Mechanics of porous media with phase transformations and periodical structures

1. Method of asymptotic averaging

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Abstract. – In the present paper a method is developed of asymptotically averaging processes in porous media with phase transformations. The advantage of the method is the possibility of determining not only the macroscopic characteristics of processes in porous media but also the microscopic characteristics in each of the phases. To calculate the characteristics of microscopic processes with the help of this method, special mathematical "problems over a periodicity cell" with periodic boundary conditions are formulated. © Elsevier, Paris

1. Introduction

The theory of porous media is widely used in different fields of science and engineering, from ground mechanics to chemical technologies and composite materials. Currently porous media with phase transformations are of great interest. One example of these media is composite materials under high temperatures, wherein there occurs a growth in quantity and size of pores which are simultaneously filled with gases generated under great intrapore pressure. This phenomenon is called the pyrolyse of composites. Empirical methods of describing processes in composite materials under high temperatures without the consideration of microscopic processes in the material were developed in Nigmatulin (1994), Dimitrienko (1995a), Dimitrienko (1995b), and Dimitrienko (1995c).

The method of asymptotically averaging processes in solid deformable media without phase transformations was suggested in Sanchez-Palencia (1980), Bakhvalov and Panasenko (1989), and Pobedyra (1984). The concept of using asymptotic methods in a theory of multiphase media was initiated in Dimitrienko (1991). In the present paper this theory is developed to porous media with phase transformations of the type: solid phase → gas (fluid).

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2. Main assumptions

Let us consider a porous medium consisting of two phases: a solid phase and pores filled with gas (fluid), where one of the phases is "old" and the other is "new". In the pyrolysis of a composite its solid matrix is the "old" phase and the gaseous products of pyrolysis in pores are the "new" phase.

It is assumed that

a) each of the phases occupies a finite volume \( V_s \) or \( V_g \), and \( V = V_s \cup V_g \), where \( V \) is the volume of the whole medium;

b) a phase transformation is considered as the process of continuously decreasing the volume of one of the phases \( V_s(t) \) or \( V_g(t) \) and increasing the volume of the other phase so that the total volume \( V \) of the medium does not change, i.e. it can change only due to deformations;

c) the porous medium has a periodical structure, i.e. the elementary recurring volume \( V_\xi \) can be extracted; this volume is called a periodicity cell and the whole medium consists of the cells \( V = NV_\xi \), where \( N \) is the number of periodicity cells in the whole medium and \( N \gg 1 \);

d) the deformations of the solid phase are small; and

e) the motion of gas in pores is inertialess.

Let us denote by \( \mathbf{x} \) the radius-vector in Descartes coordinates, by \( x_0 \) the characteristic size of the whole medium \( V \) considered and by \( l_0 \) the characteristic size of the periodicity cell \( V_\xi \) of the structure. Due to assumption (c) we can introduce small parameter \( \varkappa \):

\[
(1) \quad \varkappa = \frac{l_0}{x_0}, \quad \varkappa \ll 1.
\]

Let us also introduce a so-called radius-vector of "local" coordinates \( \xi \):

\[
(2) \quad \xi = \frac{x}{\varkappa},
\]

which can change within the limits of periodicity cell \( V_\xi \), where \( \bar{x} = x/x_0 \) are the dimensionless global coordinates changing inside the whole region \( V \) occupied by the medium.

All functions \( \Omega \) describing processes in such a periodic structure model are assumed to be quasiperiodic, i.e. they depend on coordinates \( \mathbf{x} \) and \( \xi \) the differentiation of such functions is performed by the rule for differentiating a composite function:

\[
(3) \quad \nabla \Omega(\mathbf{x}, \xi) \longrightarrow \nabla_\mathbf{x} \Omega + (1/\varkappa) \nabla_\xi \Omega.
\]

where \( \nabla_{x,\xi} \) are nabla-operators over coordinates \( \mathbf{x} \) and \( \xi \); \( V_{\xi g} \) and \( V_{\xi s} \) are the intersections of the regions \( V_s \) and \( V_g \) with the periodicity cell \( V_\xi \); \( \Sigma_{\xi g}(t) \) is the mobile boundary of
gas and solid phases (Fig. 1) moving with speed $D$; and $\Sigma_{\xi s g}$ is a part of this surface in the periodicity cell $V_\xi$.

We also assume that:

- at each time $t \geq 0$ the domains $V_g$ and $V_\xi$ are one-connected (i.e. the porosity of the medium is “open”); this assumption can be realized only in a three-dimensional space. It should be noted that Figure 1 shows only a two-dimensional cross-section of a three-dimensional porous medium. Therefore a one-connected structure of both domains $V_s$ and $V_g$ is not seen and can not be exhibited Sanchez-Palencia (1980).

- the phase separation boundary $\Sigma_{s g}$ is smooth and without corner points.

