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CHARACTERISTICS OF POROUS MEDIA USED FOR MODELING OF FILTRATION COMBUSTION

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Models that can be used in calculating the transport parameters of a porous medium are considered. Despite their simplicity, the models qualitatively and quantitatively characterize popular classes of porous media and are not given in the literature in the context in question, as far as the authors know. Certain aspects of determination and evaluation of the parameters of radiative transfer in a porous medium are discussed.

Filtration combustion is a complex physicochemical process of combustion in a porous medium, which is accompanied by the filtration of gases and combined heat and mass exchange [1–3]. Filtration combustion includes, in a broad sense, the gasification of solid hydrocarbons, combustion in a peat bed, the sintering of ores, self-propagating high-temperature synthesis, and other processes. Interest in filtration combustion has recently grown because of the prospect for converting efficiently hydrocarbon fuels to synthesis gas and hydrogen [4–8] and owing to the investigations of gas and liquid scrubbing by the method of oxidation in superadiabatic filtration-combustion waves [9–11]. The demand for reliable modeling of such systems with the aim of optimizing the structure, scaling, and predicting the parameters, regimes, etc. has risen [12].

Experience gained in numerical and experimental investigation of filtration-combustion systems [3, 5, 8] shows that the largest uncertainty (error) in the modeling is introduced, in addition to chemical kinetics, by the incorrect assignment of structural parameters and related parameters of heat and mass transfer in a porous medium. The latter is the most important in numerical optimization and selection of a porous medium for the assigned process or setup.

A mathematical model for description of filtration combustion in the regime of strong thermal coupling with the skeleton (low-velocity regime) has been approved and is constructed on heat- and mass-balance equations, filtration equations, and those of state [2, 3, 5, 8]. The most important structural parameters of porous media are porosity, specific surface, characteristic dimension of solid-phase particles, and quantum free path. It is precisely on them that the calculation of the interphase heat and mass exchange and the radiant and effective thermal conductivity of a porous medium and dispersion diffusion and heat conduction in the gas phase is based [2, 3].

The simplest porous medium is a monodisperse spherical charge. It is completely described by two easily measured parameters: spherical diameter and average porosity. (Certain nuances are related just to the determination of effective free path, which will be shown below.) Other types of porous media (fibrous, layered, and high-porosity ones) frequently have no unambiguous and convenient description. As a rule, one easily establishes the porosity and type of medium (monodisperse, polydisperse, ordered, disordered) and packing (fibrous, layered, spongy, etc.) and one characteristic linear dimension — particle diameter, number of pores per unit length, etc. In such cases it becomes necessary to determine the relationship between the parameters measured and the remaining parameters — specific surface, characteristic dimension of solid-phase particles, and quantum free path — and to formulate the required heat- and mass-exchange models.

In this work, we describe the models of a porous medium that can be used for calculation of the interrelationship between its structural and transport parameters. The formulation of the models has been simplified as much as possible; different classes of porous media are well described. We give the basic formulas relating the structural (geometric), hydrodynamic, and thermophysical parameters of a porous medium. We briefly discuss certain methodological aspects of determination and evaluations of the parameters of radiative transfer in a porous medium.

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Relationship between the Structural Parameters of a Porous Medium and the Transport Characteristics. The basic hydrodynamic equation for porous media is the equation relating the pressure gradient and the filtration rate. Many researchers use the Forchheimer binomial equation:

$$\nabla p = -\frac{\mu}{k_0} u_g - \frac{\rho_g}{k_1} \left| u_g \right| u_g ,$$

where $k_0 = \dfrac{m^3 d_p}{150(1-m)^2}$, $k_1 = \dfrac{m^3 d_p}{170(1-m)}$ [13] and the medium is characterized by the average diameter of solid-phase particles d_p and the porosity m.

