

MATHEMATICAL MODELING OF RHEOLOGICAL PROPERTIES OF CLAYS AND CLAY ROCKS

M. G. Khramchenkov

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A mathematical model of the rheological properties of water-saturated clays has been considered. The model is built upon the combination of the theory of filtrational consolidation and the theory of stability of lyophobic colloids, which is based on the concept of disjoining pressure as excess pressure compared to the hydraulic one which is due to surface forces and which acts in water films between clay particles. It is shown that the problem of shrinkage of a clay layer in deformation can be reduced to the known problem of N. N. Verigin. An approximate solution of pressing-out of water from the clay layer has been analyzed. The obtained approximate solution necessarily results in the introduction of the concept of an ultimate shear stress for clays. Special features of the model which are of importance for explaining characteristic features of transport processes in clays (the possibility of abnormally high pressures in subconsolidated clays) have been studied. It is shown that the solutions obtained are in good agreement with the experimental results.

Introduction. Traditionally clays are an object of extensive study in mechanics and geomechanics by virtue of those functions which they perform and the presence of specific properties (capability of swelling, plasticity in the moist state, and others) inherent in them. Thus, weakly permeable clay rocks usually play the role of acquicludes for water- or oil-bearing strata, act as a natural buffer in contamination of underground waters, and are the raw material for construction and other branches of industry.

The properties of clays and clay rocks as well as the occurrence of different processes in them depend on a number of factors, which makes mathematical modeling of them a rather complex problem. It is physically obvious that distinguishing features of clays are caused by the presence of clay minerals in their compositions, between whose particles surface forces act [1]. The most developed and productive concept, which refers to the action of surface forces, is the concept of disjoining pressure between colloid particles [2]. In the present work, we give a description of the physico-mechanical properties of clays, which is based on the methods of the theory of filtrational consolidation [3] and the theory of stability of lyophobic colloids (the Derjaguin–Landau–Verwey–Overbeek (DLVO) theory) invoking the concept of disjoining pressure [2].

Mechanics of Clays and Clay Rocks. Clay rocks owe their specific features to the presence of clay minerals in their composition. The latter represent hydrous aluminosilicates of calcium, magnesium, potassium, and sodium and are styled as thin sheet particles (about 50–100 nm in diameter and 1-nm high). Due to isomorphic substitution in the crystal lattice of clay minerals, these particles usually carry an electric charge (negative as a rule) which is compensated by cations absorbed on the surface of particles and capable of complete or partial dissociation in hydration and of formation of a double diffusion layer [1].

Preparatory to theoretical consideration of mechanical properties of clays, we first describe the simplest structure of clay rocks. We assume that they represent a solid porous skeleton (not necessarily bound) whose pores are not completely filled by clay particles [1]. Thus, any process related to deformation of clay rocks can be divided into two stages:

- 1) free porosity (fraction of the volume of pores not occupied by clay particles and their interlayer gaps) is not zero;
- 2) free porosity is zero, i.e., all pores are filled by clay particles and interlayer water films.

We begin with consideration of the first stage. Here we assume that filtration occurs only through a free part of the pores. We write the equation of mass-balance of the liquid and solid phases:

Kazan' State University, Kazan', Russia; email: Maxim.Khramchenkov@ksu.ru. Translated from *Inzhenerno-Fizicheskii Zhurnal*, Vol. 76, No. 3, pp. 159–164, May–June, 2003. Original article submitted September 18, 2002.

$$\frac{\partial (m\rho_f)}{\partial t} + \operatorname{div} (\rho_f m \mathbf{V}_f) + j = 0 ,$$

$$\frac{\partial (m_c \rho_f)}{\partial t} + \operatorname{div} (\rho_f m_c \mathbf{V}_c) - j = 0 ,$$

$$\frac{\partial [(1 - m - m_c) \rho_s]}{\partial t} + \operatorname{div} [\rho_s (1 - m - m_c) \mathbf{V}_s] = 0 .$$