3. Main equations

3.1. Conservation equations

The following are equations of continuity, momentum and energy in region $V_g$:

\begin{equation}
\frac{\partial \rho_g}{\partial t} + \nabla \cdot \rho_g \mathbf{v}_g = 0; \quad \mathbf{x} \in V_g,
\end{equation}

\begin{equation}
\nabla \cdot \sigma_g = 0;
\end{equation}

and

\begin{equation}
\frac{\partial}{\partial t} \rho_g c_g \theta_g + \nabla \cdot \rho_g \mathbf{v}_g c_g \mathbf{e}_g \theta_g = \nabla \cdot (\lambda_g \nabla \theta) - \nabla \cdot \sigma_g \mathbf{v}_g. \quad \mathbf{x} \in V_g.
\end{equation}

For the solid phase, the strains of which are small, the momentum and heat transfer equations have the form

\begin{equation}
\rho_s \frac{\partial^2 \mathbf{u}_s}{\partial t^2} = \nabla \cdot \sigma_s, \quad \mathbf{x} \in V_s,
\end{equation}

EUROPEAN JOURNAL OF MECHANICS. A/SOLIDS. VOL. 17, No. 2, 1998
and

\[ \rho_s c_s \frac{\partial \theta_s}{\partial t} = \nabla (\lambda_s \cdot \nabla \theta_s) - \alpha_s \theta_s \frac{\partial \sigma_s}{\partial t} + W^*_s, \]

Function \( W^*_s \) describes the dissipation of energy in the solid phase due to mechanical factors.

3.2. **Constitutive relations**

Constitutive relations for solid and gaseous components have the following form: For the gas phase,

\[ \sigma_g = -p \delta + \kappa \tau_g; \]

\[ \tau_g = \nu_g \delta \nabla v_g + k_g (\nabla \otimes v_g + (\nabla \otimes v_g)^T); \]

\[ \frac{1}{\rho_g} = \frac{\partial \mu_g}{\partial p} = R \theta_g = \frac{R \theta_g}{\rho}, \quad \text{and} \quad \mu_g = \mu_g^0 (\theta_g) + R \theta_g \ln \frac{p}{p_0}; \]

and for the solid phase:

\[ \varepsilon = -\rho_s \frac{\partial \mu_s}{\partial \sigma_s} = \alpha_s (\theta_s - \theta_0) + \Pi_s : \sigma_s; \]

\[ \mu_s = \mu_s^0 (\theta_s) + \mu_s'; \quad \text{and} \quad \mu_s' = \frac{-1}{2 \rho_s} \sigma_s : \Pi_s : \sigma_s - \frac{1}{\rho_s} \sigma_s : \alpha_s (\theta_s - \theta_0); \]

i.e. gas is assumed to be linear-viscous and its viscosity is "small", as the viscous stress tensor \( \tau_g \) contains a small parameter \( \kappa \). A solid phase is assumed to be linear-elastic, wherein \( \Pi_s \) is the elasticity compliances tensor and \( \alpha_s \) is the tensor of heat expansion. Here \( \mu_s \) and \( \mu_g \) are chemical potentials (free Gibbs energies) of the solid and gas phases respectively, \( R \) is the gas constant, \( p \) is the pressure in the gas phase, \( p_0 \) is the pressure of the initial state of the gas phase, and \( \sigma_s \) and \( \sigma_g \) are stress tensors of the solid and gas phases respectively. The expression for deformation tensor \( \varepsilon_s \) as a derivative of Gibbs free energy tensor \( \mu_s \) was given in Christensen (1980); for the problem considered this expression has form (12).

3.3. **Kinematic relations**

Solid phase strain tensor \( \varepsilon \) is connected to displacement vector \( u \) by the Cauchy relations:

\[ \varepsilon = \frac{1}{2} (\nabla \otimes u + (\nabla \otimes u)^T). \]
3.4. Conditions at the Phase Interface

Boundary conditions at the phase transformation surface $\Sigma_{sg}$ are written as follows:

(15) \[ [\rho] \mathbf{D} + \rho_y \mathbf{v}_y \cdot \mathbf{n} = 0; \]

(16) \[ -\rho_s \mathbf{D} \mathbf{v}_g + [\sigma] \cdot \mathbf{n} = 0; \]

(17) \[ \rho_s \mathbf{D} [e^0 + c \theta] - \mathbf{n} \cdot [\sigma \cdot \mathbf{v}] + \mathbf{n} \cdot [\lambda \cdot \nabla \theta] = 0; \]

and

(18) \[ [\theta] = 0; \]

where $[\Omega]$ is the jump of a function through a separation surface: $[\Omega] = (\Omega_s - \Omega_y) |_{\Sigma_{sg}}$. Here condition (15) is the continuity equation, (16) is the equilibrium equation, (17) is the balance energy equation, (18) is the additional equation of homothermality, and $D$ is the linear rate of motion of the surface $\Sigma_{sg}$ which is called a rate of phase transformation. The expression for $D$ will be given below.

Besides conditions (15)-(18), there is a so-called Gibbs principle at the phase transformation boundary $\Sigma_{sg}$ that consists in the equality of chemical potentials of phases $\mu_s$ and $\mu_y$:

(19) \[ [\mu] = 0. \]

For phase transformations of the gas-fluid type (or gas-gas, or fluid-fluid), the Gibbs principle is the consequence of the equation for entropy jump through the phase interface and also of assumptions on the absence of entropy generation (energy dissipation) at the phase interface.

For phase transformations of the type: solid phase with small deformations $\rightarrow$ gas phase, the Gibbs principle is written in the form

(20) \[ \mu_s^0 = \mu_y, \quad x \in \Sigma_{gs}. \]

If the contribution of mechanical energy $\mu_s'$ of the solid phase is much less than heat energy $\mu_s^0$, then: $\mu_s' \ll \mu_s^0$.