To determine the heat-transfer coefficient we use the expression of the Nusselt number by the dimensionless Reynolds and Prandtl numbers: Nu = f(Re, Pr) [14, 15]. The equivalent pore-channel diameter d_0 is used for computation of the Nu and Re numbers in considering the internal problem: Nu = hd_0/λ and Re = $u_g d_0/\nu$, whereas the average particle diameter d_p is used in considering the external problem. According to definition, the equivalent diameter of the pore channel is the inside diameter of a cylindrical tube having the same porosity and specific area of the interior surface as those in the porous medium:

$$d_0 = \frac{4m}{S} . \tag{1}$$

We note that the diameter d_0 determined in such a manner bears no direct relation to the geometric parameters measured — the pore diameter d_{por} (which can be determined as the diameter of a sphere inscribed into the pore), the average distance between the centers of the pores, and others.

Let us give the empirical formulas of Aérov and Todes [16] and of Wakao and Kaguei [17] that are most frequently used in computational-theoretical investigations of filtration combustion

$$\mathrm{Nu} = 0.395 \left(\frac{2m}{3\,(1-m)} \right)^{-0.36} \mathrm{Re}^{0.64} \mathrm{Pr}^{1/3} , \quad \mathrm{Re} > 65 , \tag{2}$$

$$\mathrm{Nu} = 2 + 1.1 m^{0.6} \mathrm{Re}^{0.6} \mathrm{Pr}^{1/3} . \tag{3}$$

The coefficient of volume heat exchange α directly appearing in the heat-balance equations is found as the product of the coefficient of surface heat exchange and the specific surface of the porous medium: $\alpha = hS$. The specific surface of the porous medium is expressed by the specific surface of an individual particle S_p and the porosity:

$$S = S_p (1 - m) . \tag{4}$$

Dispersive transfer in the gas phase is the most important mechanism of transfer. It is equivalent to the diffusion mechanism and is determined by the space- and time-averaged stochastic "sputtering" of gas particles. To calculate dispersive diffusion most researchers use semiempirical formulas of the following type [17, 18]:

$$D_{\parallel} = \frac{D_g m}{\tilde{T}} + 0.5 d_p u_g , \tag{5}$$

$$D_{\perp} = \frac{D_g m}{\tilde{T}} + 0.1 d_p u_g , \tag{6}$$

where the longitudinal (5) and transverse (6) dispersion are differentiated. In [3], it has been shown that for isotropic media and filtration-combustion problems, it is physically justified to use the same values of the coefficients for longitudinal and transverse dispersion

$$D_{\perp} = D_{\parallel} = \frac{D_g m}{\tilde{T}} + 0.1 d_p u_g \,.$$

The reason is that the relaxation component of dispersion is insignificant for formation of a quasistationary concentration profile of the front. The dispersion component related to the velocity pulsation (mechanical dispersion) cannot be substantially anisotropic in isotropic media. However, this important issue has yet to be discussed in the scientific literature. We note that, in view of the predominance of the second terms in Eqs. (5) and (6), the exactness of the values of the porosity and the crookedness of channels exerts no substantial influence on the general exactness of the expression.

Radiative transfer in a porous medium is the dominant mechanism of heat transfer at high temperatures in the wave $T > 1000^{\circ}C$. The radiative-heat-conduction model widely used for calculation of radiant heat fluxes gives, for the coefficient of radiative heat conduction, the expression

$$\lambda_{rad} = \frac{16\sigma\varepsilon l_0 T^3}{3} \,. \tag{7}$$

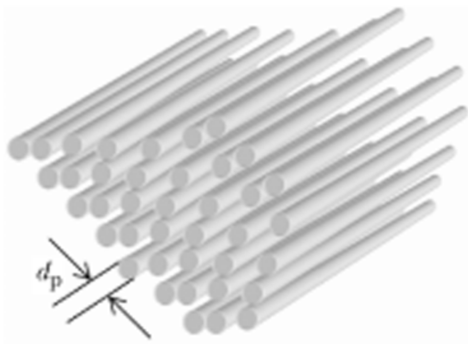
The quantum mean free path l_0 is in essence the geometric characteristic of a porous medium, which is equal to the mean distance between the surface points of the solid phase within the line-of-sight range. We have the distinctive feature of the transfer model, first indicated in [3] and lying in the fact that the radiative-heat-conduction model implies the localizability and isotropy of quantum emission and absorption (porous medium — a "gray gas"), whereas this is not observed in the actual porous medium. For formal application of the "gray-gas" model (meeting the requirement of isotropy and localizability of emission and absorption) to a porous medium we should assume that emission and absorption are distributed in the particle volume and do not occur at a specific surface point of the solid phase, and the emission temperature corresponds to the mean particle-surface temperature. However, in this case the quantum effective free path l_0 appearing in (7) must be larger than the quantum geometric free path l by a value of the order $d_p/2$. (This reasoning is true of any other model of radiative transfer in a porous medium that assumes the "gray-gas" approximation.) A comparison with experimental data on the radiative heat conduction of solid spherical packings [3] shows the physical justifiability of this reasoning and the higher accuracy of corresponding models.

