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Mathematical modeling of hydrodynamic processes in high-porous open cell ceramic foams

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Abstract

On the basis of equations of Navier-Stokes using the method of final elements, the hydrodynamic stream structure in a cell and in a layer of open-cell foam is considered. Hydrodynamic resistance of highly porous cellular material is determined during the transfer of liquid and gaseous media. Experimental data are compared.

Keywords: porous media, ceramic foam, pressure drop, hydrodynamic, mathematical modeling.

1. Introduction

Highly porous open cell materials (foam materials) are a new type of metal- and nonmetal based porous materials with ultimately high porosity and permeability of the cellular lattice structure of the porous space. Cellular materials are a special class of porous permeable materials with a specific structure (Fig. 1a) characterized by such

(a) (b)

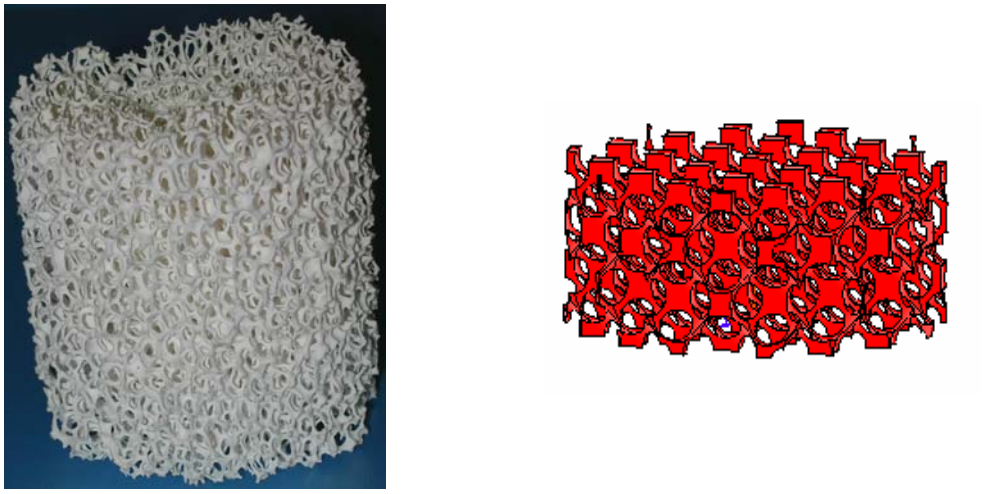

Fig.1. (a) Real and (b) modeled structure of a highly porous cellular material.

parameters as macro-porosity, cell window diameter, and equivalent diameter of a cell. Open cell foams have a good collection of physicochemical and performance characteristics: high porosity, gas permeability, thermal stability, dust capacity, filtering ability, corrosion resistance, low hydraulic resistance, high (at a given porosity) structural strength, and rigidity. Foam materials hold promise as catalyst supports, filters for removing dust and harmful emissions from industrial waste gases, and packings for liquid distribution and mass-transfer processes (distillation, adsorption). Experimental investigations of the hydraulic and filtration characteristics of open cell materials are not always possible; therefore, the problem of calculation of their hydraulic resistance arises. However, none of the solutions proposed to date is universal for calculation of the hydraulic resistance of foam media.

2. Representation of the structure of foam materials

High-porous open cell foams are produced by duplication of a cellular lattice polymer matrix with subsequent removal of the polymer matrix by thermal destruction. The polymer matrix can be produced from a wide range of materials, such as metals (nickel, copper), alloys (Invar, Nichrome), and ceramic materials (celsian electrical porcelain, perthallite porcelain, cordierite ultraporcelain, and silicon carbide). As a structure-forming matrix in highly porous cellular materials, open-cell foamed polyurethane is used. Hence, the structure of a foam material is determined by the structure of foamed polyurethane. This structure is a three-dimensional lattice at each node of which four edges meet. The cross section of each of the edges is a curvilinear triangle. The spatial arrangement of nodes is nonrandom and ordered to an extent; therefore, the free space within a highly porous cellular material can be regarded as a set of unit cells the shape of each of which is quite close to a regular dodecahedron.