On substituting the expression for chemical potentials $\mu_y$ and $\mu_s^0$ into equation (20), we obtain the expression for the pressure $p$ of the gas phase:

(21) \[ p = p^0 \exp \left( -\frac{\Delta \mu}{R \theta} \right), \quad \Delta \mu = \mu_y^0 - \mu_s^0; \]

where

\[ p^0 = p_0 \exp \left( \frac{\mu_s'}{R \theta_s} \right). \]
3.5. RATE OF PHASE TRANSFORMATION

The equation to determine the phase transformation surface $\Sigma_{\mu = \xi}$ has the form

$$
\frac{\partial f}{\partial t} + D \left( \nabla f \cdot \nabla f \right)^{1/2} = 0; \quad f(x, 0) = f^0(x),
$$

where $f(x, t) = 0$ is the equation of surface $\Sigma_{\xi = \eta}$. Here $D$ is the rate of phase transformation. The expression for $D$ can be obtained from equations (15) and (16):

$$
D = \frac{1}{\rho_s} \left( \frac{n \cdot [\sigma] \cdot n}{[1/\rho]} \right)^{1/2},
$$

but in place of pressure $p$ we should substitute expression (21). In this case equation (22) is not identical to formulae (15) and (16), and the final expression for $D$ takes the form

$$
D = \frac{\sqrt{p^0 \rho_s}}{\rho_s \sqrt{R \theta}} \exp \left( -\frac{\Delta \mu}{2R \theta} \right) \left( \frac{1 - \frac{p_0}{p_s} \exp \left( -\frac{\Delta \mu}{R \theta} \right) + \frac{\Delta \mu}{R \theta} + \frac{n \cdot \tau^e_s}{p_s} \cdot n}{1 - \frac{p_0}{R \theta \rho_s} \exp \left( -\frac{\Delta \mu}{R \theta} \right)} \right)^{1/2},
$$

where $p_s = -n \cdot \sigma \cdot n$ is the normal pressure of the solid phase. For phase transformations of the type: solid phase $\rightarrow$ gas, the following relation between pressures $p_s$ and $p^0$ is usually satisfied:

$$
p_s \approx p^0 \approx p_e, \quad \frac{p_0}{R \theta \rho_s} \ll 1,
$$

where $p_e$ is the external pressure on the porous medium.

When a pyrolise process occurs to components, usually under heating temperatures up to 1000° C the condition

$$
\exp \left( -\frac{\Delta \mu}{R \theta} \right) \ll 1
$$

is also satisfied, and the expression for $D$ can be rewritten in the simple form

$$
D = D_0 \exp \left( -\frac{E_a}{R \theta} \right) \left( 1 - \frac{p_e}{p_0} \exp \left( -\frac{2E_a}{R \theta} \right) \right)^{1/2};
$$

$$
D_0 = \frac{p_e}{\rho_s \sqrt{R \theta}}; \quad \text{and} \quad E_a = \frac{\Delta \mu}{2}, \quad \Delta \mu = \mu^0_{\eta} - \mu^0_{\xi};
$$

where $E_a$ is the activation energy of the phase transformation, and $D_0$ is the pre-exponential multiplier. Dependence (26), without taking account of the third multiplier, is called the Arrhenius law. Parameters $D_0$ and $E_a$ are usually given empirically or found in experiments. The derivation given above allows us to find their analytical expressions.
3.6. Boundary and Initial Conditions

Conditions at the external boundary $\Sigma$ of the porous media as a whole are formulated as follows:

\begin{equation}
\sigma_s \cdot n = S_e, \quad x \in \Sigma_\sigma; \quad \sigma_g \cdot n = S_e, \quad x \in \Sigma_g;
\end{equation}

\begin{equation}
u = u_e, \quad x \in \Sigma_u; \quad \text{and} \quad v_g = v_e, \quad x \in \Sigma_v;
\end{equation}

where $\Sigma_\sigma$, $\Sigma_u$, and $\Sigma_g$, $\Sigma_v$ are parts of surface $\Sigma$: $\Sigma = \Sigma_g \cup \Sigma_u = \Sigma_\sigma \cup \Sigma_g$.

Initial conditions are

\begin{equation}
 t = 0 : \quad \rho_g = \rho_{g0}, \quad \theta_g = \theta_{g0}; \quad \theta_s = \theta_{s0}; \quad \text{and} \quad f = f^0.
\end{equation}

3.7. Dimensionless Equations

Let us introduce typical magnitudes of the functions: $t_0$ for the durations of all the processes, $\rho_0$ for the densities of the phases, $\theta_0$ for the temperatures of the phases, $v_0 = x_0/t_0$ for the velocities of the phases, $u_0 = x_0$ for the displacements of the solid phase, $\sigma_0 = \rho_0 x_0^2/t_0^2$ for the stresses of the phases, $D_0 = l_0/t_0$ for the rate of the phase transformation, $\epsilon_0 = \sigma_0/\rho_0 \theta_0$ for heat capacities, $\lambda_0 = x_0^2 \rho_0 \epsilon_0/l_0$ for heat conductivity, and $\epsilon_0 = c_0 \theta_0$ for the internal energy of the phases. Then, introducing the corresponding dimensionless values of the functions

\begin{equation}
\bar{\rho}_g = \rho_g/\rho_0, \quad \bar{\rho}_s = \rho_s/\rho_0, \quad \bar{\theta}_g = \theta_g/\theta_0, \quad \bar{\theta}_s = \theta_s/\theta_0,
\end{equation}

