous media. There are only approximate solutions for simple cases of porous media comprising periodically arranged cylinders [7–11], which we consider in this paper. Mostly in practice, the Kozeny–Carman relation between the permeability and geometrical parameters of porous media is used [12, 13]:

$$K = \frac{\phi^3}{6s^2}$$

where φ is the porosity and s is the specific surface area. However, this relation was obtained for simple porous medium which constructed by the parallel capillaries with circular cross-section and this relation does not consider the microstructure of the porous medium.

This paper presents the results of numerical simulation of incompressible viscous flow in porous media at the pore-scale level. This simulation is based on the numerical solution of incompressible Navier-Stokes equations in irregular domains using the projection method on staggered grids, where the irregular boundary is represented by its level-set function [14–16]. When the fluid flow obeys Darcy's law, the permeability of these porous media was numerically calculated and compared with the previous works based on the numerical solution of the lattice-Boltzmann equation in irregular domains [17], and also the artificial compressibility relaxation algorithm was applied [18].

Experimental

Definition of the problem. A porous medium of volume V is represented in the form of the domain D which consists of two sub-domains: domain of voids D_0 with volume of fraction φ and domain of solid phases D_1 with volume of fraction 1- φ. The voids are called pores, and these pores form a pore space. Fluids that occupy these pores can flow if these pores are connected with each other [12, 13]. The minimum value of volume fraction φ at which fluid flows through a porous medium is called a threshold value [19]. A slow laminar flow through a porous medium is the problem that needs to be solved on a microscopic level. The microstructure of two-phase porous medium D is described in detail by the characteristic $I(\vec{x})$ function:

$$I(\vec{x}) = \begin{cases} 0 \; for \; \vec{x} \in D_0 \\ 1 \; for \; \vec{x} \in D_1 \end{cases} \tag{2}$$

The considering model is based on the numerical solution of Navier-Stokes equations for incompressible fluid flow through porous medium which is described by the $I(\vec{x})$ (equation (2)):

$$\left(\frac{\partial \vec{u}(\vec{x},t)}{\partial t} + (\vec{u}(\vec{x},t)\cdot\nabla)\vec{u}(\vec{x},t)\right) = \rho\vec{g} - \nabla p(\vec{x},t) + \mu\nabla^2\vec{u}(\vec{x},t), \vec{x} \in D_0 \tag{3}$$

$$\nabla\cdot\vec{u}(\vec{x},t) = 0, \vec{x} \in D_0 \tag{4}$$

No-slip boundary conditions are applied on the pore-matrix interface ∂D_0:

$$\vec{u}(\vec{x},t) = 0, \vec{x} \in \partial D_0 \tag{5}$$

The cubic porous medium domain D with size a is considered and the periodic boundary conditions are applied on its faces:

$$\vec{u}\left(\overrightarrow{x_C} - \frac{a}{2}, t\right) = \vec{u}\left(\overrightarrow{x_C} + \frac{a}{2}, t\right) \tag{6}$$

where $\overrightarrow{x_C}$ is the position of center of cubic domain D.

To find the permeability of porous medium, the steady state solution of equations (3, 4) with boundary conditions (5, 6) is found using the projection method on staggered grids [15]. This solution is averaged over the porous medium domain:

$$\vec{U} = \frac{\int_D \vec{u}(\vec{x})dV}{V}. \tag{7}$$

Then the Reynolds number ($Re = \frac{\rho UL}{\mu}$, where L is the characteristic length) is found below which the fluid flow in porous medium obeys Darcy's law for permeability calculation using the equation (1).

