cp) capillary; md) mold; sat) saturation; nom) nominal; v) vapor; s.m) superheating of the melt; m) melt; c) centripetal; cf) centrifugal; max) maximal.

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NONISOTHERMAL RHEODYNAMICS IN SHS PRESSING OF POWDER MATERIALS

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The article deals with thermal and rheodynamic processes of SHS pressing (SHS stands for self-propagating high-temperature synthesis) of viscous compressible materials. It presents numerical calculations of the nonisothermal kinetics of compaction with different thermal and technological parameters. Conditions are found for the realization of qualitatively different regimes of compacting SHS materials.

One of the topical problems of the theory and practice of SHS pressing (the same as in hot pressing) of powdered high melting materials is the study of the state of stress of the products of synthesis under the effect of applied external forces. It is usual to apply the macrorheological approach to the description of the behavior of porous materials suggested in [1-3] which makes use of the model of a viscous compressible liquid. Buchatskii et al. [3] and Stolin et al. [4] found an analytical solution of the problem of one-sided compression of such systems for the case when there is no temperature distribution in the material. Buchatskii et al. [5] made a qualitative analysis of different thermal regimes of compaction on the assumption that in the process a thermal gradient is not involved. The obtained analytical solution of the problem made it possible to evaluate the conditions of realization of a quasiisothermal regime of compaction where the process of pressing is not accompanied by a noticeable change of temperatures. However, in practice the nonuniformity of the temperature regime in the material and the conditions of heat exchange have a substantial effect on the distribution of densities, speeds, and stresses, and consequently also on the quality of the finished products. The aim of the present work is a numerical analysis of the temperatures, densities, speeds, and stresses within the bulk of viscous porous material in the process of its one-sided compression in dependence on the initial distribution of temperature and density throughout its volume.

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As a rule material is pressed in a cylindrical mold, and the equations contained in the statement of the problem will therefore be written henceforth in a system of cylindrical coordinates. It is assumed that flow is unidimensional, with one velocity component v_z (henceforth the subscript z will be omitted) and opposed to the direction of the z axis. It was shown in [2, 3] that the Reynolds number is small on account of the great viscosity of the incompressible base of the material (from 10^7 to 10^{10} Pa·sec), and the equations of motion can therefore be replaced by the conditions of equilibrium. With the mentioned assumptions the problem reduces to the solution of the following system of equations of rheodynamics and heat exchange:

$$\frac{\partial\rho}{\partial t}+\frac{\partial}{\partial z}(\rho v)=0,$$

$$\frac{\partial\sigma_{zz}}{\partial z}=0,$$

$$\sigma_{zz}=\left(\frac{4}{3}\mu+\xi\right)\frac{\partial v}{\partial z},$$

$$\sigma_{rr}=\sigma_{\theta\theta}=\left(-\frac{2}{3}\mu+\xi\right)\frac{\partial v}{\partial z},$$

$$c\left[\frac{\partial(\rho T)}{\partial t}+\frac{\partial(\rho vT)}{\partial z}\right]=\frac{\partial}{\partial z}\left[\lambda(\rho)\frac{\partial T}{\partial z}\right]-\frac{2\alpha}{r_0}(T-T_0).$$

Here it is assumed that the temperature across the section z = const of the pressed compact is constant because its transverse dimension is small in comparison with the length, and that the thermophysical properties of the material do not depend on the temperature. Heat removal in the transverse direction is taken into account by the last term of the equation of heat conduction.

The dependences of shear viscosity $\mu(\rho, T)$ and bulk viscosity $\xi(\rho, T)$ on the density and temperature of the compressible material are adopted in the following form:

$$\mu(\rho,\ T)=\mu_1(T)\,\mu_2(\rho)=\mu_0\exp(U/RT)\,\rho^m,$$

$$\xi(\rho,\ T)=\frac{4}{3}\mu(\rho,\ T)\frac{\rho}{1-\rho}=\frac{4}{3}\mu_0\frac{\rho^{m+1}}{1-\rho}\exp(U/RT).$$

The dependence of viscosities on density is taken from published data [1, 2] where the empirical parameter m is chosen on the basis of an experiment. We choose the boundary conditions:

$$-\lambda(\rho)\frac{\partial T}{\partial z}=\begin{cases}-\alpha_1(T-T_0), & z=0,\\ \alpha_2(T-T_0), & z=z_0,\end{cases}$$

$$v|_{z=0}=0,\quad \sigma_{zz}|_{z=z_0}=-P.$$

At the initial instant the distribution of density and temperature in the material is specified:

$$\rho(z,0)=\rho_0(z),\ T(z,0)=T_*(z).$$

The dependence of thermal conductivity on density is adopted in the form of a power law [6]:

$$\lambda(\rho)=\lambda_0[\rho/\rho_0]^k,$$

where k is an empirical parameter.