\begin{equation}\bar{\sigma}_g = \sigma_g/\sigma_0, \quad \bar{\sigma}_s = \sigma_s/\sigma_0, \quad \bar{D} = D/D_0, \quad \bar{f} = f/x_0, \quad \bar{\epsilon}_g = \epsilon_g/\epsilon_0, \quad \bar{\epsilon}_s = \epsilon_s/\epsilon_0, \quad \bar{c}_g = c_g/c_0, \quad \bar{c}_s = c_s/c_0, \quad \text{etc.},
\end{equation}

we obtain equations for the dimensionless functions which have the same form as the corresponding equations for dimensional functions (4)-(14), (18), (28), and (29). Boundary conditions (15)-(17) take the forms

\begin{equation}(15a) \quad \kappa \bar{\rho}_g \bar{D} + \bar{\rho}_g \bar{v}_g \cdot n = 0;
\end{equation}

\begin{equation}(16a) \quad \kappa \bar{\rho}_s \bar{D} \bar{v}_g + [\bar{\sigma}] \cdot n = 0;
\end{equation}

and

\begin{equation}(17a) \quad \kappa \bar{\rho}_s \bar{D} [\bar{e}^0 + \bar{c} \bar{\theta}] - n \cdot [\bar{\sigma} \cdot \bar{v}] + n \cdot [\bar{\lambda} \nabla \bar{\theta}] = 0.
\end{equation}

The small parameter in (15a)-(17a) appears to be due to the fact that the typical magnitude of the phase transformation rate $D_0$ has an order of $l_0/t_0$ and the characteristic magnitude of the gas velocity is $v_0 = x_0/t_0$.

Below we will use the system (4)-(14), (15a)-(17a), (18), (28), and (29) in the dimensionless form, and the bars over symbols will be omitted.
4. Asymptotic averaging for processes in porous media

4.1. Asymptotic expansions

Equation system (4) - (8) and (22) with constitutive relations (9)-(13), conditions (15)-(18) at the phase interface and (28) at the external boundary of the medium, and initial conditions (29) forms the problem of determining ten functions \( u, v_{\bar{y}}, \rho_{\bar{y}}, \theta_s, \theta_y \) and \( f \) of coordinates \( x, \xi \) and time \( t \). This problem contains small parameter \( \varkappa \).

An asymptotic solution of the problem is sought in the following form:

\[
\begin{align*}
    u &= u^{(0)}(x, t) + \varkappa u^{(1)}(x, \xi, t) + \varkappa^2 \ldots; \\
    v_{\bar{y}} &= v_{\bar{y}}^{(0)}(x, \xi, t) + \varkappa v_{\bar{y}}^{(1)}(x, \xi, t) + \varkappa^2 \ldots; \\
    \rho_{\bar{y}} &= \rho_{\bar{y}}^{(0)}(x, t) + \varkappa \rho_{\bar{y}}^{(1)}(x, \xi, t) + \varkappa^2 \ldots; \\
    \theta_s &= \theta_s^{(0)}(x, t) + \varkappa \theta_s^{(1)}(x, \xi, t) + \varkappa^2 \ldots; \quad i = 1, 2; \\
    \theta_y &= \theta_y^{(0)}(x, t) + \varkappa \theta_y^{(1)}(x, \xi, t) + \varkappa^2 \ldots; \\
\end{align*}
\]

and

\[
    f = f^{(0)}(x, \xi, t) + \varkappa f^{(1)}(x, \xi, t) + \varkappa^2 \ldots.
\]

On substituting functions (30) into governing equations (9)-(14), the rest of the functions of the problem are obtained in the asymptotic form:

\[
\begin{align*}
    (30a) \quad \Omega = \Omega^{(0)}(x, \xi, t) + \varkappa \Omega^{(1)}(x, \xi, t) + \varkappa^2 \ldots, \quad \Omega = \{\rho_{\bar{y}}, \nu, \tau_{\bar{y}}, \sigma_s, \varepsilon, \mu_s, \mu_{\bar{y}}, D\}.
\end{align*}
\]

4.2. Problems "over periodicity cell" of "zero" level

Having substituted expansions (30) into equations (4) and (5), then having collected terms of the same powers of \( \varkappa \) and putting terms at the lowest powers of \( \varkappa \) equal to zero, we obtain the local problem of the zero level "over the periodicity cell":

\[
\begin{align*}
    \nabla_\xi \cdot v_{\bar{y}}^{(0)} &= 0; \\
    -\nabla_p^{(1)} + \nabla_\xi \cdot \tau_{\bar{y}}^{(0)} &= \nabla \rho_{\bar{y}}^{(0)}; \quad \xi \in V_{\xi\xi}; \\
    \tau_{\bar{y}}^{(0)} &= \nu_{\bar{y}} \delta \nabla_\xi \cdot v_{\bar{y}}^{(0)} + k_{\bar{y}} (\nabla_\xi \otimes v_{\bar{y}}^{(0)} + (\nabla_\xi \otimes v_{\bar{y}}^{(0)})^T); \\
    p^{(1)} &= R \left( \rho_{\bar{y}}^{(1)} \theta_{\bar{y}}^{(0)} + \rho_{\bar{y}}^{(0)} \theta_{\bar{y}}^{(1)} \right); \\
    v_{\bar{y}}^{(0)} |_{\Sigma_{\xi\xi}} &= 0, \quad \text{and} \quad \langle \rho_{\bar{y}}^{(1)} \rangle_{\bar{y}} = 0;
\end{align*}
\]

the solution of which is functions \( v_{\bar{y}}^{(0)} \) and \( \rho_{\bar{y}}^{(1)} \) and the rest of functions contained in (31), \( p^{(1)} \) and \( \theta^{(0)} \) are assumed to be known "initial data" of the problem.