Assuming ρ_f and ρ_s constant and summing up the equations of the system, we obtain the relation

$$\operatorname{div} \mathbf{V}_s + \operatorname{div} [m (\mathbf{V}_f - \mathbf{V}_s)] - \operatorname{div} [m_c (\mathbf{V}_c - \mathbf{V}_s)] = 0 .$$

which, after the redesignation $\operatorname{div} \mathbf{V}_s = \dot{\theta}$, $m(\mathbf{V}_f - \mathbf{V}_s) = \mathbf{q}$ and use of the condition $\mathbf{V}_c = \mathbf{V}_s$ for clay particles (the condition means that the clay particles can move only with the solid skeleton), leads to the equation

$$\dot{\theta} + \operatorname{div} \mathbf{q} = 0 . \quad (1)$$

We now write the conditions of mechanical equilibrium. We assume that outer load G is applied to the clay. Then the load distribution between the medium components results in the equation

$$G_{ij} = (1 - m - m_c) \sigma_{ij}^s - m_c (p + \Pi) \delta_{ij} - m p \delta_{ij} = (1 - m - m_c) (\sigma_{ij}^s + p \delta_{ij}) - m_c \Pi \delta_{ij} - p \delta_{ij} ,$$

which, after the designation $(1 - m - m_c)(\delta_{ij}^s + p \delta_{ij}) = \sigma_{ij}^f$, takes the form

$$G_{ij} = \sigma_{ij}^f - m_c \Pi \delta_{ij} - p \delta_{ij} . \quad (2)$$

Here Π is the disjoining (additional to hydraulic) pressure in water interlayers between clay particles; a physical sense of the introduction of σ_{ij}^f will be disclosed in what follows.

In description of the thermodynamic equilibrium we express free energy of the solid phase in terms of the macroparameters σ^f , m , m_c , θ , and Π . For this sake we write the first and second laws of thermodynamics for the solid phase:

$$dU_s = \delta Q^{(e)} + \delta A^{(i)} , \quad T dS_s = \delta Q^{(e)} + \delta Q' .$$

Under isothermal conditions $\delta A^{(i)} = dU_s - \delta Q^{(e)} = dU_s - T dS_s + \delta Q' = dF_s + \delta Q'$. In the absence of mass forces we have

$$\frac{\delta A^{(i)}}{dt} = \dot{F}_s + \frac{\delta Q'}{dt} = \int_{V_s} \sigma_{ij}^s \frac{\partial u_i}{\partial x_j} dV = \int_{V_s} \frac{\partial \sigma_{ij}^s u_i}{\partial x_i} dV ,$$

where u_i are the components of the vector of displacement of the skeleton particles. In the last relation we transform the volume integral to the surface one:

$$\begin{aligned} \frac{\delta A^{(i)}}{dt} &= \int_{\Sigma_s} \sigma_{ij}^s n_j u_i ds = \int_{S_e^s} i_{ij}^s n_j u_i ds + \int_{S_e^s} (-\sigma + p) u_i n_i ds + \int_{S_e^s} -p u_i n_i ds + \int_{S_{s-w}} -p u_i n_i ds - \int_{S_{s-c}} (p + \Pi) u_i n_i ds = \\ &= \int_{S_e^s} i_{ij}^s n_j u_i ds + \int_{S_e^s} (-\sigma + p) u_i n_i ds - \int_{\Sigma_s} p u_i n_i ds - \int_{S_{s-c}} \Pi u_i n_i ds . \end{aligned}$$

Here $\sigma = -(1/3)\sigma_{ij}^s$ is the pressure in the solid phase. Passing on to the mean over the representative volume, we obtain

$$\frac{\delta A^{(i)}}{dt} = \int_{V_0} \frac{\partial (\sigma_{ij}^f \langle u_i \rangle)}{\partial x_i} dV_0 + (-p) \int_{\Sigma_s} u_i n_i ds + (-\Pi) \int_{S_{s-c}} u_i n_i ds, \quad (3)$$

where $\sigma_{ij}^f = (1 - m - m_c)(\langle i_{ij}^s \rangle - \langle \sigma - p \rangle \delta_{ij})$ is the tensor of effective stresses which corresponds to (2). It is obvious that $\int_{\Sigma_s} u_i n_i ds = \dot{V}_s$ is the rate of change in the volume of the solid phase. Then, from the condition $\rho_s V_s = M_s = \text{const}$

it follows that

$$(-p) \int_{\Sigma_s} u_i n_i ds = V_0 (1 - m - m_c) p \frac{\dot{\rho}_s}{\rho_s}.$$