Numerical methodology. The solid surface is determined by introducing the level-set function for solid phase. For example, if the solid phase is a single sphere with diameter d, then its level-set function is as follows:

$$F(x, y, z) = (x - x_C)^2 + (y - y_C)^2 + (z - z_C)^2 - \frac{d^2}{4},$$

where x_C, y_C, z_C are the coordinates of the center of sphere. After introducing the level-set function for solid phase the characteristic function $I(\vec{x})$ (equation (2)) can be determined:

$$I(x, y, z) = \begin{cases} 0 \; if \; F(x, y, z) > 0, \\ 1 \; if \; F(x, y, z) \leq 1. \end{cases}$$

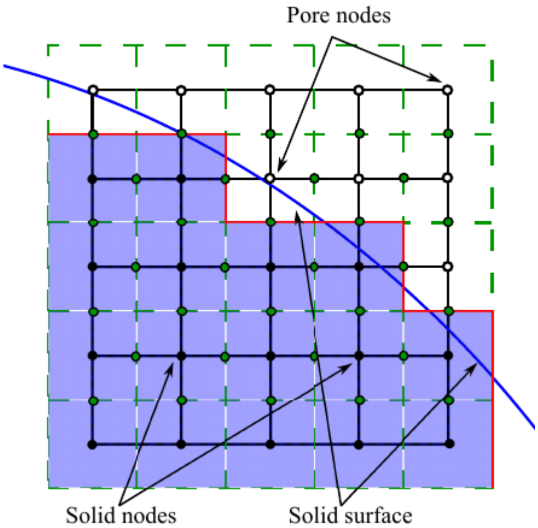

Figure 1. Representation of the staggered grid and solid surface

Porous medium domain D is approximated by generating a uniform, structured mesh that incorporates nodes of solid phase (or rock phase) D_1 and pore D_0 domains (example of the 2D structured mesh is shown in Figure 1 as black, solid lines).

The volume of solid phase of a porous medium can be calculated using the level-set function of solid phase:

$$V_{i,j,k} = \begin{cases} 0 \; if \; I(x_i, y_j, z_k) = 0 \\ \Delta^3 \; if \; I(x_i, y_j, z_k) = 1 \end{cases} \tag{8}$$

where i, j, k are the indexes of the mesh nodes in x, y, z direction, respectively, Δ and $V_{i,j,k}$ are the size and volume of the cells which circumscribed around the mesh nodes, respectively.

The total volume of the solid phase of a porous medium is:

$$V_s = \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_y-1} \sum_{k=0}^{N_z-1} V_{i,j,k}, \tag{9}$$

where N_x, N_y and N_z are the number of the mesh nodes in x, y, z direction, respectively.

The total volume of pores of a porous medium is:

$$V_p = V - V_s.$$

The volume fraction of pores (or porosity) of a porous medium is:

$$\phi = \frac{V_p}{V} = 1 - \frac{V_s}{V}.$$

Also, the solid surface (blue line in Figure 1) can be calculated using the level-set function of solid phase:

$$S_{i,j,k} = \begin{cases} \Delta^2 \; if \; (I_{i+1,j,k} = 1 \; or \; I_{i,j,k} = 1) \; and \; I_{i+1,j,k} I_{i,j,k} = 0, \\ \Delta^2 \; if \; (I_{i,j+1,k} = 1 \; or \; I_{i,j,k} = 1) \; and \; I_{i,j+1,k} I_{i,j,k} = 0, \\ \Delta^2 \; if \; (I_{i,j,k+1} = 1 \; or \; I_{i,j,k} = 1) \; and \; I_{i,j,k+1} I_{i,j,k} = 0, \\ 0 \; otherwise. \end{cases} \quad (10)$$

The total value of the solid surface is (red line in Figure 1):

$$S = \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_y-1} \sum_{k=0}^{N_z-1} S_{i,j,k} \quad (11)$$

The specific surface is:

$$s = \frac{S}{V}.$$

Calculation of the cross-sectional area and perimeter of a cylinder. The solid surface of a cylinder with the periodic structure (Figure 2) is determined by introducing the following level-set function:

$$F(x,y) = (x - x_C)^2 + (y - y_C)^2 - \frac{d^2}{4}, \quad (12)$$

where d is the diameter of a cylinder.

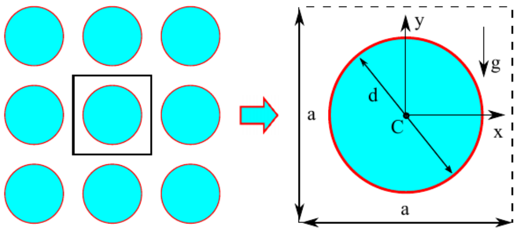

Figure 2. Two-dimensional rectangular area (d is the diameter of cylinder)

The area and perimeter of the cross-section of a cylinder are numerically calculated using equations (8, 9, 10, 11, 12). The comparison of numerical values of cross-sectional area and perimeter of a cylinder with exact values are shown in the Table 1, where a cylinder's diameter is d=0.6 (exact value of the area is $S = \frac{\pi d^2}{4} = 0.282743$ and the perimeter is $P = \pi d = 1.884956$).