The movement of the upper boundary of the specimen under the effect of the plunger of the press is taken into account in the model in the following way: $U_p = \partial z_0/\partial t$.

To simplify the initial system of equations and to be able to compare the results of numerical calculations with the analytical solution of the isothermal problem of one-sided compression obtained earlier on [4], we also go over the Lagrangian mass system of coordinates in which the time t_L is the same as time t, and the mass coordinate q has the meaning of relative mass of the material in a volume from 0 to z:

$$q=\int_0^z \rho(z,\ t)\,dz.$$

In view of the adopted equality of times t and t_L we henceforth omit the subscript L. The statement of the problem in the Lagrangian system of coordinates with boundary and initial conditions has the form:

$$\frac{\partial\rho}{\partial t}+\rho^2\frac{\partial v}{\partial q}=0,\ \frac{\partial\sigma_{zz}}{\partial q}=0,$$

$$\sigma_{zz}=\left(\frac{4}{3}\mu+\xi\right)\rho\frac{\partial v}{\partial q},\ \sigma_{rr}=\sigma_{\theta\theta}=\left(-\frac{2}{3}\mu+\xi\right)\rho\frac{\partial v}{\partial q},$$

$$\frac{\partial T}{\partial t}=\frac{\partial}{\partial q}\left[\ \lambda(\rho)\rho\ \frac{\partial T}{\partial q}\right]\frac{\lambda_0}{c\rho_1}-\frac{2\alpha}{c\rho\rho_1 r_0}(T-T_0), \tag{1}$$

$$-\lambda(\rho)\rho\frac{\partial T}{\partial q}=\begin{cases}-\alpha_1(T-T_0),\ q=0,\\ \alpha_2(T-T_0),\ q=q_0,\end{cases}$$

$$\sigma_{zz}|_{q=q_0}=-P,\ v|_{q=0}=0,$$

$$\rho(q,\ 0)=\rho_0(q),\ T(q,\ 0)=T_*(q).$$

When the force on the plunger of the press is specified, we obtain from the condition of equilibrium: $\sigma_{zz} = -P(t)$. Taking into account the correlation between stress σ_{zz} and velocity, we obtain an equation for determining the flow velocity of the material

$$\frac{\partial v}{\partial q}=-\frac{1}{\rho}\frac{P}{\frac{4}{3}\mu+\xi}. \tag{2}$$

Substituting (2) into the equation of continuity, we write the expression for determining the density

$$\frac{\partial(\ln\rho)}{\partial t}=\frac{P}{\frac{4}{3}\mu+\xi}.$$

We convert the problem to dimensionless form by introducing the following variables and criteria:

$$\theta=\frac{U}{RT_*^2}(T-T_*),\ \bar{q}=q/q_0,$$

$$\bar{\mu}=\mu/\mu_1(T_*),\ \bar{\xi}=\xi/\mu_1(T_*),$$

$$\bar{v}=v/v_m,\ \tau=\mathrm{Fo}=\frac{\lambda_0}{c\rho_1 q_0^2}t,\ \bar{\alpha}=\frac{2\alpha q_0^2}{\lambda_0 r_0},$$

$$\mathrm{Bi}_{1,2}=\frac{\alpha_{1,2}q_0}{\lambda_0},\ V=\frac{v_m\rho_1 c q_0^2}{\lambda_0 z_0},\ \mu_1(T_*)=\mu_1\exp\left(\frac{U}{RT_*}\right),$$

$$P_1=\frac{c\rho_1 q_0^2 P}{\lambda_0\mu_1(T_*)},\ P_2=\frac{q_0 P}{\mu_1(T_*)v_m}.$$

The statement of the problem in dimensionless form is finally written as follows:

$$\frac{\partial(\ln\rho)}{\partial\tau}=\frac{P_1}{\frac{4}{3}\bar{\mu}+\bar{\xi}}, \tag{3}$$

$$\frac{\partial \bar{v}}{\partial \bar{q}} = \frac{P_2}{\left(\frac{4}{3}\bar{\mu} + \bar{\xi}\right)\rho}, \tag{4}$$