In the first stage of deformation till complete disappearance of the transportation pores, the water in the interlayers between the clay particles does not perceive effective stresses of the skeleton and is in thermodynamic equilibrium with the water in transportation pores, i.e., it corresponds to the equation $\Pi = 0$. Therefore, in the first stage we have from (3)

$$\frac{1}{V_0} \left(\dot{F}_s + \frac{\delta Q}{dt} \right) = \sigma_{ij}^f e'_{ij} + \frac{(1 - m - m_c)}{\rho_s} \dot{\rho}_s p,$$

where e_{ij} is the tensor of deformation rates. We consider an elastic skeleton, i.e., the case of $\delta Q/dT = 0$. Then from the last equation we obtain $\dot{F}_s = T_{ij} e'_{ij} - \sigma^f \dot{\theta} + (1 - m - m_c) p \dot{\rho}_s / \rho_s$. Here e'_{ij} is the deviator of the tensor of deformation rates. Since the disjoining pressure Π is a function of the thickness of the water interlayer h between clay particles, the condition $\Pi = 0$ is equivalent to the condition $h = \text{const}$. This means that the volume V_c occupied by the clay particles and the interparticle water films is preserved. We write this in the form $m_c V_0 = V_c = \text{const}$. Then, from the last equation we have $\dot{m}_c / m_c = -\dot{V}_0 / V_0 = \theta$, such that

$$m_c = m_c^{(0)} \exp(-\theta). \quad (4)$$

Since $(1 - m - m_c) \rho_s V_0 = \text{const}$,

$$\frac{d [\ln V_0 + \ln \rho_s + \ln (1 - m - m_c)]}{dt} = 0,$$

and with account for (4) we obtain one equation for three variables. In the simplest case, where $\rho_s = \text{const}$, we represent this equation as

$$\frac{1 - m - m_c}{1 - m^{(0)} - m_c^{(0)}} = 1 + \theta. \quad (5)$$

Then for free energy we have the dependence $F_s = F(J_2', \theta, \rho_s)$, where J_2' is the second invariant of the deviator of the tensor of deformations. Thus

$$\dot{F}_s = \frac{\partial F}{\partial J_2'} \varepsilon'_{ij} e'_{ij} + \frac{\partial F}{\partial \theta} \dot{\theta} + \frac{\partial F}{\partial \rho_s} \dot{\rho}_s.$$

Having compared the right-hand sides of the equations for \dot{F}_s , we obtain

$$T_{ij} = 2 \frac{\partial F}{\partial J_2'} \varepsilon'_{ij}, \quad -\sigma^f = \frac{\partial F}{\partial \theta}, \quad p \frac{1-m-m_c}{\rho_s} = \frac{\partial F}{\partial \rho_s}.$$

If we take the specific form of F for an elastic solid skeleton [4]

$$F = \frac{\lambda}{2} \theta^2 + \mu J_2' - \nu \theta \sqrt{J_2'},$$

where λ , μ , and $\nu = \text{const}$, then

$$-\sigma^f = \lambda \theta - \nu \sqrt{J_2'}, \quad T_{ij} = \left(2\mu - \frac{\nu \theta}{\sqrt{J_2'}} \right) \varepsilon'_{ij}. \quad (6)$$

Equations (6) play the role of the rheological relations which allow obtaining of the closed system of equations for filtration consolidation of clays in the first stage.

In the second stage $m = 0$ and it is necessary to specify the law of filtration in this system, since till now we neglected filtration of water between clay particles (in the first stage it was assumed that the Darcy law holds for \mathbf{q}). In this case, for the elementary work of internal surface forces we have

$$\frac{\delta A^{(i)}}{dt} = \int_{S_e^s} i_{ij} n_j \mu_i ds + \int_{S_e^s} (-\sigma + p) u_i n_i ds - \int_{S_e^s} p u_i n_i ds + \int_{S_{s-c}} -(\Pi + p) u_i n_i ds,$$

since there is no free water in the system. Then, passing on to the mean, we obtain the same relation (3), but now we must take into account the contribution of Π to F . The second term on the right-hand side of (3), as previously, gives $(1-m-m_c)p\dot{\rho}_s/\rho_s$. The third term describes pressing-out of water from the porous space completely occupied by clay particles:

$$\frac{\Pi}{V_0} \int_{S_{s-c}} u_i n_i ds = -\frac{\Pi}{V_0} \dot{V}_c = -m_c \Pi \frac{\dot{V}_c}{V_c} = -m_c \Pi \frac{d \ln V_c}{dt} = -\Pi m_c \frac{d \ln (m_c V_0)}{dt} = -\Pi (\dot{m}_c + \dot{\theta} m_c).$$