Substituting expansions (30) into equations (7) and (8) and conditions on the phase interface (16), and then collecting terms of the same powers of \( \varkappa \) in these equations,
we put terms at $(1/\kappa)$ in equation (2) and terms at $\lambda^0$ in equations (8) and (12) equal to zero, and then we obtain the local contact problem of solid body mechanics within the “periodicity cell”:

\begin{equation}
\nabla_{\xi} \cdot \sigma^{(0)} = 0;
\end{equation}

\begin{equation}
\varepsilon^{(0)} = \alpha(\theta^{(0)} - \theta_0) + \Pi : \sigma^{(0)},
\end{equation}

\begin{equation}
2\varepsilon^{(0)} = 2\varepsilon + \nabla_{\xi} \otimes \mathbf{u}^{(1)} + (\nabla_{\xi} \otimes \mathbf{u}^{(1)})^T, \quad \xi \in \mathbf{V}_{\xi s},
\end{equation}

\begin{equation}
\sigma^{(0)}_n \cdot \mathbf{n}^{(0)} = -p^{(0)}_n, \quad \xi \in \Sigma_{\xi s g};
\end{equation}

\begin{equation}
\langle \varepsilon^{(0)} \rangle_s = \varepsilon; \quad \text{and} \quad 2\varepsilon = \nabla_{\xi} \otimes \mathbf{u}^{(0)} + (\nabla_{\xi} \otimes \mathbf{u}^{(0)})^T.
\end{equation}

Functions $\theta^{(0)}$ and $\mathbf{u}^{(0)}$ are also assumed to be known data of the problem. Function $\mathbf{u}^{(1)}$ depends on $\mathbf{u}^{(0)}$ and $\theta^{(0)}$ parametrically.

At last, let us substitute expansions (30) into equations (6) and (8) and conditions (17) and (18) and collect terms of the same powers of $\kappa$. Then setting terms at $(1/\kappa)$ in equations (6) and (8) and terms at $\lambda^0$ in the boundary conditions equal to zero, we obtain

\begin{equation}
\nabla_{\xi} \cdot \mathbf{q}^{(0)}_s = 0; \quad \xi \in \mathbf{V}_{\xi s},
\end{equation}

\begin{equation}
\nabla_{\xi} \cdot \mathbf{q}^{(0)}_g = 0; \quad \xi \in \mathbf{V}_{\xi g},
\end{equation}

\begin{equation}
\mathbf{q}^{(0)}_s = \lambda_s(\nabla_{\xi} \theta^{(0)} + \nabla_{\xi} \theta^{(1)}), \quad \mathbf{q}^{(0)}_g = \lambda_g(\nabla_{\xi} \theta^{(0)} + \nabla_{\xi} \theta^{(1)}),
\end{equation}

\begin{equation}
[\mathbf{q}^{(0)}] \cdot \mathbf{n}^{(0)} = 0;
\end{equation}

\begin{equation}
\langle \theta^{(1)} \rangle = 0; \quad \xi \in \Sigma_{\xi s}, \quad \text{and} \quad \langle \theta^{(1)} \rangle = 0;
\end{equation}

that is, the local contact stationary problem on heat-conductivity in the periodicity cell—to determine periodic functions $\theta^{(1)}_s$ and $\theta^{(1)}_g$. Here $\mathbf{q}^{(0)}_g$ and $\mathbf{q}^{(0)}_s$ are heat fluxes in the gas and solid phases. Functions $\theta^{(1)}_s$ and $\theta^{(1)}_g$ depend on $\theta^{(0)}$ parametrically.

The following average values for phases are introduced:

\begin{equation}
\langle \Omega_s \rangle_s = \frac{1}{\varphi_s|V_{\xi}|} \int_{V_{\xi s}} \Omega_s dV_{\xi s};
\end{equation}

\begin{equation}
\langle \Omega_g \rangle_g = \frac{1}{\varphi_g|V_{\xi}|} \int_{V_{\xi g}} \Omega_g dV_{\xi g};
\end{equation}

\begin{equation}
\langle \Omega \rangle = \varphi_s \langle \Omega \rangle_s + \varphi_g \langle \Omega \rangle_g;
\end{equation}

\begin{equation}
\varphi_s = \frac{1}{|V_{\xi}|} \int_{V_{\xi s}} dV_{\xi s}; \quad \text{and} \quad \varphi_g = 1 - \varphi_s.
\end{equation}

A solution of all three problems for functions $\rho^{(1)}_g$, $\nu^{(0)}_g$, $\mathbf{u}^{(1)}$, $\theta^{(1)}_s$, and $\theta^{(1)}_g$ is sought in the class of functions which are periodic in $\xi$ coordinates.
The phase interface $\Sigma_{\xi \sigma}$ within the periodicity cell is described by function $f^{(0)}(x, \xi, t) = 0$. The equation for $f^{(0)}$ is found on substituting asymptotic expansions (30) into (22):

$$\frac{\partial f^{(0)}}{\partial t} + D^{(0)}(\nabla_{\xi} f \cdot \nabla_{\xi} f)^{1/2} = 0; \quad \text{and} \quad f^{(0)}(x, \xi, 0) = f^{0}(x, \xi);$$

where $D^{(0)}$ is the rate of the phase transformation in the zeroth approximation:

$$D^{(0)} = D_0^{(0)} \exp \left( -\frac{E_a}{R\theta^{(0)}} \right) \left( 1 - \frac{p^{(0)}}{p_0} \exp \left( -\frac{2E_a}{R\theta^{(0)}} \right) \right)^{1/2}; \quad D^{(0)} = \frac{p^0}{\rho_s \sqrt{R\theta^{(0)}}}.$$