The deviation between the numerical value of area and exact value is:

$$E.A. = |numerical\ value - exact\ value|.$$

The relative error is:

$$R.E.A. = \frac{E.A.}{exact\ value}.$$

Table 1

The comparison of the numerical values of cross-sectional area and perimeter of a cylinder with exact values (cylinder's diameter is d=0.6)

Number of the mesh nodes	S (cross sectional area)	E.A.	R.E.A.	P (cross-sectional perimeter)	E.P.	R.E.P.
16x16	0.269531	0.013212	0.046728	2.250000	0.365044	0.193662
32x32	0.286133	0.003389	0.011988	2.375000	0.490044	0.259977
64x64	0.281494	0.001249	0.004418	2.437500	0.552544	0.293134
128x128	0.283020	0.000277	0.000979	2.406250	0.521294	0.276555
256x256	0.282486	0.000257	0.000910	2.390625	0.505669	0.268266
512x512	0.282825	0.000082	0.000290	2.398438	0.513482	0.272411

Permeability calculation. There are many theoretical predictions of the permeability of fibrous porous media with the periodic structure [8–11].

John Happel [8] found the theoretical estimation of the permeability of these media by solving the Stokes equation for a fluid flow around a cylinder with no-slip boundary conditions at the surface of cylinder and periodic boundary conditions at the domain boundary. His theoretical prediction of the permeability of a fibrous porous medium is:

$$K_1^* = \frac{K_1}{d^2} = \frac{1}{32\varphi}\left[ln\left(\frac{1}{\varphi}\right) - \frac{1-\varphi^2}{1+\varphi^2}\right],$$

where K_1 is the permeability of fibrous porous media, d is the diameter of cylinders and $\varphi = \frac{d^2}{a^2}$, where a is the distance between centers of cylinders (see Figure 2). The main inaccuracy in his calculation is that the solution was based on solving the Stokes equation in a cylindrical coordinate system, and hence the boundary of its domain does not coincide with the real boundary.

In the work of Hasimoto [9], the exact solution of the Stokes equation for fluid flow around a cylinder in the form of infinite series is used to predict the permeability of fibrous porous media. He found the theoretical prediction of the permeability of fibrous porous media using only the terms of lowest order of this series:

$$K_2^* = \frac{K_2}{d^2} = \frac{1}{32\varphi'}\left[ln\left(\frac{1}{\varphi'}\right) - 1.476 + 2\varphi'\right] + O(\varphi'),$$

where $\varphi' = \frac{\pi d^2}{4a^2}$.

Later Sangani and Acrivos (1982) [20] improved the theoretical prediction of permeability of fibrous porous media using the terms of the highest order of the series presented in the work of Hasimoto [9]:

$$K_3^* = \frac{K_3}{d^2} = \frac{1}{32\varphi'}\left[\ln\left(\frac{1}{\varphi'}\right) - 1.476 + 2\varphi' - 1.774\varphi'^2 + 4.078\varphi'^3\right] + O\left(\varphi'^3\right).$$

The value of K_3 is close to exact value when φ' is close to 0, so the numerical value of permeability can be validated by comparing with the value of K_3 when φ' is close to 0. They also presented the numerical method to calculate the permeability for all values of the porosity in the work [10].

In the work [11], the porous medium is considered as "unit cell" and there is a unidirectional flow with a parabolic velocity profile. Their theoretical prediction of the permeability of fibrous porous medium is:

$$K_4^* = \frac{K_4}{d^2} = \frac{1}{3\varphi'} \cdot \frac{(1-\varphi)^{\frac{5}{2}}}{\left(2(\varphi+2) + 4\frac{(1-\sqrt{\varphi})(1-\varphi)^2}{\sqrt{\varphi}}\right)\frac{\sqrt{1-\varphi}}{\sqrt{\varphi}} + 12arctan\left(\frac{1+\sqrt{\varphi}}{\sqrt{1-\varphi}}\right)}.$$

The projection method on the staggered grid was applied to solve the incompressible Navier-Stokes equations and all numerical calculations were performed using PARIS simulator [21]. The results of numerical calculation of permeability were validated by comparing with theoretical estimations of the permeability of porous media like porous medium which consist of periodically arranged cylinders [7–11].