We use expression (5) for $m = 0$:

$$m_c = \beta - (1-\beta)\theta, \quad \beta = m_c^{(0)} + m^{(0)}, \quad (7)$$

so $\dot{m}_c = -(1-\beta)\dot{\theta}$. Then for the elastic porous medium we have

$$\dot{F} = T_{ij} \dot{\varepsilon}'_{ij} - \left\{ \sigma^f + [m_c - (1-\beta)] \Pi \right\} \dot{\theta} + \frac{1-m_c}{\rho_s} p \dot{\rho}_s$$

and instead of (6) we obtain

$$-\sigma^f - [m_c - (1-\beta)] \Pi = \lambda \theta - \nu \sqrt{J_2'}, \quad T_{ij} = \left(2\mu - \frac{\nu \theta}{\sqrt{J_2'}} \right) \varepsilon'_{ij}. \quad (8)$$

Since the first equation of (8) involves the term containing the disjoining pressure, which in turn depends on the thickness of the interparticle film of water, we must find the form of the function $h(\theta)$, i.e., relate the microparameter h to the macrovariables of the process. On the one hand, we have relation (7) for m_c . On the other hand, $m_c =$

$S_c h/V_0$, $S_c = \text{const}$. Here S_c is the half-area of the surface of clay particles in the volume V_0 . We differentiate the left- and right-hand sides of the latter relation with respect to time:

$$\dot{m}_c = \frac{S_c \dot{h}}{V_0} - \frac{S_c h \dot{V}_0}{V_0^2} = m_c \frac{\dot{h}}{h} - m_c \dot{\theta}.$$

Having integrated this equation we obtain

$$m_c = m_c^{(1)} \frac{h}{h^{(1)}} \exp(-\theta), \quad m_c^{(1)}, \quad h^{(1)} = \text{const},$$

or, with account for (6),

$$h = \frac{h^{(1)}}{m^{(1)}} [\beta - (1 - \beta) \theta] \exp(\theta). \quad (9)$$

The constants $h^{(1)}$ and $m_c^{(1)}$ provide "joining" of the first and second stages. The latter relation becomes physically more transparent if we recall that the shrinkage $\theta < 0$. Thus, the process of clay consolidation in the second stage determines the quantity h and, consequently, the disjoining pressure as a function of shrinkage. In this case, disjoining pressure can make an additional contribution to the hydrostatic pressure depending on the value of the shrinkage. This fact can explain the nature of abnormally high bed pressures in deep-lying, clay-containing reservoirs.

Rheological Properties of Clays and Clay Rocks. We study the rheology of clays by an example of the one-dimensional problem of clay-layer shrinkage under the effect of constant outer load. From (1), (2), (6), and the Darcy law we obtain for the first stage of the process of water pressing-out

$$\sigma^f - p = G, \quad \frac{\partial q}{\partial z} + \dot{\theta} = 0, \quad \sigma^f = \lambda \theta, \quad q = -\frac{k}{\eta} \frac{\partial p}{\partial z}. \quad (10)$$

The system (10) can easily be reduced to the equation $\frac{\partial \theta}{\partial t} = \frac{\lambda}{\eta} \frac{\partial}{\partial z} \left(k \frac{\partial \theta}{\partial z} \right)$ the solution of which requires assignment of the function $k(\theta)$. Usually, for this purpose the known Archi empirical relation is used [5]:

$$k = A \exp((n \ln 10)/0.03), \quad A = \text{const}, \quad (11)$$

where $n = m_c + m$ is the porosity of clays related to shrinkage θ by the relationship

$$n = \beta - \theta(1 - \beta) = \beta_0,$$

which follows from (4) and (5). It is obvious that keeping only the first term of expansion in terms of θ we can write $k = k_0 - \alpha\theta$, $\alpha = \text{const}$. Then, designating $1 - \alpha\theta/k_0 = \varphi$ and allowing for the fact that $\alpha\theta/k_0 \ll 1$, for φ we obtain the equation of heat conduction

$$\frac{\partial \varphi}{\partial t} = \chi \frac{\partial^2 \varphi}{\partial z^2}, \quad \chi = \frac{k}{\eta \lambda}, \quad (12)$$

where the parameter χ can be treated as the effective coefficient of piezoconductivity [6]. It is obvious that, due to the linear relation between φ and θ , the same equation can also be written for shrinkage θ .