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial}{\partial \bar{q}}\left(\lambda(\rho)\rho\frac{\partial \theta}{\partial \bar{q}}\right) - \frac{\bar{\alpha}}{\rho}(\theta - \theta_0),$$

$$\frac{d\bar{z}_0}{d\tau} = \bar{U}_p V, \quad \sigma_{zz} = \sigma_{\theta\theta} = -\left(-\frac{2}{3}\bar{\mu} + \bar{\xi}\right)P\Big/\left(\frac{4}{3}\bar{\mu} + \bar{\xi}\right); \tag{5}$$

the boundary conditions:

$$-\lambda(\rho)\rho\frac{\partial \theta}{\partial \bar{q}} = \begin{cases} -\mathrm{Bi}_1(\theta - \theta_0), & \bar{q} = 0, \\ \mathrm{Bi}_2(\theta - \theta_0), & \bar{q} = 1, \end{cases} \tag{6}$$

$$\bar{v}|_{\bar{q}=0} = 0,$$

the initial conditions:

$$\rho(\bar{q},\ 0) = \rho_0(\bar{q}), \quad \theta(\bar{q},\ 0) = 0. \tag{7}$$

For solving the equation of heat conduction (5) together with the boundary (6) and initial (7) conditions we use the method of balance [7, 8], the conservative implicit difference schema, and for solving the finite-difference equations we use the method of matching and the iteration method [9, 10]. Equation (3) is solved by the finite difference method with the use of the implicit four-point difference schema, and Eq. (4) is solved either by Euler's method or by some other single-step method. As a result of the numerical solution of the problem we find the distribution of temperature, density, velocity, and stresses in the pressed material at any instant.

Analysis of the Numerical Results. Figure 1 shows the dependences of density on time obtained analytically [4] (curve a) and numerically (b, c), corresponding to different conditions of heat exchange on the boundaries of the region (b to adiabatic conditions, Bi = 0, c to substantial heat exchange with the environment, Bi > 1). Numerical calculations are in good agreement with the analytical solution of the isothermal problem solely under adiabatic conditions. If there is heat exchange between them, there is a considerable discrepancy. An analysis of the numerical calculation showed that with nonisothermal pressing the following qualitatively different regimes of compaction are realized: 1) without compaction, 2) maximal compaction, 3) insufficient compaction. The decisive factor in the realization of a certain regime of pressing are the initial viscosity (at the combustion temperature) and the range of its change within the characteristic temperature interval (from the combustion temperature to the viable temperature). Let us consider each regime separately.

Regime without Compaction. In this case there is no noticeable compaction of the material. Figure 2a (curve 1) shows the characteristic shape of the dependence of density on time for $\mu_1 = 10^9$ Pa·sec. The regime without compaction is realized when the viscosity of the solid base is sufficiently high. Numerical calculations can establish the critical value of μ_* above which this regime is realized. For selected parameters of the problem it was found that μ_* is equal to $5 \cdot 10^8$ Pa·sec (the dashed line in Fig. 2b). If the initial viscosity is higher than the critical one and is a weak function of the temperature (Fig. 2b, curve 1), then $\mu_1(T) > \mu_*$, and the regime without compaction is always realized. Under these condi-

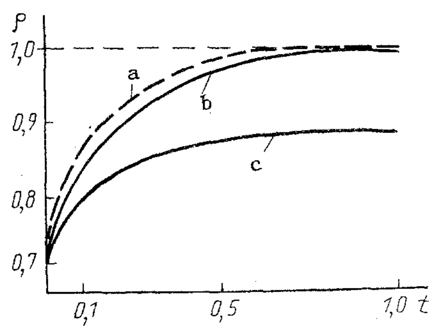

Fig. 1. Dependence of the density of material on time: a) analytical curve; b) curve plotted from the results of numerical calculation on condition that the process proceeds adiabatically; c) numerical curve with specified heat exchange Bi > 1. Parameters: $P = 10^8$ Pa, $\mu_1 = 10^7$ Pa·sec, $q_0 = 0.04$ m. t, sec.

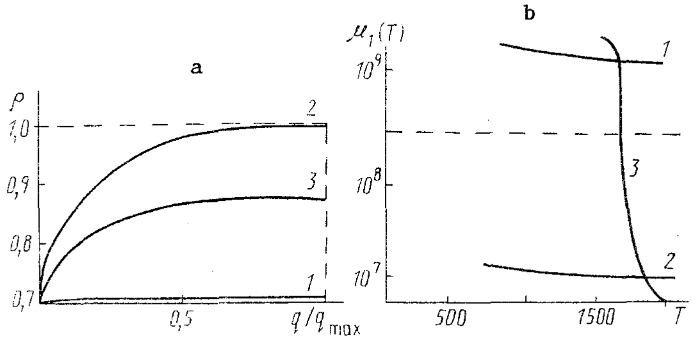

Fig. 2. Different regimes of compacting material: 1) regime without compaction ($\mu_1 = 10^9$ Pa·sec); 2) regime of maximal compaction ($\mu_1 = 10^7$ Pa·sec); 3) regime of insufficient compaction; a) distribution of density ρ along the mass coordinate q; b) dependence of the viscosity of the solid phase μ_1 on the temperature T. Parameters: P = 10^8 Pa, $t_d = 0$, $\Pi_0 = 0.3$. T, K.