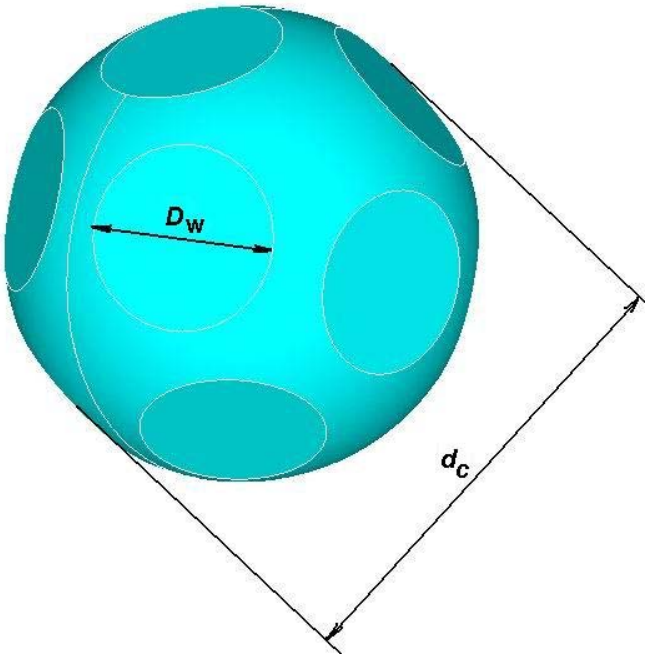

Fig. 2.Unit cell of a highly porous cellular material.

However, the angles between faces of a regular dodecahedron are such that space cannot be filled by a regular packing of dodecahedra. A unit cell of a highly porous cellular material can be represented as being formed from a sphere by cutting off twelve spherical segments so that space can be filled by a regular packing of the unit cells obtained (Fig. 2). The cell is characterized by the diameter of its forming sphere (d_c) and the degree of cutting (or the degree of overlap - p, i.e., the distance from the center of the cellforming sphere to the plane that cuts off a spherical segment divided

by the cell diameter). The degree of overlap affects the diameter of a window, i.e., the circle that is the intersection of the spherical surface with the cutting plane, and, consequently, influences the porosity of the foam material obtained. The window diameter is related to the cell diameter and the degree of overlap by the expression:

$$D_w = \sqrt{d_c^{\,2} - 4(p \cdot d_c)^2}.$$

To eliminate the overlap of neighboring windows, the degree of overlap is limited by a certain minimal value calculated from the cell geometry:

$$p_{\min} \approx 0.433.$$

The maximal value of p, at which the cutting planes are only tangent to the sphere surface, is

$$p_{\max} = 0.5.$$

For modeling the hydrodynamics using the program package Ansys, it is necessary to specify the geometry of the flow forming in channels of the highly porous cellular material. To represent the lattice of the porous material, it is necessary to subtract a set of cells communicating with each other through windows from a certain space. The cylindrical foam material layer obtained by this operation is shown in Fig. 1b.

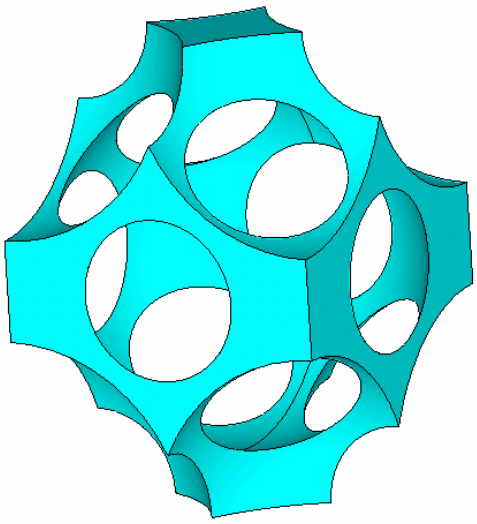

Fig. 3. Part of the structure of a highly porous cellular material that characterizes the geometric properties of the model.