If due to the choice of the boundary condition at the open end of the layer, the value of p is such that the shrinkage θ is higher than is admissible in the first stage, a zone is formed where, according to (2), (8), and (9), the first and third equations in (10) must be replaced by more complex ones. However, linearizing the function in front of $\partial\theta/\partial z$, we obtain an equation similar to (12) with the only difference that another coefficient χ is present in it. Thus,

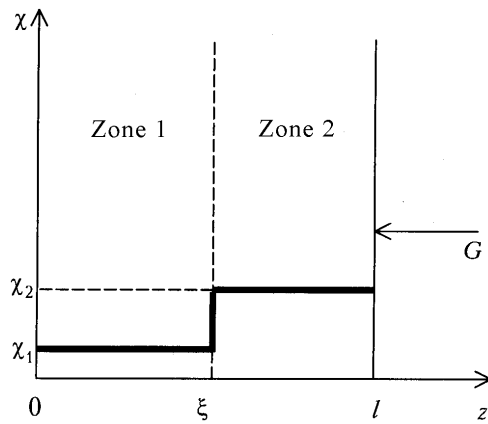


Fig. 1. Formation of two shrinkage zones with different values of piezoconductivity (χ_1 and χ_2) and the movable boundary between them. The bold line indicates the jump of the coefficient of piezoconductivity.

in our case, the problem of water pressing-out from the clay layer was reduced to the known Verigin problem [7]. The process of clay shrinkage and water pressing-out occurs in two zones — "fast" and "slow" — with different coefficients χ_1 and χ_2 . When shrinkage in the "fast" zone reaches some value θ_0 (determined from (4) and (5) at $m = 0$), the coefficient χ_2 of the "fast" zone attains, in a jumpwise manner, a value of χ_1 in the "slow" zone. Thus, the boundary between two zones is movable (see Fig. 1).

We consider this problem in more detail. The process of shrinkage for two zones is described by Eq. (12). The motion of the boundary between the zones is determined from the condition of equality of filtration flow rates. Thus, for the first and second zones we write

$$\begin{aligned} \frac{\partial \theta_1}{\partial t} &= \chi_1 \frac{\partial^2 \theta_1}{\partial z^2}, \quad 0 \leq z < \xi; \\ \frac{\partial \theta_2}{\partial t} &= \chi_2 \frac{\partial^2 \theta_2}{\partial z^2}, \quad \xi < z \leq l, \end{aligned} \quad (13)$$

where θ_1 and θ_2 are shrinkages in the first and second zones, respectively. For $0 < t < \tau$ we have the following boundary conditions:

$$\theta_1(z=0) = \theta_{\max}, \quad \theta_2(z=l) = 0. \quad (14)$$

On the contact boundary of two zones the following conditions hold:

$$\theta_1(\xi) = \theta_2(\xi) = \theta_0, \quad \theta_0 = \text{const}, \quad \chi_1 \frac{\partial \theta_1}{\partial z}(\xi) = \chi_2 \frac{\partial \theta_2}{\partial z}(\xi). \quad (15)$$

Exact solutions of the problem (13)–(15) are unknown; therefore, we can speak only of approximate solutions. The method of integral relations seems to be promising here [8]. Another simplification is the use of a simpler equation $\partial^2 \theta / \partial z^2 = 0$ instead of the second equation of (13), due to the fact that the process in the first ("slow") zone occurs more slowly and during this period a steady-state regime is established in the second zone. In this case, the problem (13)–(15) can easily be solved by the function erf [9].

We refer to a rougher approximation of the process, which, nevertheless, allows one to reveal and study a number of its physically important features. We neglect filtration between clay particles when shrinkage reaches a value θ_0 . Thus, θ_0 is a limiting value of shrinkage. We note that this case is also described by the system (13) with one proviso. Water pressure in the clay does not decrease to zero upon attainment of $\theta = \theta_0$ but becomes equal to

some constant value p_0 , which can be considered as a limiting stress of flow with an opposite sign [10]. The value of θ_0 is determined directly from (4) and (5) and the first equation of (10) takes the form $\lambda\theta_0 - p_0 = G$. It involves two empirical constants, λ and p_0 , and, consequently, can be used for determining one of them by the other, which is known. In such a formulation, (13), with the above-mentioned proviso relative to p_0 , is a classical one-dimensional problem of filtrational consolidation of grounds, and its solutions have been studied adequately [11]. We use the relation for shrinkage of a ground layer of thickness l , which was obtained in [11]:

$$\theta \approx \theta_{\text{fin}} \left(1 - \frac{8}{\pi^2} \exp(-N) \right), \quad N = \frac{\pi\chi}{4l^2 t}.$$