Using the expression $n = \nabla_{\xi} f [\nabla_{\xi} f]^{-1}$, the vector $n$ normal to the separation surface $\Sigma_{\xi \sigma}$ is obtained as follows:

$$n = n^{(0)} + \kappa n^{(1)};$$

$$n^{(0)} = \nabla_{\xi} f^{(0)} [\nabla_{\xi} f^{(0)}]^{-1}, \quad n^{(1)} = - (\nabla_{\xi} f^{(0)} + \nabla_{\xi} f^{(1)} [\nabla_{\xi} f^{(0)}]^{-1};$$

and

$$[\nabla_{\xi} f^{(0)}] = (\nabla_{\xi} f \cdot \nabla_{\xi} f)^{1/2}.$$

4.3. Problems “over the periodicity cell” of the “first” level

Having collected terms in equations (4) and (5) at the next powers of $\kappa$ we obtain local problems over the first level cell:

$$\nabla_{\xi} \cdot (\rho_{g}^{(0)} v_{y}^{(1)} + \rho_{g}^{(1)} v_{y}^{(0)}) = - \left( \frac{\partial \rho_{g}^{(0)}}{\partial t} + \nabla_{\xi} \cdot \rho_{g}^{(0)} v_{y}^{(0)} \right);$$

$$- \nabla_{\xi} \rho^{(2)} + \nabla_{\xi} \tau_{g}^{(1)} = \nabla_{\xi} \tau_{g}^{(0)};$$

$$\tau_{g}^{(0)} = \nu_{g}^{(0)} \delta \nabla_{\xi} \cdot v_{g}^{(1)} + k_{g}^{(0)} (\nabla_{\xi} \otimes v_{g}^{(1)} + (\nabla_{\xi} \otimes v_{g}^{(1)})^{T});$$

$$\rho^{(2)} = R^{(2)} \beta_{g}^{(1)} + \rho_{g}^{(1)} \beta_{g}^{(2)};$$

$$(\rho_s - \rho_g^{(0)}) D^{(0)} + (\rho_g^{(0)} v_{y}^{(1)} + \rho_g^{(1)} v_{y}^{(0)}) \cdot n^{(0)} + \rho_g^{(0)} v_{y}^{(0)} \cdot n^{(1)} = 0; \quad \xi \in \Sigma_{\xi \sigma};$$

and

$$\langle \rho_g^{(2)} \rangle_g = 0.$$

Functions $\rho_g^{(2)}$ and $v_{y}^{(1)}$ in this problem are unknown, and the rest are “initial data”.

Similarly to the above, collecting terms of higher powers of $\kappa$ in equations (7) and (8), we obtain

$$\nabla_{\xi} \cdot \sigma_{s}^{(1)} = - \left( \rho_s \frac{\partial^2 u^{(0)}}{\partial t^2} - \nabla_{\xi} \cdot \sigma_{s}^{(0)} \right), \quad \xi \in V_{\xi \sigma};$$

EUROPEAN JOURNAL OF MECHANICS, A/SOLIDS, VOL. 17, NO 2, 1998
(39) \[-\rho_s \nu_y^{(0)} D^{(0)} + [\sigma^{(0)}] \cdot n^{(1)} + [\sigma^{(1)}] \cdot n^{(0)} = 0; \quad \xi \in \Sigma_{sx};\]

and

\[\langle u_s^{(2)} \rangle_s = 0\]

- a local contact problem on solid mechanics of the “first” level of determining functions \(u_s^{(2)}\).

On collecting terms of powers of \(x^0\) in equations (6) and (8) and conditions (17) at the phase interface, we obtain

\[(40) \quad \nabla \xi \cdot (\lambda_s \cdot (\nabla \nabla \theta_s^{(1)} + \nabla \theta_s^{(2)})) + \nabla \xi \cdot (\lambda_s \cdot \nabla \theta_s^{(1)}) = -\rho_s c_s \frac{\partial \theta_s^{(0)}}{\partial t} - \nabla \xi \cdot (\lambda_s \cdot \nabla \theta_s^{(0)}) - \alpha_s \frac{\partial \theta_s^{(0)}}{\partial t} + W_s^{(0)}; \quad \xi \in \xi_s;\]

\[\nabla \xi \cdot (\lambda_g \cdot (\nabla \nabla \theta_g^{(1)} + \nabla \theta_g^{(2)})) + \nabla \xi \cdot (\lambda_g \cdot \nabla \theta_g^{(1)}) = -\frac{\partial}{\partial t} \rho_s c_y \theta_s^{(0)} - \nabla \xi \cdot (\rho_s c_y \theta_s^{(0)}) - \nabla \xi \cdot (\rho_s^{(0)} \nabla \theta_s^{(0)} + \rho_s^{(1)} \nabla \theta_s^{(1)} + \rho_s^{(0)} \nabla \theta_s^{(0)} - \nabla \xi (\sigma_{s1} \cdot v_s^{(0)} + \sigma_{s1} \cdot v_s^{(1)}), \quad \xi \in \xi_g;\]

\[\rho_s [c_s \theta_s^{(0)}] D^{(0)} - n^{(0)} \cdot \sigma_{s1}^{(0)} + \sigma_{s1}^{(1)} \cdot v_s^{(1)} + n^{(1)} \cdot \sigma_{s1}^{(0)} + v_s^{(1)} + n^{(1)} \cdot \lambda \cdot (\nabla \theta_s^{(1)} + \nabla \theta_s^{(2)}) + n^{(1)} \cdot \lambda \cdot (\nabla \theta_s^{(0)} + \nabla \theta_s^{(1)})] = 0; \quad \xi \in \Sigma_{sx};\]

and

\[\langle \theta_s^{(2)} \rangle_s = 0;\]

- a local problem on heat-conductivity of the “first” level of determining functions \(\theta_s^{(2)}\).