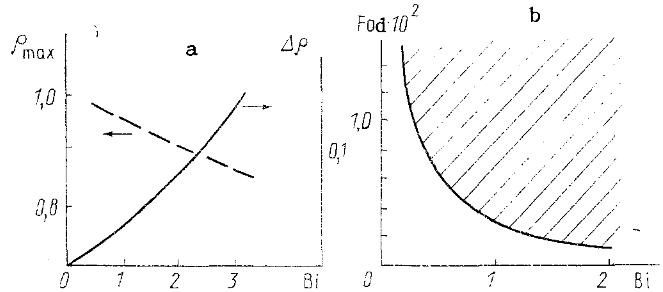

Fig. 3. Effect of the conditions of heat exchange (Bi) on: a) the heterodensity in the material $\Delta\rho = \rho_{max} - \rho_{min}$ and the maximal density; b) the dimensionless delay time Fo_d (the hatched area in which, with the given parameters of the problem, a compact product cannot be obtained). Parameters: P = 10^8 Pa, $\mu_1 = 10^8$ Pa·sec, q_0 = 0.04 m.

tions the initial value of porosity does not have a substantial effect on the maximal value of density in compaction. The decisive factor here is in particular the viscosity of the solid phase or, in other words, the ductility of the grains of the solid carcass. This factor determines the resistance to deformation in compaction, and consequently also the intensity of this process. We note that in this regime the thermal processes and the processes of compaction weakly affect each other, i.e., they proceed practically independently of each other. In that case the earlier thermal model of SHS pressing [11] can be used (without taking the rheodynamic factors into account).

Regime of Maximal Compaction. A characteristic feature of this regime is the change of density from the initial value to 1 (curve 2, Fig. 2a). This regime is realized when the initial viscosity of the solid base during the entire process remains lower than the critical one, i.e., $\mu_1(T) < 5 \cdot 10^8$ Pa·sec, e.g., as shown in Fig. 2b (curve 2), when a change of temperature entails only a small change of viscosity. If the temperature changes only slightly (coming close to the adiabatic case), compaction proceeds quasiisothermally, and the process is well described by the isothermal formulas of compaction [1]. However, when the temperature is uniformly distributed throughout the bulk of the material, model [5] can be used. In that case the processes of compaction do not depend on the temperature but the thermal processes depend on density (on account of the dependence of the thermophysical properties on this variable).

Regime of Insufficient Compaction. In such a regime density increases noticeably at the beginning of the process only, when the material still has retained its ability of plastic

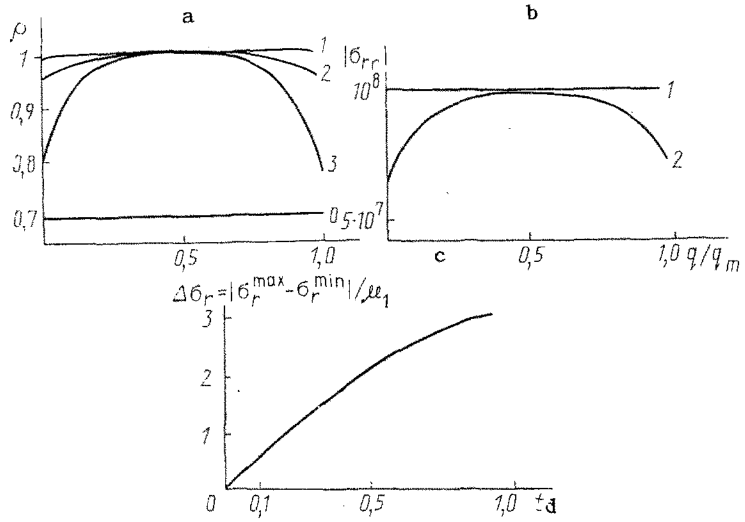

Fig. 4. Distribution over the specimen in dependence on the delay time: a) of density (curves 1, 2, 3 correspond to the delay times 0, 5, and 10 sec); b) of the radial stresses (curve 1 corresponds to the case of compaction without delay of pressure supply, curve 2 corresponds to a delay time of 10 sec); c) of the stress gradient. Parameters of the problem: $\mu_1 = 10^7$ Pa·sec, $P = 10^8$ Pa, $\Delta\rho_0 = 0.01$.

deformation. Later the material "freezes" because it is cooled, it loses its viability, and density does not change any more (curve 3 in Fig. 2a). This regime is realized when the initial value of viscosity of the incompressible base is lower than the critical μ_* but higher in the course of the process than the critical value in consequence of the strong dependence on the temperature (curve 3 in Fig. 2b). Under the conditions of this regime the thermal processes and the processes of compaction proceed correlatively. Thus, variation of parameters of the temperature dependence of the viscosity of the solid base alone ensures a continuous transition from one regime of compaction to another.