To compare the model structure of the cellular material with the real one, a relationship between one of the geometric parameters of the model (degree p of overlap) and a parameter of the real structure (porosity) was determined. To find the porosity of the model structure, a rectangular parallelepiped of volume V was singled out. This parallelepiped includes a part of the structure of volume V_{str} that characterizes the geometric properties of the model (Fig. 3). The porosity is found from the formula:

$$\Pi = 1 - \frac{V_{str}}{V}$$

The values of the porosity Π at different degrees of overlap and the specific internal surface of the layer of the highly porous cellular material with d_c= 0.9 mm are presented below:

p	Π	S_{sp}, m^2
0.434	0.963	1567.4
0.44	0.951	2026.2
0.45	0.927	2706.1
0.46	0.898	3293.9
0.47	0.863	3800.9
0.48	0.825	4237.9
0.49	0.784	4612.3
0.499	0.745	4903.1
0.4999	0.741	4930.6

where S_{sp} is a specific surface area of an open cell foam material.

3. Mathematical modeling of the flow pattern in a layer of an open cell foam material

To simplify the model and reduce the time of calculation of the velocity of a gas or liquid flow through the layer of the foam material, the model was restricted to an ensemble of 13 unit cells. The central cell communicates through 12 windows with the 12 other cells. It is assumed that this cell has the properties of real cells in a layer of a highly porous material. A steady-state flow induced by an applied constant pressure drop is considered. For an incompressible liquid ($\rho = \text{const}$) of constant viscosity ($\mu = \text{const}$), the continuity (incompressibility) equation has the form

$$\operatorname{div} \bar{v} \equiv \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0$$

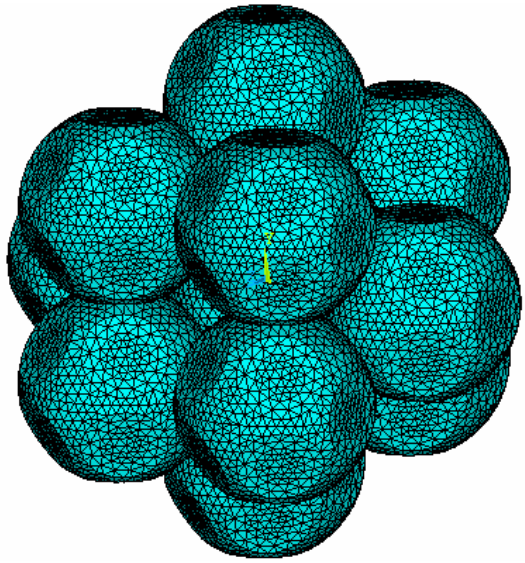

Fig. 4. Ensemble of 13 unit cells and tetrahedral finite element mesh.

The system of Navier–Stokes equations is written as

$$\frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \upsilon \nabla^2 v_x$$

$$\frac{\partial v_y}{\partial t} + v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial y} + \upsilon \nabla^2 v_y$$

$$\frac{\partial v_z}{\partial t} + v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial z} + \upsilon \nabla^2 v_z,$$

where $\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is the Laplace operator and $\upsilon = \mu/\rho$ is the kinematic viscosity.

A constant pressure drop across the inlet and outlet windows of the ensemble is preset, which induces the steady-state flow of the medium. The inlet pressure is $P = \Delta P$, and the outlet pressure is $P = P_0 = 0$.

On the surface of the ensemble of 13 unit cells, an adhesion condition is preset: $v_x = 0$, $v_y = 0$, $v_z = 0$. The velocity gradients at the inlet and outlet windows of the ensemble are

$$\frac{dv_x}{x} = 0, \quad \frac{dv_y}{y} = 0, \quad \frac{dv_z}{z} = 0.$$

The Navier–Stokes equations cannot be solved in the general form but can be solved numerically, e.g., by the finite-element method. In this case, a region under consideration is divided into geometrically simple subregions, which are called finite elements. In the one-dimensional case, they are segments; in the two-dimensional case, triangles or quadrangles; and in the three-dimensional case, tetrahedra or hexahedra. In each of such subregions, the sought solution of the problem is represented as a polynomial of a given degree with unknown coefficients. Thereby, solving a set of differential equations reduces to solving a set of algebraic equations.

In our case, the finite-element mesh is constituted by tetrahedral elements packed freely (for the finite-element mesh to fill the entire space occupied by the ensemble). Such an approach allows one to rapidly and accurately construct a mesh the size of elements of which depends on only one parameter—the tetrahedron edge length. The mesh contains a total of 60122 points and 323345 elements (Fig. 4).