The issue of the correspondence of the radiative-heat-conduction model to the radiative transfer of heat in a porous medium is discussed in [3] in greater detail. Below, we give expressions for the quantum geometric free path in a porous medium l and those recommended for calculation of the radiative thermal conductivity l_0. Thus, for close packings of particles, the higher accuracy is ensured by the quantum effective free path calculated as the mean distance between the centers of neighboring particles:

$$l_0 = d_p \left(\frac{\pi/6}{1 - m} \right)^{1/3} . \tag{8}$$

Models of Porous Media. ***Charge of Spheres of Close Dimensions.*** A packing (charge) of identical spheres is the simplest and universal model used in the case where the porous medium represents a packing of solid particles with a small distribution by size $d_{max}/d_{min} < 2$ [16]. The porosity of random packings is $m \sim 0.4$, as a rule. Formulas for the structural characteristics in this model are as follows:

$$S = \frac{6\,(1 - m)}{d_p} , \quad d_0 = \frac{2}{3} \frac{m}{1 - m} d_p , \quad l = \frac{2}{3} \frac{m}{1 - m} d_p \tag{9}$$



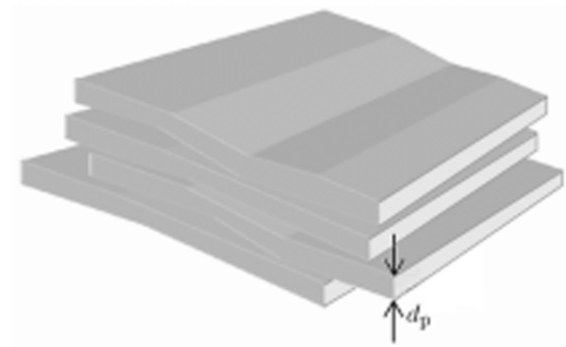


Fig. 1. Porous medium formed by a packing of parallel fibers.

Fig. 2. Packing of parallel sheets — a porous-medium model.

(d_0 is taken from the determination of the equivalent pore channel, and l is taken from [19]). We can calculate the quantum effective free path by two methods: using either formula (8) or the expression obtained in [3]:

$$l_0 = \frac{2}{3}\frac{m}{1-m} d_p + \frac{2}{3} d_p = \frac{2}{3\,(1-m)} d_p\,.$$

Packings of Parallel Fibers. This model corresponds to porous systems made up of fibers or particles with a large dimensional ratio from approximately 10 to infinity (Fig. 1). Formulas for the characteristics of such a medium are as follows:

$$S = \frac{4\,(1-m)}{d_p}\,, \quad d_0 = \frac{m}{1-m} d_p\,, \quad l = \frac{\pi d_p}{4\,(1-\varepsilon)}\,.$$

The last formula has been taken from [20] where intersecting bundles of fibers were considered.

Packings of Parallel Sheets. This model describes porous media made up of plates or particles with a large ratio of large dimensions in relation to a smaller dimension (10 or more) (Fig. 2). Formulas for the characteristics of a porous medium in this model are as follows:

$$S = \frac{2\,(1-m)}{d_p}\,, \quad d_0 = \frac{2m}{1-m} d_p\,, \quad l_\perp = \frac{m}{1-m} d_p\,.$$

In calculating the quantum mean free path in the direction parallel to the planes $l_\parallel$, the parallelism of the layers and the distance between the layers are determining, since these characteristics assign the maximum quantum path in this direction $l_{\parallel\max}$. It can be shown that $l_\parallel \approx \frac{m}{1-m} d_p \ln\,(l_{\parallel\max}/l_\perp)$. In actual media, we have $l_\parallel \approx 2\text{–}3 l_\perp$.

