Two-scale modeling of spatial flows of gas and weakly compressible liquid in porous composite structures

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Abstract. The paper proposes a physico-mathematical model of a weakly compressible fluid and a two-scale model of the spatial flow of a weakly compressible fluid that displaces the gas medium in a porous composite structure. The model is based on an asymptotic analysis of the three-dimensional Navier-Stokes equations. Algorithms for the numerical solution of local problems of the spatial flow of liquid and gas on the periodicity cells of composite structures and the algorithm for calculating the permeability tensor are developed. A numerical algorithm for solving the global liquid flow problem that displaces gas from a porous composite structure is developed. Examples of numerical modeling of local spatial flows of liquid and gas on the periodicity cell of typical composite structures are given, and also results of numerical modeling of the macroscopic flow of a liquid binder displacing the gas medium in a typical porous composite structure are obtained.

1. Introduction

Liquid and gas filtration processes play an important role in the production of modern composite materials and structures based on LCM (Liquid Composite Molding) methods, which consist of impregnating the reinforcing filler with a liquid binder in the mold. The quality of the composite structures obtained by these methods depends to a large extent on the parameters of the manufacturing technology. In this connection, it is extremely important to adequately model the flow of a liquid binder in porous composite structures having a complex spatial geometric shape, simultaneously with the movement of gas (air) displaced by the liquid.

The problems of modeling various processes in porous systems, in particular with reference to the mechanics of composite materials, are of considerable interest today. For example, the stability of non-steady plane water evaporation fronts, arising in vertical flows with phase transition in horizontally extended domains of a porous medium is studied in [1]. Various aspects of modeling the technological processes of composite materials production are considered in [2-8].

We note that in the vast majority of publications, the study of fluid flow processes in porous structures is studied in the framework of the phenomenological filtration theory, which is based on the Darcy law and its modifications [9, 10]. In this case, the permeability coefficients of a porous medium are determined either experimentally or by using various empirical and approximate relationships to describe local filtration processes. In this case, rather rough estimates of real processes occurring inside pores with complex geometry are obtained, which leads to large deviations in the determination of permeability. Therefore, an important part of the filtration study is the analysis of local processes of
the fluid spatial flow in a single pore using the solution of the Navier-Stokes equations and the derivation of the averaged filtration equations "from the first principles", rather than on the basis of phenomenological theories.

This approach to the modeling of filtration in porous structures is called a two-scale simulation, which is a joint study of the flow of liquid and gas medium in individual pores (a local problem) and in a porous system as a whole (a global problem). For the mathematical justification of the two-scale modeling of the filtration process in a porous system, the asymptotic homogenization method \[11\] based on the asymptotic analysis of processes in periodic structures is used in this paper. This method makes it possible to obtain mathematically justified averaged equations for homogenized medium on the basis of an asymptotic analysis of the exact initial equations of continuum mechanics ("from the first principles"). The asymptotic homogenization method has proved itself well in modeling local transport processes in porous systems \[12\], determining the strength characteristics of reinforced composites \[13\], the theory of plates and shells \[14, 15\].

2. General formulation of the problem of the motion of a gas and a weakly compressible fluid in a porous medium

In this paper we consider the slow Stokes (inertialess) motion of medium in a porous system. It is assumed that the liquid and gas are isotropic linearly viscous compressible medium, the liquid is assumed to be weakly compressible, the porous skeleton is not deformable and its motion is not considered, the motion of the liquid and gas is isothermal, mass forces are absent. The dimensionless phase state equations were formulated as follows:

\[ p_m = A_m \rho_m + \delta_{ml} (p_{0|l} - \bar{K}), \]  

where the index \( m = l \) corresponds to the liquid phase, and \( m = g \) – the gas phase; \( \rho_m \) – density; \( p_m \) – pressure; \( A_m = \left( \frac{\tilde{R} \theta_g}{\tilde{p}} \right) \delta_{mg} + \left( \frac{\bar{K}}{\rho_{0l}} \right) \delta_{ml} \) – dimensionless constant; \( \rho_{0l} \) – density of the liquid at the initial instant of time; \( \bar{K} \) – fluid volume compression module; \( p_{0l} \) – hydrostatic part of the pressure in the fluid, responsible for the change in pressure without changing the density of the liquid. In the overwhelming majority of cases, the last function is given in the form of a certain empirical constant.