4.4. AVERAGED EQUATIONS

The averaging operation of quasiperiodic functions \(\Omega(x, \xi, t)\) over coordinate \(\xi\) was introduced by formula (34). To derive averaged equations, the following properties of the averaging operation will be used:

\[(41) \quad \int_{V_{\xi_s}} \frac{\partial \Omega}{\partial t} dV_\xi = \frac{\partial}{\partial t} \Omega_\varphi (\langle \Omega \rangle_s) - \int_{\Sigma_{\xi_s}} \Omega D^{(0)} d\Sigma_\xi;\]

\[\nabla \xi \cdot \nabla \Omega dV_\xi = \nabla \xi \cdot \varphi (\langle \Omega \rangle_s) + \int_{\Sigma_{\xi_s}} \Omega n^{(1)} d\Sigma_\xi;\]

and

\[\Omega_\varphi (\langle \Omega \rangle_s) = \int_{\Sigma_{\xi_s}} \Omega n^{(0)} d\Sigma_\xi;\]

For the averaging operation of function \(\Omega\) over \(V_{\xi_s}(t)\) we should change the sign before the integral over the phase interface \(\Sigma_{\xi_s}\).

Let us average now the first equation from (38) over \(V_{\xi_s}\) and momentum equation (39) over \(V_{\xi_s}\) and sum the latter with the first equation of (31) averaged over \(V_{\xi_s}\). Equation
(40) is averaged over $V_{\xi_s}$ and $V_{\xi_y}$ respectively and these equations are then summed with each other. As a result we obtain the system of averaged equations:

\begin{equation}
\frac{\partial \varphi_s}{\partial t} = -J;
\end{equation}

\begin{equation}
\frac{\partial \varphi_y \rho_y^{(0)}}{\partial t} + \nabla_x \cdot \varphi_y \rho_y^{(0)} \langle \mathbf{v}_y^{(0)} \rangle_y = J;
\end{equation}

\begin{equation}
\rho_s \varphi_s \frac{\partial^2 \mathbf{u}^{(0)}}{\partial t^2} = \nabla_x \cdot \varphi_s \sigma_s - \nabla_x \varphi_y \rho_y^{(1)};
\end{equation}

\begin{equation}
\rho c \frac{\partial \theta^{(0)}}{\partial t} + \varphi_y \rho_y^{(0)} c_y \langle \mathbf{v}_y^{(0)} \rangle_y \cdot \nabla_x \theta^{(0)} = \nabla_x \cdot (\bar{\lambda} \cdot \nabla_x \theta^{(0)}) - \bar{\varphi}_y \mathbf{v}_y^{(0)} \cdot \nabla_x \rho_y^{(0)} - J \Delta c;
\end{equation}

to determine functions $\varphi_s$, $\rho_y^{(0)}$, $\mathbf{u}^{(0)}$ and $\theta^{(0)}$, where the following designations for parameters of phase interchange $J$ and $\Delta c$ are introduced:

\begin{equation}
\Delta c = [\Delta c^{(0)}] + [\varepsilon] \theta^{(0)},
\end{equation}

and

\begin{equation}
J = \rho_s D^{(0)} \int_{\Sigma_{\xi_s}} d\Sigma_{\xi}.
\end{equation}

Equation (42) is an evident consequence of properties (41) if $\Omega = 1$.

In equations (42)-(45) we introduce the following notation for functions $\bar{\sigma}_s$, $\bar{\varepsilon}$, $\bar{q}$ and $\bar{\rho c}$, which are averaged values over the periodicity cell:

\begin{equation}
\bar{\sigma}_s = \langle \sigma_s^{(0)} \rangle_s,
\end{equation}

\begin{equation}
\bar{q} = \langle \lambda \cdot (\nabla_{\xi} \theta_s^{(1)} + \nabla_x \theta_s^{(0)}) \rangle_s;
\end{equation}

\begin{equation}
\bar{\varepsilon} = \frac{1}{2} \left( \nabla_x \otimes \mathbf{u}^{(0)} + (\nabla_x \otimes \mathbf{u}^{(0)})^T \right);
\end{equation}

and

\begin{equation}
\bar{\rho c} = \rho_s \varphi_s \sigma_s + \rho_y^{(0)} \varphi_y c_y.
\end{equation}

These averaged values of functions are connected with relations:

\begin{equation}
\bar{\varepsilon} = \alpha (\bar{\theta}_s - \theta_0) + \Pi : \bar{\sigma}_s - \frac{1}{2} \langle \nabla_{\xi} \otimes \mathbf{u}^{(1)} + (\nabla_{\xi} \otimes \mathbf{u}^{(1)})^T \rangle_s;
\end{equation}
and

\[ \bar{q} = \bar{\lambda} \cdot \nabla_{\xi} \theta, \]

where \( \bar{\lambda} \) is the effective tensor of heat-conductivity which can be determined from the second equation (47a), into which the expression for \( \bar{q} \) from (47b) and the expression for \( \nabla_{\xi} \theta^{(0)} \) in terms of function \( \nabla_{\xi} \theta^{(0)} \) should be substituted. The dependence \( \nabla_{\xi} \theta^{(1)}(\nabla_{\xi} \theta^{(0)}, \xi) \) can be determined from equations (33).