Media with a Higher-Than-Average Porosity. Media with a porosity higher than that of a random spherical packing ($m > 0.45$) are formed in the presence of internal cavities and hollows in the particles (e.g., packings of rings, saddle-shaped particles, and perforated particles) or in solid materials of the spongy type. In the latter case the porosity may attain $m \sim 0.95$ or more. The specific surface of media consisting of standard (geometrically definite) particles is easily calculated with the use of (4) and the porosity measured. The specific surface and other parameters are indicated by suppliers of standard particles.

Spongy Porous Medium (Model of Hollow Spheres). *Media with a medium porosity ($m < 0.6$).* It is difficult to determine the dimension of the solid-phase "element" d_p for continuous porous media not made up of individual grains (spongy and foam ones). In practice one can measure the pore diameter (maximum inside dimensions) d_{por}, the mean diameter of the pore cross sections d_{por} ($d_{por} = \pi d_{por}/4$ for spherical pores), the number of pores per unit length, etc. In certain cases the dimension is calculated from the measured specific surface and porosity. Parameters

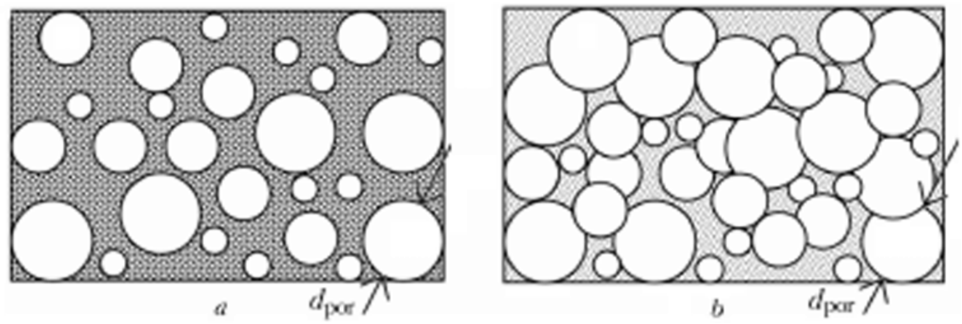


Fig. 3. Spongy medium: a) model of nonintersecting hollow spheres, b) model of intersecting hollow spheres.

measured directly and those calculated are significantly different, and to determine the relationship between them and to find the specific surface, the quantum free path, and other characteristics in terms of them, one must use the porous-medium models.

The model of hollow spheres distributed in a solid medium can be used as a geometric model for moderately high porosities ($m < 0.6$) (Fig. 3a). It is assumed that the medium's geometric structure is determined mainly by isolated pores (although they can be interconnected.) The model is convenient in that the basic structural-geometric relations are somehow analogous (inverse) to those of a standard porous medium — a spherical packing. An expression for the specific surface area is obtained from (9):

$$S = \frac{6m}{d_{por}} .$$

From relation (1) it follows that

$$d_0 = \frac{2}{3} d_{por} .$$

Formulas for the remaining structural characteristics in this model have the form

$$\bar{d}_{por} = \frac{\pi}{4} d_{por} ,$$

$$d_p = \frac{2}{3} \frac{1-m}{m} d_{por} , \tag{10}$$

$$l = \frac{2}{3} d_{por} , \quad l_0 = \frac{2}{3} d_{por} + \frac{d_p}{2} . \tag{11}$$

Media with a High Porosity ($m > 0.6$). The model of hollow spheres can also be used for description of a porous medium with a high porosity. The "intersection" of cavities and related formation of "windows" between the pores and decrease in the specific surface should be taken into account. Such media can be represented by the model of intersecting hollow spheres (Fig. 3b).