In this paper we propose a generalized model of a weakly compressible fluid in which the function \( p_{0l} \) is regarded as an unknown value, which is determined from the solution of a separate auxiliary problem. However, in this case the initial system of Stokes equations for a weakly compressible fluid turns out to be non-closed. To close it, the functions of pressure, density, and velocity were represented in an additive form:

\[ p_l = p_{0l} + p_{1l}, \quad \rho_l = \rho_{0l} + \rho_{1l}, \quad v_l = v_{0l} + v_{1l}, \]  

where \( \rho_{0l} \) and \( p_{0l} \) are defined above. After substituting (2) into the original Stokes system and dividing it into two systems, we obtain the statement of the problem for the case of a generalized model of a weakly compressible fluid. The systems obtained are closed: the first of them is the formulation of the problem of the motion of an incompressible fluid with respect to the functions \( p_0 \), \( v_{0l} \), and the second is the statement of the problem with respect to functions \( p_1 \), \( v_{1l} \), and the functions \( p_0 \) and \( v_{0l} \) in it are treated as input data. If both systems are carried out, then also the initial system is automatically carried out.

3. Statement of local filtration problems

The application of the classical procedure of the asymptotic homogenization method to the initial systems of equations for gas and liquid leads to local filtration problems on the periodicity cell. It is noteworthy that the local problems of gas filtration and the generalized weakly compressible fluid
have the same form and can be written in the form of classical systems of differential equations in 1/8 of the periodicity cell:

\[
\begin{align*}
\mathbf{W}^{(a)}_{iij} &= 0, \\
(\mathbf{p}^{(a)}_{iij} - \mathbf{W}^{(a)}_{ij}) &= \delta^{(a)}_{ij}, \quad \xi_i \in V_{vp}; \\
\mathbf{W}^{(a)}_{i} &= 0, \quad \xi_i \in \Sigma_{vp}; \\
i &= 1, 3, \quad j = 1, 3, \quad \alpha = 1, 3
\end{align*}
\]

(3)

This system is supplemented by boundary conditions on opposite faces of the periodicity cell, which satisfy the periodicity conditions. Each of problems (3) is a stationary flow problem for some dummy linearly viscous incompressible medium. The solution of problems depends only on the internal geometry of the pores, and therefore their formulation is applicable to calculations of the filtration of any gases and liquids within the framework of the assumptions made.

4. Statement of global filtration problem

Averaging of the local equations allows one to obtain the classical Darcy filtration law:

\[
\mathbf{W} = \frac{1}{\mu_m} \mathbf{K} \cdot \nabla_x \bar{p},
\]

where \( \mathbf{W} = \mathbf{v}^{(0)} \) – the filtration velocity, \( \mathbf{K} = \mathbf{v}^{(0)} \) = const – the components of the permeability tensor of the porous medium.

Averaging the local equations of continuity of the first level, taking into account the equations of state of the gas and a weakly compressible fluid, we obtain general nonlinear equations for unsteady phase filtration. A special feature of the global problem is the presence of previously unknown boundaries of the interacting mediums interface, the position and shape of which varies with time. Within the framework of the present paper we use the method of introducing dynamic independent coordinates in which the position of the interface does not change: \( X_1 = x_1, \ X_2 = x_2, \ X_3 = x_3(\alpha x_1 + \beta) \). The coefficients \( \alpha \) and \( \beta \) are determined from the conditions

\[
X_1(L) = L; \ X_3(x_3) = f_0(x_1, x_2), \ X_3 = f(x_1, x_2, t).
\]

For the case in which the interface between the liquid and gas phases moves in a plane-parallel manner, the formulation of the global problem of the displacement of a gas by a weakly compressible fluid in dynamic variables takes the form:

\[
\frac{\partial \mathbf{p}}{\partial t} - \nabla_x \cdot (\mathbf{A}_m \cdot \nabla_x \bar{p}) - \mathbf{b}_m \cdot \nabla_x \bar{p} = f_m, \quad m = l, g
\]

(5)

– general nonlinear equation of unsteady phase filtration;

\[
\mathbf{p}_{\Sigma g} = \rho_{eg}, \quad \mathbf{p}_{\Sigma l} = \rho_{el}; \quad \mathbf{n} \cdot \mathbf{A}_l \cdot \nabla_x \bar{p}_{\Sigma l} = 0, \quad \mathbf{n} \cdot \mathbf{A}_g \cdot \nabla_x \bar{p}_{\Sigma g} = 0;
\]

\[
\bar{p}_t = \bar{p}_g, \quad \mathbf{n} \cdot (\mathbf{A}_l \cdot \nabla_x \bar{p}_l - \mathbf{A}_g \cdot \nabla_x \bar{p}_g) = 0, \quad \mathbf{x} \in \Sigma_{ig}; \quad \bar{p}_t = \rho_{ot}, \quad \mathbf{x} \in \mathbf{V}_t, \quad \bar{p}_g = \rho_{og}, \quad \mathbf{x} \in \mathbf{V}_g, \quad t = 0
\]

– boundary and initial conditions;

\[
\frac{df}{dt} = F(t, f(t), \mathbf{p}) = -\frac{K_1}{\varrho_1 \mathbf{p}_0} \left( f_0 - L \right) \frac{\partial \bar{p}}{\partial X_3}, \quad f(0) = f_0
\]