In our case, $\theta_{\text{fin}} = \theta_0$. We differentiate the latter relation with respect to t :

$$\dot{\theta} = \frac{2\chi\theta_0}{\pi l^2} = \frac{2\chi}{\pi l^2 \lambda} (G - G_0), \quad (16)$$

where the notation $G_0 = -p_0$ is introduced; this relation corresponds to the agreement of signs of stress in the mechanics of continua. Equation (16) is the law of flow with a limiting shear stress (the Bingham body), which, as a limiting case, describes the rheology of clays observed in experiments [12]. Thus, following the above-developed model we succeed in deriving a theory of the rheological properties of clays which is in agreement with the experiment.

CONCLUSIONS

Problems using in one form or another the rheological models of clays or clay rocks are of rather frequent occurrence in technology or hydro- and engineering geology. As a rule, one hypothesis or another on the rheology of clays, e.g., the Bingham rheology, are built into these models. It was of importance for us to suggest such a model of the physico-mechanical properties of clays which would not *a priori* use any assumptions on the rheology of the medium but was based on the known facts related to the properties of the minerals constituting clays and clay rocks.

This model has been developed by combining the theory of filtrational consolidation and the Derjaguin–Landau–Verwey–Overbeek theory. Using this model we solved the simplest problem of clay-layer shrinkage under loading and showed that the model allows correct description of the experimentally observed rheology of clays and clay rocks.

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NOTATION

$A^{(i)}$, work of internal surface forces; G , outer load; G_{ij} , tensor of outer load; G_0 , limiting shear stress for clay; e_{ij} , tensor of deformation rates; F , free energy of the body with microdamages; F_s , free energy of the solid phase of the skeleton; i_{ij}^s , deviator of G_{ij}^s ; j , exchange flow between the clay and transportation pores; h , thickness of the interparticle film of water in the clay; k , permeability of clays; l , thickness of the clay layer; M_s , mass of the solid phase; m , free (transportation) porosity; m_c , fraction of film (interlayer) water in the representative volume; n , total porosity of the medium; \mathbf{q} and q , filtration rate and its modulus; p , pressure in the liquid phase; $Q^{(e)}$ and Q' , external and non-compensated heat; T , temperature; t , time; S_c , specific surface of clay particles; S_s , entropy of the solid phase; S_e^s , free surface of solid-phase particles; S_{s-w} , surface of the contact between the skeleton and water; S_{s-c} , surface of the contact between the skeleton and clay film; ds , area element; T_{ij} , deviator of the tensor of effective stresses; U_s , internal energy of the solid phase; u_i , components of the vector of the displacement velocity of skeleton particles; dV , volume element; V_0 , representative volume; V_c and V_s , volume of the clay and the solid phase; \mathbf{V}_f and \mathbf{V}_c , fluid velocity in the transportation pores and the clay; \mathbf{V}_s , velocity of the solid phase; x , coordinate; z , vertical axis; χ , coefficient of piezoconductivity; ε_{ij} , tensor of deformation; δ_{ij} , Kronecker symbol; η , water viscosity; λ , μ , and ν , elastic constants; τ , time of formation of complete shrinkage; Π , disjoining pressure; θ , shrinkage; $\dot{\theta}$, shrinkage rate; ρ_f and ρ_s , density of the fluid and the solid phase; G_{ij}^s , tensor of effective stresses; σ^f , trace of the tensor of effective stresses; σ_{ij}^s , tensor of intrinsic stresses of the skeleton; σ , trace of the tensor of intrinsic stresses of the skeleton; Σ_s , total surface of the

solid phase; ξ , boundary of the contact between the two deformation zones. Indices: c, clay; e, external; f, liquid phase; 0, initial state; s, solid phase; w, water; i, j , projection on the coordinate axes; (i), inner; (e), outer; (1), refers to the parameters of porosity and the thickness of the interlayer film of water in clay on change-over of the first stage of deformation to the second one; dot, partial time-derivative; prime, deviator of the corresponding tensor; fin, final value; max, maximum value; sub- and superscripts c, f, s, e, and 0 have the same meaning.

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