Permeability calculation in periodic porous medium based on rhombohedral structure

D E Igoshin, A S Gubkin, P A Ignatev and A A Gubaidullin

Tyumen Branch of Khristianovich Institute of Theoretical and Applied Mechanics SB RAS, Tyumen State University, Tyumen, Russia

E-mail: igoshinde@gmail.com

Abstract. A method for calculating the permeability of a porous medium is proposed and realized using the example of a rhombohedral porous structure. The method is based on the Darcy equation, while the flow rate is found by numerical simulation of a three-dimensional flow of a viscous incompressible fluid in a pore channel. Computational experiments are performed using open SALOME-OpenFOAM packages. The results of the calculations allow estimating the accuracy of previously obtained analytical estimates of permeability.

1. Introduction

Models of periodic porous media are widely used in describing the properties of nanomaterials [1-4], in geophysics [5] and in geology [6, 7]. Mathematical modeling of porous media by periodic structures has several advantages: the porosity of the medium can be specified analytically; in numerical simulation of the filtration, it is sufficient to find a solution in the volume of the pore of a single rhombohedron. The main parameter that determines the filtration is the permeability of the porous medium. In [8-9], approaches were developed to obtain analytical estimates of the permeability of periodic porous media. In this paper, we propose a method for calculating permeability using the Darcy equation, where the fluid flow is found by numerical simulation of a three-dimensional flow of a viscous incompressible fluid in a pore channel. The method is illustrated by examples of calculating the permeability of periodic rhombohedral porous structures.

2. Porosity and permeability the rhombohedral periodic structure

Permeability of porous media is determined not only by porosity, but also by the structure of pore channels [10]. Previously, a model of a porous medium with three parameters \( L, \alpha, \theta \) based on a periodic rhombohedral structure was developed [11]. Within the framework of the model, the porosity of the medium is determined by the expression

\[
m = \frac{V_n}{V} = 1 - \frac{V_c}{V} = 1 - \frac{\pi [2 - 3\alpha^2 (3 - \alpha) - 3\alpha_2^2 (3 - \alpha_2)]}{12 (1 - \alpha)^3 (1 - \cos \theta) \sqrt{1 + 2 \cos \theta}},
\]

\[
\alpha = \frac{r - r_0}{r}, \quad r_0 = \frac{L}{2}, \quad r_* = \frac{r_0}{\cos(\theta/2)},
\]

\[
\alpha_2 = 1 - 2(1 - \alpha) \sin(\theta/2) \quad \text{при} \quad \alpha > 1 - \frac{1}{2 \sin(\theta/2)}.
\]
where $L$ is the lattice period, $r$ is the radius of the spherical segments, $r_0$ is the radius in the case of tangent of balls, $r_*$ is the radius in the case of closed pores, $\theta$ is the acute angle on the rhombohedron face, $\alpha$ is the dimensionless parameter of the degree of intersection of the spheres, and $\alpha_2$ is the dimensionless parameter of the degree of intersection of the spheres located on opposite vertices of the rhombus.

Isolines of porosity for various values of the parameters $\theta$ and $\alpha$ (porosity does not depend on $L$) are shown in figure 1. It can be seen that the porosity increases with increasing $\theta$ for a fixed $\alpha$ and decreases with increasing $\alpha$ at a fixed $\theta$. The line MN corresponds to the boundary of the region $(\theta, \alpha)$, at which the pores are closed.

![Figure 1](image.png)

**Figure 1.** The isolines of the porosity of the rhombohedral structure for different values of the angle $\theta$ and the degree of intersection of the spheres $\alpha$.

The main parameter that determines the filtration is the permeability of the porous medium. To calculate the permeability of the model structure, we use the Darcy equation.

$$\frac{Q}{S} = \frac{k}{\mu} \frac{\Delta p}{H},$$

where $Q$ is the volumetric flow through a porous medium with a cross-section $S$, $k$ is the permeability, $\Delta p$ is the pressure drop, $\mu$ is the dynamic viscosity of the liquid, and $H$ is the extent of the porous medium. The values of $H, S$ can be expressed in terms of the parameters of the model $L, \theta$

$$H = L \sqrt{1 - \left( \frac{\cos \theta}{\cos(\theta/2)} \right)^2}, \quad S = L^2 \sin \theta.$$

Then, from the Darcy equation, one can find the permeability of the model medium at a given pressure drop and the corresponding flow rate.
The flow $Q$ is determined from the results of a numerical solution of the system of equations for a 
stationary three-dimensional flow of a viscous incompressible fluid

$$
\nabla \vec{v} = 0,
$$

$$
(\nu \nabla) \vec{v} = -\nabla p + \mu \Delta \vec{v}.
$$

The periodicity of the model rhombohedral structure allows us to confine ourselves to the solution 
for the pore space of an individual rhombohedron. As the boundary conditions, we take the condition 
of "slipping" "no-slip" on the wall of the pore channel, and at the inlet and outlet to the channel we set 
the pressure. On the other faces of the rhombohedron, we impose periodic boundary conditions that 
ensure the continuity of the flow (figure 2).

\begin{align*}
\text{inlet:} & \quad \frac{dv}{dn} = 0, \quad p = p_{in}, \\
\text{outlet:} & \quad \frac{dv}{dn} = 0, \quad p = p_{out}, \\
\text{wall:} & \quad v = 0, \quad \frac{dp}{dn} = 0, \\
\text{cyclic:} & \quad \text{periodic boundary conditions}.
\end{align*}

3. **Numerical simulation of flow**

For the numerical solution of problem (2) - (3), the simpleFoam solver included in the standard 
package of the OpenFOAM was used. The computational domain was covered with an unstructured 
tetrahedral mesh with condensations, taking into account the features of geometry. Calculation of the 
convective part of the acceleration was carried out using a TVD-scheme with a vanLeer limiter. To 
calculate the Laplace operator, a linear scheme with a non-orthogonal correction was used. For solving 
the conservation equations SIMPLE-procedure with optimal relaxation factors was used: 0.3 — for 
pressure equation and 0.9 — for velocity equation. The relaxation parameters were selected from a 
series of calculations for a single structure and subsequently used for other structures. As a method of 
solving a system of linear algebraic equations (SLAE) for pressure, a multigrid method was used, and 
the method of bi-conjugate gradients was used for the velocity. The preconditioning of SLAE for 
pressure was carried out by the method of incomplete decomposition of Cholesky, and for speed — by 
the method of incomplete LU-factorization.