(7)

– problem for determining the position of the interface in the new coordinate system;

\[
\nabla_x \cdot (\mathbf{A}_n \cdot \nabla_x \bar{p}_0) + \mathbf{b}_n \cdot \nabla_x \bar{p} = 0; \quad \mathbf{p}_0|_{\Sigma l} = \rho_{ot}, \quad \mathbf{p}_0|_{\Sigma g} = \rho_{og}(t). \quad \mathbf{n} \cdot \mathbf{A}_n \cdot \nabla_x \bar{p}_0|_{\Sigma l} = 0
\]

(8)

– a problem for calculating the field of hydrostatic pressure in a fluid.

5. Numerical problem definition

For numerical solution of local problems of liquids and gases flow in a separate periodicity cell, the classical procedure of the finite element method [16, 17] based on the Hellinger-Reissner variational principle is applied. Ten nodal tetrahedral finite element with 34 degrees of freedom was used: three velocity components at each node and one pressure value at each vertex of the tetrahedron.
Numerical solution of non-stationary nonlinear macroscopic equations of fluid and gas motion was performed using the Newton-Raphson method in combination with the finite element method.

6. Results
In the work, a numerical simulation of the two-scale flow of liquid and gas medium in porous composite structures was carried out. In the case of modeling local filtration processes, the pore formed by the interlacing of fibers was considered. Examples of the microfields distribution of pressure pulsations $\tilde{P}^{(i)}$ and the component $\tilde{W}_1^{(i)}$ of the velocity vector obtained by solving a local problem for a porous structure with a dimensionless fiber radius of 0.125 are shown in Figures 1-2. The dimensionless permeability coefficients $K_1^i$ and $K_3^i$ for this structure were also equal, respectively, $2.047 \cdot 10^{-3}$ and $1.385 \cdot 10^{-3}$ with a porosity of 0.555.

![Figure 1](image1.png) Distribution of pressure $\tilde{P}^{(i)}$ in 1/8 of the tissue structure periodicity cell

![Figure 2](image2.png) Distribution of the velocity component $\tilde{W}_1^{(i)}$ in 1/8 of the tissue structure periodicity cell

When solving the global filtration problem, the impregnation time of the reinforcing filler was evaluated by a binder using a generalized model of a weakly compressible liquid. The sample in the form of a parallelepiped had dimensions $0.5 \times 0.15 \times 0.02$ m. At the initial time, the interface between the liquid and gas phases was located in the position $x_i = 0.05$ m. The filler was a fiberglass cloth laid in several layers. Therefore, in solving the global problem, the permeability coefficients obtained from solving local problems were used. The small parameter of the problem was assumed to be equal $\kappa = 1 \cdot 10^{-4}$. As a binder, an unsaturated polyester resin with a viscosity $\mu_1 = 0.2$ Pa·s and a compressibility factor $\beta = 2.2 \cdot 10^{-10}$ m²/N was considered. In the role of gas, air with a viscosity $\mu_3 = 1.81 \cdot 10^{-5}$ Pa·s was adopted. The movement of the binder occurred under the influence of pressure drop $0.9 \cdot 10^5$ Pa on opposite faces of the sample in the direction of the interface movement. The time step was 27 seconds. Examples of pressure distribution curves obtained for the case of a generalized model of a weakly compressible liquid are shown in Figure 3. The time for impregnation of the reinforcing material by the binder in the case of using the generalized model was 40.5 min.

7. Conclusions
The proposed method allows to calculate the distribution of pressure microfields and the filtration velocity components within a single pore, and also to calculate numerically the permeability coefficients of a porous medium without carrying out any additional empirical studies. For this purpose, on the basis of the asymptotic homogenization method, local problems of the spatial flow of a weakly compressible fluid and gas in the periodicity cells and the global problem of the flow of a liquid displacing gas from a porous composite structure are formulated. In this case, the model of weak compressibility of a liquid is based on a new equation of state requiring the calculation of hydrostatic pressure by solving a separate auxiliary problem.

The results of numerical modeling of liquid and gas local spatial flows on the periodicity cell of fabric composite structures are obtained, showing the effectiveness of the proposed algorithm for solving local problems and calculating the porous medium permeability tensor. The results of
numerical modeling of the macroscopic flow of a liquid binder displacing the gas medium in a typical fabric composite structure have been obtained, showing the effectiveness of the proposed algorithm for solving problems for the model of a weakly compressible liquid.

Figure 3. Graphs of the distribution of the average cross-sectional macroscopic pressure $\bar{p}$ as a function of the longitudinal coordinate for different instants of time and for the corresponding positions of the phase interface in the case of the generalized model of a weakly compressible liquid.

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