These equations are effective constitutive relations for porous media.

To the equation system (42)-(45) we should add the equations connecting a mean velocity of gas phase flow \( \langle \mathbf{v}^{(0)} \rangle_{y} \) with pressure \( p^{(0)} \). This relation is found from the solution of problem (31) over the periodicity cell: 

\[ \rho_{g}^{(0)} \langle \mathbf{v}^{(0)} \rangle_{y} = \mathbf{V}_{g}(\xi) \cdot \nabla_{\xi} p^{(0)} \]

where function \( \mathbf{V}_{g}(\xi) \) is determined by the geometry of the pores.

Averaging this expression over \( V_{\xi y} \), we obtain

(48) \[ \rho_{g}^{(0)} \langle \mathbf{v}^{(0)} \rangle_{y} = -\mathbf{K} \cdot \nabla_{\xi} p^{(0)} \]

which is the relation known as the Darcy law.

5. Discussion

A main concept of the asymptotic averaging method described above consists of the following: With the help of assumptions on the regularity of the internal structure of a porous medium and asymptotical expansions of functions (30), the system of initial equations of thermomechanics (4)-(8) describing accurately high-temperature processes in porous media has been transformed to the system of averaged equations (42)-(45) describing the processes accurately up to small values of the order of \( \varkappa \). Resolving the system (42)-(45) is essentially simpler than resolving the initial system (4)-(8), as the domain of definition of system (42)-(45) is a "homogenized" one and the domain of definition of system (4)-(8) is the initial "nonhomogeneous" one \( V \) with a very complicated internal geometry (Fig. 2).

![Fig. 2. - A periodicity cell of a porous medium.](image-url)
As a result of the averaging procedure, the initial constitutive relations of phases (9)-(13) have been transformed to averaged constitutive relations in system (47a) connecting averaged function \( \bar{\sigma}_s \) to \( \bar{\varepsilon} \) and \( \theta^{(0)} \).

As a rule, averaged constitutive relations are determined empirically with the use of additional experimental data (Nigmatulin, 1994). The method of asymptotic averaging allows us to determine a precise expression for all these functions. For this purpose it is necessary to solve subsidiary local problems of the “zeroth” level (31)-(33). Solutions of local problems (38) and (40) are not necessary; these equations have been used only for the derivation of averaged equations (42)-(45).

Local problems of “zero th” and “first” levels are stationary equations of conservation (i.e. all derivatives of the unknown with respect to time are equal to zero). The solution of these problems is sought within the domain \( V_{\xi} \), i.e. within the first periodicity cell. In addition, requirements on the periodicity of all the unknown functions \( \rho_g^{(1)} \), \( v_g^{(0)} \), \( \theta_g^{(1)} \), \( u^{(1)} \), and \( \theta_s^{(1)} \) are imposed. Moreover, conditions of an integral type (the last line of formulae (31)-(33)) are attached to the local system of the “zero th” level. They are conditions of equality to zero of the averaged values of the functions: \( \langle \rho_g^{(1)} \rangle_{\xi} = 0 \), \( \langle \theta^{(1)} \rangle = 0 \), and \( \langle \varepsilon^{(0)} \rangle_{\xi} = \bar{\varepsilon} \). These equations are necessary for the existence of a unique solution of the problems “over the periodicity cell” (Bakhvalov and Panasenko, 1989).

In fact, as seen from system (31), if \( \rho_g^{(1)} \) is a solution of the problem, then function \( \tilde{\rho}_g^{(1)} = \rho_g^{(1)} + C(x, t) \) is also a solution, where \( C(x, t) \) is an arbitrary function independent of \( \xi \). In order to eliminate the non-uniqueness of the solution, we should give the additional integral condition \( \langle \rho_g^{(1)} \rangle_{\xi} = 0 \), which is a condition of normalizing. The consequence of equation \( \langle \rho_g^{(1)} \rangle_{\xi} = \langle \rho_g^{(2)} \rangle = \ldots = 0 \) is that the function \( \rho_g^{(0)} \) is the averaged value \( \rho_g \): \( \rho_g^{(0)} = \langle \rho_g \rangle_{\xi} \). The same occurs in functions \( u^{(1)} \) in (32) and \( \theta^{(1)} \) in (33).

6. Conclusions

In the present paper the method of asymptotic averaging for processes in porous media with phase transformations and a regular (periodic) structure has been developed.

The advantage of this method is that it allows us not only to obtain averaged equations for multiphase media but also to set the special mathematical problems “over the periodicity cell” in order to determine the microscopic characteristics of processes within each of the phases. The solution of the problems “over the periodicity cell” allows us to obtain the accurate presentation of the distribution of the main parameters such as stresses, strains, pressure, density, and temperatures inside the phases, while most up-to-date theories on multiphase media are based on the hypothesis of the uniform distribution of parameters over the phases.

In the next paper the solutions of local problems “over the periodicity cell” will be obtained, and the effect of the microscopic parameters of phases on the behaviour of the solution of the averaged equations will be analyzed.
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