As a result of the computational experiments, isolines of dimensionless permeability were 
constructed for various porous media of the rhombohedral structure (figure 3). Each point on the plane 
$(\theta, \alpha)$ corresponds to a specific porous structure. 2336 calculations (experiments) were performed with 
a step $\Delta \theta = 0.5^\circ$ with respect to the angle $\theta$ and $\Delta \alpha = 0.005$ with respect to the parameter $\alpha$. The 
number of elementary volumes in the calculation area ranged from 50 to 220 thousand. The curve MN 
in figure. 3 limits the region of impermeable porous media in the same way as the curve MN in figure. 
1 bounds the region of closed-pore media. The comparison of figures 1 and 3 shows a qualitatively 
similar dependence of porosity and permeability on the parameters $\theta, \alpha$ as the MN line approaches, 
the porosity decreases, and the permeability rapidly falls by several orders of magnitude.

Previously, the methods of analytical estimation of permeability [12-14], which can be applied to 
the rhombohedral structure, have been proposed. The results of this paper allow us to analyze the 
accuracy of these estimates. The results of the analysis are shown in figures 4 and 5 in the form of 
isolines of permeability ratios calculated by the methods of [12] and [14], to the permeabilities 
calculated in this paper for the corresponding values of $\theta, \alpha$. It can be seen that the technique [12] 
overestimates the permeability values the more, the smaller the porosity / permeability, and the 
technique [14], on the contrary, underestimates the permeability values. The degree of understatement
also increases with a decrease in porosity / permeability, however, the accuracy of the estimate by the method of [14] is higher than that of [12].

![Figure 2. Computational domain with tetrahedral mesh.](image)

![Figure 3. Isolines of the permeability of the rhombohedral structure for different values of the angle $\theta$ and the degree of intersection of the spheres $\alpha$.](image)
**Figure 4.** The isolines of the permeability ratios calculated by the method of [12] to those obtained on the basis of numerical modeling, for different values of the angle $\theta$ and the degree of intersection of the spheres $\alpha$.

**Figure 5.** The isolines of the permeability ratios calculated by the method of [14] to those obtained on the basis of numerical modeling, for different values of the angle $\theta$ and the degree of intersection of the spheres $\alpha$. 
In conclusion, we note that the experience of this paper will be applied in the future to the model of a porous medium with random microinhomogeneities, developed in [15, 16].

This work was supported by the Russian Foundation for Basic Research (Project No. 16-29-15119).

References
[1] Tretyakov Yu, Lukashin A and Eliseev A 2004 Russian Chemical Reviews 73-9 899
[2] Zakharova G, Volkov V, Ivanovskaya V and Ivanovskii A 2005 Russian Chemical Reviews 74-7 587
[3] Rempel A 2007 Russian Chemical Reviews 76-5 435
[4] Golovan L, Timoshenko V and Kashkarov P 2007 Physics-Uspekhi 50-6 595
[5] Kocharyan G, Kostyuchenko V and Pavlov D 2004 Physical Mesomechanics 7-1 5
[6] Kontorovich A, Burshtein L, Safronov P, Guskov S, Ershov S, Kazanenkov V, Kim N, Kontorovich V, Kostyreva E, Melenevskiy V, Livshits V, Malyshov N, Polyakov A and Skvortsov M 2013 Russian Geology and Geophysics 54-8 917
[7] Cherepanov S, Matyushev D and Ponomareva I 2013 Oil Industry 3 62
[8] Igoshin D E and Maksimov A Yu 2015 Tyumen State University Herald (Physical and Mathematical Modeling. Oil, Gas, Energy) 1-3 112
[9] Igoshin D E and Khromova N A 2015 Tyumen State University Herald (Physical and Mathematical Modeling. Oil, Gas, Energy) 1-4 69
[10] Igoshin D E and Khromova N A 2016 Proceedings in Cybernetics 3-23 8
[11] Igoshin D E and Khromova N A 2016 Tyumen State University Herald (Physical and Mathematical Modeling. Oil, Gas, Energy) 2-3 107
[12] Igoshin D E and Ignatev P A 2017 Proc. All-Rus. Conf. on Digital Methods of Engineering (Tula), 114
[13] Gubaidullin A A, Igoshin D E and Khromova N A 2016 Tyumen State University Herald (Physical and Mathematical Modeling. Oil, Gas, Energy) 2-2 105
[14] Gubaidullin A A, Igoshin D E and Ignatev P A 2018 Proc. All-Rus. Seminar on Dynamics of Multiphase Media (Novosibirsk) AIP Conference Proceedings 1939 020033
[15] Gubkin A S, Igoshin D E and Trapeznikov D V 2016 Tyumen State University Herald (Physical and Mathematical Modeling. Oil, Gas, Energy) 2-4 54
[16] Gubaidullin A A, Gubkin A S, Igoshin D E and Ignatev P A 2018 Proc. All-Rus. Seminar on Dynamics of Multiphase Media (Novosibirsk) AIP Conference Proceedings (American Institute of Physics) 1939 020035