The numerical calculation was performed for a liquid of density ρ = 1000 kg/m3 and viscosity μ = 0.01 Pa s, which corresponds to water at a temperature of 20°C; for air, ρ = 1.292 kg/m^3 and $\mu = 1.8\ 10^{-5}$ Pa s.

The parameters of the foam material structure for which the dependence of the pressure difference on the liquid (water) velocity was experimentally determined are the following:

$d_c = 0.9\times10^{-3}$ m; $\Pi = 0.9$ (or $p = 0.46$);

$L = 15\times10^{-3}$ m.

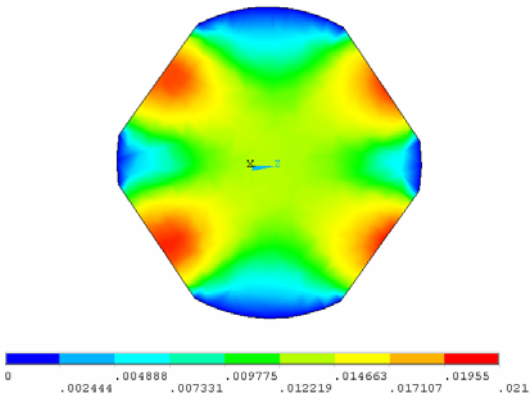

Fig. 5. Distribution of velocities through a longitudinal section of the cell.

To convert the experimental pressure difference to the pressure difference to be used in the model, it is assumed that the pressure distribution along the length (L) of a real foam material is linear and the length in the model is the distance between the parallel planes passing through the centers of the inlet and outlet windows of the ensemble. In this case

$$\Delta P = \Delta P_L \frac{3\sqrt{2}d_c p}{L}.$$

The distribution of velocities (Fig. 5) through a longitudinal section of the central cell of the ensemble at ΔP_L = 20 Pa (ΔP = 2.34 Pa) suggests that the local velocity in constrictions (windows) is three to four times higher than the linear velocity of the liquid flow through the layer of the foam material. A similar principle is implemented in reactors of the divergent–convergent type.

The volumetric liquid flow rate through the outlet windows of the central cell is calculated as the sum of the integrals over the surface of each outlet window of the central cell.

The fluid flow rate through a window is

$$Q_W = \int_{Sw} \nu_n dS = \int_0^{Dw/2} \nu_n 2\pi r dr,$$

where $\nu_n = \nu_x n_x + \nu_y n_y + \nu_z n_z$.

To calculate the volumetric liquid flow rate through the outlet windows of the central cell, we applied the surface integral calculation method used in the program package:

$$Q_c = \sum_{i=1}^{4} Q_i$$

The linear velocity of the liquid flow through the layer of the highly porous cellular material is calculated by

$$w = \frac{Q_c}{4p^2 d_c^{\,2}}$$

Fig. 6 presents the results of modeling the liquid flow through the layer of the highly porous cellular material at various pressure differences.

One can see that at low Reynolds numbers (at ΔP = 80 Pa, we have Re = 23) the dependence of the pressure difference on the rate of liquid filtration through the layer of the highly porous cellular material is linear. The relative error at ΔP = 50 Pa is 12.8%.

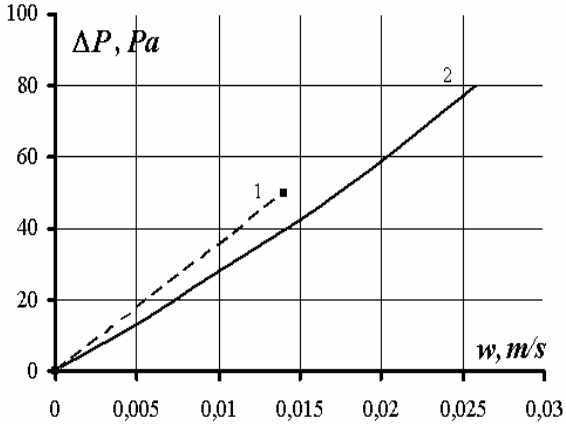

Fig. 6. Experimental (*1*) and modeled (*2*) dependences of the pressure difference on the velocity of the liquid flow through an open cell ceramic foam of porosity $\Pi = 0.9$ at a layer height of L = 15 mm and d_c = 0.9 mm.