The limit state of density and the time the material remains in the plastic state depend on the conditions of heat exchange (Biot number) and on the technological parameters. Figure 3 shows that an increase of the Biot number has a deleterious effect on the final heterodensity of the material (solid line) and on the maximal value of density (dashed line): with Bi ~ 1 the specimen remains uncompacted $\rho_{mx} < 0.9$ and then heterodensity is $\Delta\rho > 0.1$. With Bi → 0 the maximal density of the specimen is close to 1, and $\Delta\rho \to 0$.

Among the technological parameters of SHS pressing we have to lay emphasis on the delay time t_d (the time from the onset of initiation of the chemical reaction to the pressure supply) which is essential for forming the structure of the specimen and for degassing. The existence of such a time boundary separating the stages of synthesis of the material and of compaction under the effect of external pressure makes it possible to examine constantly the process of SHS pressing. In [11] it was shown that t_d has a substantial effect on the existence of a temperature gradient in the material. Instead of the delay time we will henceforth use the dimensionless criterion $Fo_d = at_d/q_0{}^2$. An analysis of the numerical results shows that a condition of the realization of the regime of compaction is some boundary curve Fo_d–Bi below which lies the working region of SHS pressing, and above which there is insufficient compaction (Fig. 3b). For real technological regimes of SHS pressing the Fo_d and Bi numbers have the following ranges of change: $0.02 \le Bi \le 2.5$; $0 \le Fo_d \le 5$. When the delay time within the range of its change becomes longer while Bi is fixed, transition across the boundary curve into the unfavorable region (the dashed region in Fig. 3b) is possible.

The present model made it possible to investigate the effect of the delay time on the distribution of density and of stresses in the material (on account of the statement of the problem the axial stresses σ_{zz} are constant, and the tangential stresses are equal to the radial ones $\sigma_{rr} = \sigma_{\theta\theta}$, henceforth we will therefore confine ourselves to dealing with the radial stresses σ_{rr}). With short delay times ($Fo_d = 0.2 \cdot 10^{-2}$) and uniform initial temperature distribution (T = 2000 K), a uniform state of stress is attained in the material within the characteristic time of compaction (Fig. 4a, curve 1), and the compressive stresses are maximal (Fig. 4b, curve 1), which is a sign of good quality of the finished product. When the delay time is longer, the gradient of radial stresses over the specimen increases in consequence of strong cooling of the material from the end faces (Fig. 4c), an ever increasing part of the material near its end faces remains incompletely compacted (Fig. 4a, b, curves 2, 3), and the maximal density of the material also becomes substantially lower. Thus, the model under consideration makes it possible to calculate the technological regimes of compacting SHS materials and to predict the quality of products from the point of view of the level of thermal gradients as well as of the state of stress of the material and of the density distribution. It is assumed that on its basis the process of SHS pressing can then be optimized.

NOTATION

t) time; r, z) transverse and longitudinal coordinate; T) temperature; r_0, z_0) radius and height of the compact, respectively; ρ_1, μ_1) density and viscosity of the incompressible base of the material, respectively; ρ) relative density of the material; ρ_0, Π_0) initial density and porosity of the compact, respectively; λ_0) thermal conductivity of the material in the uncompacted state; $q_0 = \int_0^{z_0} \rho(z, t) dz$ relative mass of the compact; σ_{rr}, $\sigma_{\theta\theta}$, σ_{zz}) radial, tangential, and axial stresses, respectively; λ, c) thermal conductivity and specific heat of the material, respectively; μ, ξ) shear and bulk viscosity of the material, respectively; T_*) characteristic temperature of the process; α, α_1, α_2) heat transfer coefficients in the transverse direction, at the upper and lower end face of the compact, respectively; v) flow velocity of the material; U_p) velocity of the plunger of the press; P) force on the press; τ) dimensionless time (Fo number); θ) dimensionless temperature; U) activation energy of the process; R) universal gas constant; T_0) ambient temperature; Bi) Biot number; v_m) absolute maximal flow velocity of the material.

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