Let us express certain parameters of a porous medium within the framework of this model. We make the following assumptions:

(1) spheres have the same diameter d_{por};

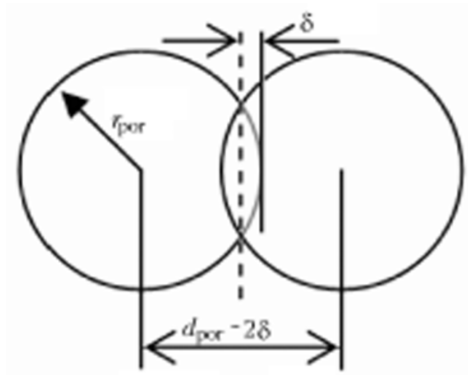


Fig. 4. Pair of hollow spheres, i.e., pores shifted toward each other to form a "window" between the pores.

(2) spheres are arranged in a relatively ordered manner so that there is no simultaneous intersection of three spheres (triple intersections); the packing is characterized by coordinate number N; it is permissible to use the model of ideal spherical packings for calculation of the mean-statistical geometric characteristics;

(3) we can take d_{por} for the characteristic pore dimension, since the high degree of intersection (>50%) is rather uncommon.

We consider a pair of neighboring spheres in the packing (Fig. 4). As the centers of the spheres approach each other by 2δ (the relative change in the distance is equal to δ/r_{por}), the area of the "window" between the pores will be $s_{win} = 2\pi r_{por}\delta$ (the window's fraction in the total spherical surface is calculated from $s_{win}/s_{por} = \delta/(2r_{por})$), and the effective volume of each sphere will decrease by $\Delta V_{por} = \pi h^2(3r_{por} - \delta)/3$ (the relative decrease in the volume is determined from $\dfrac{\Delta V_{por}}{V_{por}} = \dfrac{\delta^2(3r_{por} - \delta)}{4r_{por}^3}$).

The porosity of the system will be expressed by the parameters of the initial packing of hollow spheres m_{in}, N, and r_{por} and the value of the approach of the spheres δ:

$$m = m_{in}\frac{1 - \dfrac{3}{4}N\left(\dfrac{\delta}{r_{por}}\right)^2 + \dfrac{1}{4}\left(\dfrac{\delta}{r_{por}}\right)^3}{1 - \dfrac{3\delta}{r_{por}} + 3\left(\dfrac{\delta}{r_{por}}\right)^2 - \left(\dfrac{\delta}{r_{por}}\right)^3} \cong \frac{m_{in}}{1 - \dfrac{3\delta}{r_{por}}}. \tag{12}$$

Hence in the first approximation by δ/r_{por} we have

$$\delta = \frac{m - m_{in}}{3m} r_{por}. \tag{13}$$

Taking into account that the fraction of the windows in the pore surface is $N\delta/(2r_{por})$, we obtain

$$\Psi = \frac{Ns_{win}}{s_{por}} = N\frac{m - m_{in}}{6m}. \tag{14}$$

The quantum mean free path from (11) in such a system will be expressed by the series

$$l = \frac{2}{3}d_{por}(1 - \Psi) + \frac{4}{3}d_{por}\Psi(1 - \Psi) + \frac{6}{3}d_{por}\Psi^2(1 - \Psi) + \frac{8}{3}d_{por}\Psi^3(1 - \Psi) + \ldots .$$

After simple transformations, we obtain

$$l = \frac{2}{3\,(1-\Psi)}\, d_{por}\,. \tag{15}$$

The specific surface area per unit volume of one pore is equal to

$$S_{por} = \frac{s_{por} - N s_{win}}{V_{por} - N \Delta V_{por}} = \frac{4\pi r_{por}^2 - 2\pi N r_{por}\delta}{\frac{4}{3}\pi r_{por}^3 - N\pi\delta^2 \frac{3r_{por} - \delta}{3}} \cong \frac{6r_{por} - 3N\delta}{2r_{por}^2}\,,$$

then, for the porous medium (by analogy with formula (4)), we have

$$S = S_{por} m = m\,\frac{6r_{por} - 3N\delta}{2r_{por}^2}\,. \tag{16}$$

Let us give an example of using the model of hollow spheres. In [21], the medium is described by the porosity m = 0.87 and the number (assigned by the supplier) of pores per unit (inch) length of the secant segment n = 32 inch^{-1}. We obtain a formula for changing from this characteristic to other geometric parameters of the porous medium. According to the Cavalieri–Acker principle, m inches of the pore space and 1–m inches of the space occupied by the solid phase account for 1 inch of the secant segment in the porous medium. Thus, knowing n and m, we establish the mean length of the part of the secant segment per pore (in terms of meters): $L = 0.0254m/n$. Assuming that the pore geometry remains spherical for both the model of hollow spheres and the model of intersecting hollow spheres, we calculate the mean length of the part of the secant segment per pore as $L = 2/3d_{por}$. Equating the two expressions for L, we obtain $d_{por} = 0.0381m/n$.