Results and Discussion

The fibrous porous medium with a periodic structure is considered in this section. Fibers are located at the same distance to each other and have the same diameter. Planar flow, that is perpendicular to the axes of cylinders, is considered. The fluid flows through this porous medium by the gravitational force. The following parameters are used: fluid density ρ=1, fluid viscosity μ=1, domain size a=1.

To find the permeability, the steady-state solution of Navier-Stokes equations is averaged over the porous medium domain (equation (7)). The permeability of fibrous porous media is numerically calculated and compared with existing theoretical estimations. For the case when the value of the porosity is close to 1, the Brinkman's estimation can be used to obtain exact solution [22].

The relation between flow rate and number of mesh nodes is shown in Table 2.

Table 2

Relation between the flow rate and number of nodes of the mesh for 2D fluid flow through the fibrous porous medium when a cylinder's diameter is *d*=0.6

Number of the mesh nodes	Flow rate
16x16	1.126954E-02
32x32	1.166258E-02
64x64	1.146031E-02
128x128	1.125835E-02

The comparison of numerical and theoretical values of the permeability of fibrous porous medium is shown in Figure 3 and Table 3.

Table 3

Numerical values of the permeability of fibrous porous medium

d (diameter of the cylinders)	φ (porosity)	s (specific surface)	$K^* = \frac{K}{d^2}$ (permeability)
0.2	0.968933	0.781250	2.076525
0.3	0.929626	1.218750	0.584678
0.4	0.874207	1.593750	0.207850
0.5	0.804138	2.031250	0.080000
0.6	0.716980	2.406250	0.030931
0.7	0.614929	2.781250	0.010859
0.8	0.496765	3.218750	0.003048
0.9	0.363464	3.593750	0.000543

Figure 3 illustrates the convergence of the flow rate (equation (7)) to the steady state value for 2D fluid flow through the fibrous porous medium.

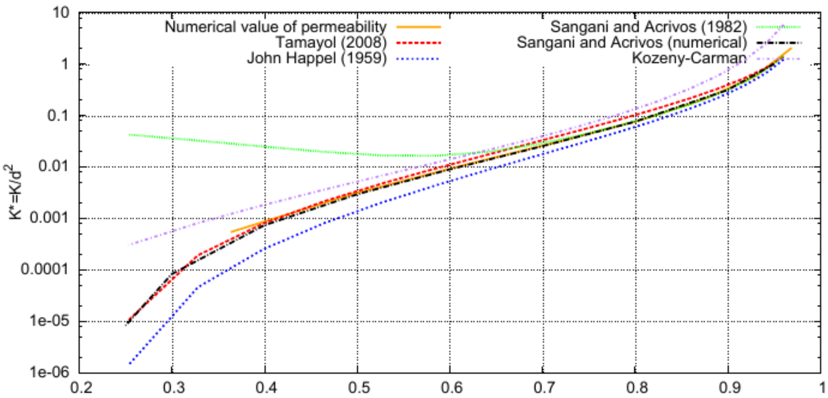

Figure 3. Comparison of the numerical and theoretical values of the permeability of fibrous porous medium

When the cylinder's diameter is small, the boundary of the domain which is considered in the work [8] almost coincide with the real boundary, so in this case the value of K_1 is close to exact value (see Figure 3).

According to Figure 3 the numerical value of the permeability is close to the value of K_3 when φ is close to 1. Thus, the error in numerical calculation of the specific surface of the fibrous porous medium has a weak effect on the numerical value of permeability.

Also, it can be seen that the numerical values of permeability presented in the work [10] are close to the numerical values of permeability for all values of the porosity where the numerical calculations were performed.