The discrepancy between the calculated and experimental data can be caused by the fact that the proposed model poorly fits the geometry of a real material because of idealizing of the model structure (assuming that the structure is ordered). As a result, the porosity of the modeled highly porous cellular material somewhat differs from the real value.

In modeling the air flow along with the laminar flow a turbulent flow was also considered. At the values of the velocity of air filtration in the layer of the highly porous cellular material that were found in the experiment, there may be a transient (i.e., undeveloped turbulent) flow. However, this flow is difficult to model and has been studied insufficiently. Therefore, to model the turbulent gas flow, we used a standard k-ε turbulence model with typical values of variables.

The turbulent kinetic energy equation has the form:

$$\frac{\partial \rho k}{\partial t}+\frac{\partial(\rho v_x k)}{\partial x}+\frac{\partial(\rho v_y k)}{\partial y}+\frac{\partial(\rho v_z k)}{\partial z}=$$

$$=\frac{\partial}{\partial x}\left(\frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial y}\right)+\frac{\partial}{\partial z}\left(\frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial z}\right)+\mu_t\Phi-\rho\varepsilon;$$

and the dissipation rate equation is written as:

$$\frac{\partial \rho \varepsilon}{\partial t}+\frac{\partial(\rho v_x \varepsilon)}{\partial x}+\frac{\partial(\rho v_y \varepsilon)}{\partial y}+\frac{\partial(\rho v_z \varepsilon)}{\partial z}=$$

$$=\frac{\partial}{\partial x}\left(\frac{\mu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{\mu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial y}\right)+\frac{\partial}{\partial z}\left(\frac{\mu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial z}\right)+C_1\mu_t\frac{\varepsilon}{k}\Phi-C_2\rho\frac{\varepsilon^2}{k},$$

where k - turbulent kinetic energy; ε —kinematic viscosity of the flow;
μ_t - turbulent viscosity; Φ - viscous dissipation (kinetic energy dissipation into heat);
σ_k, σ_ε - diffusion factors in the *k*-ε turbulence model; C_1 and C_2 - constants.
The solution of the turbulence equations is used for calculating the effective viscosity $\mu_e=\mu+C\,\rho\frac{k^2}{\varepsilon}$, where C is a constant.

Then, this formula is substituted into the set of Navier–Stokes equations instead of μ.

Fig. 7 shows that, in the air flow through the layer of the highly porous cellular material, the velocities calculated under the assumption that the flow is laminar differ significantly from the experimental data (Fig. 7), whereas line *2* for the turbulent flow quite accurately describes the dynamics of increase in the air velocity with an increase in the pressure difference.

Probably, the small discrepancy between the experimental and calculated data for the turbulent flow is due to the presence of sharp edges in the model geometry (Fig. 3), which give rise to zones of additional turbulization of the flow. The relative errors at ΔP = 15000 Pa are 9.5 and 3.9% for the models assuming the laminar and turbulent flows, respectively.

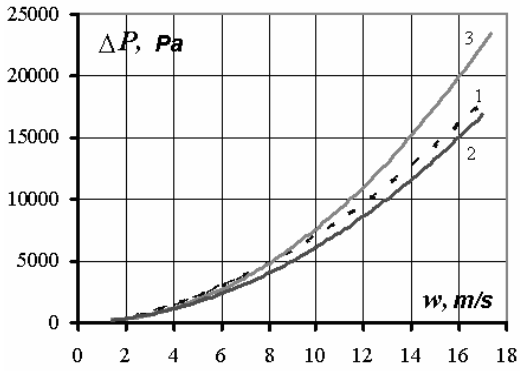

Fig. 7. Experimental (*1*) and modeled (*2*, *3*) dependences of the pressure drop on the velocity of the turbulent (*2*) and laminar (*3*) gas (air) flow through an open cell ceramic foam of porosity $\Pi = 0.9$ at a layer height of L = 70 mm and d_c = 2.1 mm.

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