Thus, for the ceramics investigated in [21] (m = 0.875 and n = 32 inch^{-1}), we have d_{por} = 1mm. According to (14)–(16), for the basic close hexagonal packing (N = 12 and m_{in} = 0.74), the fraction of windows in the pore surface is Ψ = 0.31, the quantum mean free path is $l = 0.96\ d_{por}$, and the specific surface is S = 3500 m^2/m^3. If the basic packing is random (N = 8 and m_{in} = 0.6), we have Ψ = 0.42, $l = 1.15\ d_{por}$, and S = 2900 m^2/m^3. We note that we have $\delta/r_{por} \sim 0.05$ in the first case and ~0.1 in the second case. To determine the dispersion, the permeability coefficients, and the quantum effective free path $l_0 = l + d_p/2$ we must evaluate the characteristic dimension of particles (elements) of the solid phase. According to (10), we obtain $d_p = \frac{2}{3}\,\frac{1-m}{m}\,d_{por}$ = 0.1 mm.

CONCLUSIONS

1. We have systematized and given the formulas for calculation of the structural characteristics of variously structured porous media. The model of hollow spheres (variants of intersecting and nonintersecting hollow spheres) has been proposed for description of the structural characteristics of high-porosity media of the spongy ("foam") type. With these models, we have obtained formulas relating the structural characteristics of porous media and the characteristic of heat and mass exchange.

2. We have discussed the methodological issues of formulations of models of dispersive and radiative transfer in porous media: inclusion of the relaxation component into the dispersion and evaluation of the quantum effective free path in considering a porous body as a homogeneous gray medium.

3. The data of the present work can be used for scientific and engineering-technical calculations of thermochemical reactors, gas generators, and different chemical reactors and units, where porous media are used as the working media.

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NOTATION

d, diameter, m; d_p, mean diameter of particles (elements) of the solid phase, m; d_0, effective (equivalent) diameter of the pore channel, m; d_{por}, mean diameter of the pores of a porous medium, m; D, diffusion coefficient, m^2/sec; h, surface coefficient of interphase heat exchange, $W/(m^2 \cdot K)$; k_0 and k_1, permeability coefficients of a porous medium in the Forchheimer formula, m; L, mean length of the part of the secant segment per pore, m; l, quantum geometric mean free path, m; l_0, quantum effective mean free path in a porous medium, m; m, porosity; n, number of pores per unit length of the secant segment, 1/inch; N, coordination number of a packing; Nu, Nusselt number; p, pressure, Pa; Pr, Prandtl number; r, radius, m; Re, Reynolds number; s, surface area, m^2; S, specific surface area, m^2/m^3; T, temperature, K; $\tilde{T}$, crookedness of filtration channels; u, velocity (rate), m/sec; V, volume, m^3; ΔV_{por}, change in the pore volume on the formation of a "window," m^3; α, volume coefficient of interphase heat exchange, $W/(m^3 \cdot K)$; δ, half the approach of the centers of the pores, m; ε, emissivity factor of the surface of a porous medium; λ, thermal conductivity, $W/(m \cdot K)$; μ, coefficient of dynamic viscosity, Pa·sec; ν, coefficient of kinematic viscosity, m^2/sec; σ, Stefan–Boltzmann constant, $W/(m^2 \cdot K^4)$; ρ, density, kg/m^3; Ψ, fraction of "windows" in the pore surface. Subscripts: g, gaseous; in, initial; max, maximum; min, minimum; p, particle; por, pore; rad, radiative; win, "window;" $\parallel$, longitudinal; $\perp$, transverse; $\bar{\ }$, for the cross sections of the pores at section.

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