Conclusions

This paper presents the results of numerical simulation of incompressible viscous flow in porous media at the pore-scale level. To find the Reynolds number below which the fluid flow obeys Darcy's law, the incompressible Navier-Stokes equations are numerically solved using the projection method on staggered grids. The main reason for choosing this method is the possibility of finding the steady-state solution of Navier-Stokes equations more quickly than such methods as Lattice-Boltzmann, Smoothed-Particle Hydrodynamics, etc. However, this method becomes ineffective when the value of the porosity is small or is close to 1. The comparison of numerical and theoretical values of permeability shows that this method is sufficiently accurate for porosity values φ=0.2–0.8.

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Кеуекті ортадағы сұйықтық ағынын кеуек масштабында модельдеу тұрақсыз аймақтардағы сығылмайтын сұйықтық үшін Навье-Стокс теңдеулеріне проекциялау әдісін қолдану

Мақалада периодты орналастырылған цилиндрлерден тұратын кеуекті ортадағы тұтқыр сығылмайтын сұйықтықтың ағынын сандық модельдеудің нәтижелері келтірілген. Бұл модельдеу шахмат торларындағы проекциялық әдісті қолдана отырып, тұрақты емес аудандардағы сығылмайтын сұйықтық үшін Навье–Стокс теңдеулерін сандық шешуге негізделген, мұнда тұрақты емес шекара масштабты деңгейде деңгей орнату функциясымен ұсынылған. Кеуекті орта арқылы сұйықтық ағынын сандық есептеудегі негізгі мәселе кеуектілік мәні 1 немесе шекті мәнге жақын болған кезде пайда болады. Мұндай жағдайларда қосымша есептеу қуатын қажет ететін өте аз сандық торды пайдалану керек, сонымен қатар, есептеу уақытын арттырады. Периодты орналастырылған цилиндрлермен тұратын кеуекті орта сияқты кеуекті ортаның қарапайым түрлеріне нақты аналитикалық шешімдер бар. Мақала авторлары бұл кеуекті орталардың кеуектілігін сандық түрде есептеп, оларды сұйықтық ағыны Дарси заңына бағынатын кезде біркелкі емес аймақтардағы Больцман тор теңдеуінің сандық шешіміне негізделген алдыңғы жұмыстармен салыстырған. Кеуектіліктің сандық және теориялық мәндерін салыстыру бұл әдістің φ = 0,2–0,8 кеуектілік мәндері үшін өте дәл екенін көрсетеді.

Кілт сөздер: Навье-Стокс теңдеулері, сандық модельдеу, проекция әдісі, талшықты кеуекті орта, өткізгіштік, кеуектілік, тор, тұрақсыз шекара, сұйықтық ағыны, кеуектер кеңістігінің геометриясы.

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Поромасштабное моделирование течения жидкости в пористых средах с использованием проекционного метода для несжимаемых уравнений Навье–Стокса в нерегулярных областях

В статье представлены результаты численного моделирования течения вязкой несжимаемой жидкости в пористой среде, которая состоит из периодически расположенных цилиндров. Данное моделирование основано на численном решении уравнений Навье–Стокса для несжимаемой жидкости в нерегулярных областях с использованием проекционного метода на шахматных сетках, где нерегулярная граница представлена ее функцией установки уровня на поромасштабном уровне. Основная проблема при численном расчете течения жидкости через пористую среду возникает, когда значение пористости близко к 1 или к пороговому значению. В таких случаях необходимо использовать очень мелкую численную сетку, что требует дополнительных вычислительных мощностей, а также увеличивает время вычислений. Существуют точные аналитические решения для простых типов пористых сред, таких как пористые среды, которые состоят из периодически расположенных цилиндров. Авторами статьи пористости указанных пористых сред были численно рассчитаны и сравнены с предыдущими работами, основанными на численном решении решеточного уравнения Больцмана в нерегулярных областях, когда течение жидкости подчиняется закону Дарси. Сравнение численных и теоретических значений пористости показывает, что данный метод достаточно точен для значений пористости φ = 0,2–0,8.

Ключевые слова: уравнения Навье-Стокса, численное моделирование, проекционный метод, волокнистая пористая среда, проницаемость, пористость, сетка, нерегулярная граница, течение жидкости, геометрия порового пространства.