Simulation of heat and moisture transfer in a porous material

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Abstract. The aim of this paper is to present the results of a self-consistent model, which allows describing the evolution of temperature and humidity distributions in a spherical sample of porous clay-like material in drying and cooling processes. Due to the isotropy of the studied material, the solutions obtained are nonlinear radial distributions that change with time. The results are in good agreement with the experimental results obtained in the works of other authors.

1. Introduction
Clay is a fine-grained rock, which, in some cases, contains grains of gold. Today, even after thorough industrial processing, gold pieces with an effective radius of $R_0 < 40 \mu m$ are not extracted from the rock. In other words, half of the gold from gold-bearing clay is thrown away. To effectively extract precious metals from clay, it is necessary to study the porous material itself.

In clay, as in other porous materials, the pores are often filled with moisture. Moisture and its characteristics determine the properties of the clay sample, on which the course of the thermal processes occurring in the sample [1,2], such as drying or cooling [3], will depend.

Industrial drying is one of the most important types of material processing, widely used in industry [4]. If more power is applied to the drying apparatus, the clay sample in it will be significantly deformed [5-9]. Although for most practical applications such a phenomenon turns out to be extremely harmful, it can be used to crush clay and to further extract precious metals from its pores. To study the drying process, it becomes necessary to build a numerical model that describes the heating of the porous rocks.

Thermal and diffusion processes occurring in porous materials under the influence of an external heat source are extremely complex [2]. The drying process is a process of simultaneous mass and energy transfer. This process affects both the areas inside the sample and the interaction of its surface with the environment. Drying is characterized by internal transfer mechanisms: thermal diffusion, capillary flows, moisture diffusion, Knudsen diffusion, as well as evaporation and condensation. Moisture diffusion is the most important transfer process in a sample of porous clay, and Fick's law can be used to describe it. The transfer of heat can be described by the Fourier law.

In [10], the authors of this paper described the processes of heating and freezing of a spherical clay sample using a numerical model; however, that model did not take into account moisture transfer as a result of heat exchange. Moisture transfer was taken into consideration in [11]. The current paper is a logical continuation of work [11]. This paper presents a numerical model that calculates a one-dimensional nonlinear temperature distribution in a spherical clay sample for the processes of drying...
and freezing under various initial and boundary conditions taking into account changes in the moisture distribution.

2. Model

To simplify the calculations some simplifications are made. The clay sample is considered as an isotropic sphere. The evaporation of the liquid occurs only from the surface of the clay sphere. During heating, only the kinetics associated with the solid and liquid phases is considered, and these phases are assumed to be incompressible and have the same temperature. The influences of external forces, as well as the dissipation of heat are neglected.

In this paper, the distribution of heat and moisture in the clay sample is described by the equations:

\[ \rho c \frac{\partial T}{\partial t} = \text{div}[\lambda_{\text{eff}} \cdot \text{grad}T], \]

(1)

\[ \frac{\partial U}{\partial t} = \text{div}[D_{\text{eff}} \cdot \text{grad}U], \]

(2)

where \( \rho \) and \( c \) are density and specific heat of the material, \( \lambda_{\text{eff}} \) and \( D_{\text{eff}} \) are effective thermal conductivity and effective water diffusion coefficients, \( \rho = \rho(U,T), \ c = c(U,T), \ \lambda_{\text{eff}} = \lambda_{\text{eff}}(U,T), \ D_{\text{eff}} = D_{\text{eff}}(U,T) \), \( U \) is local moisture content, \( T \) is local temperature.

Specific heat is determined by the formula:

\[ c = \frac{C_{p,s} + UC_{p,l}}{1 + U}, \]

(3)

where \( C_{p,s} = 1.1 \text{ kJ/kg/K}, \ C_{p,l} = 4.22 \text{ kJ/kg/K} \) are the heat capacities of the solid and liquid phases, respectively.

The density of the sample \( \rho \) is the function of the moisture content \( U \) and expressed through the mass of solid dry sample \( m_0 \), its volume \( V \) and initial moisture content \( U_0 \):

\[ \rho = \frac{m_0 (1 + U)}{V (1 + U_0)}, \]

(4)

where \( m_0 \) is the sample initial mass, \( V \) the sample volume, \( U_0 \) is the sample initial moisture.

Effective thermal conductivity is given by

\[ \lambda_{\text{eff}}(U,T) = (1 - \phi) \lambda_s + \phi \lambda_l, \]

(5)

where \( \phi = \frac{U_p}{\rho_p} / (\rho_l + U_p) \) is the sample porosity, \( \rho_s = 2600 \text{ kg/m}^3 \) is the solid phase density, \( \rho_l = 1000 \text{ kg/m}^3 \) is the liquid phase density, \( \lambda_s = 1.178 \text{ W/m/K} \) is the thermal conductivity coefficient of the solid phase and \( \lambda_l = 0.597 \text{ W/m/K} \) is the thermal conductivity coefficient of the liquid phase.

Effective diffusion coefficient \( D_{\text{eff}} \) is defined in the form [8,12]:

\[ D_{\text{eff}}(U,T) = 5.61 \times 10^{-10} \left( 7.5 + \exp \left( \frac{44U}{1.6 + U} \right) \right) \exp \left( -\frac{510}{T} \right). \]

(6)

Heat flux density \( q_T \) and moisture flux density \( q_U \) are defined as:

\[ q_T = -\lambda_{\text{eff}} \cdot \text{grad}T, \]

(7)

\[ q_U = -D_{\text{eff}} \cdot \text{grad}U. \]

(8)

The heat flux on the surface of a sphere is defined as the sum of the convective term \( q_T \) and the heat term \( q_m \), associated with condensation (evaporation) of moisture on (from) the surface of the sample:

\[ q_T = h_v (T_s - T_m) + h_w q_U, \]

(9)

where \( q_U \) is the evaporation rate from sample surface (kg/m²/s), \( h_v = 2500 \text{ kJ/kg} \) is the latent heat of water evaporation, \( h_w = 40 \text{ W/m}^2/\text{K} \) is the convection heat transfer coefficient, \( T_s \) is the sample surface temperature, and \( T_m \) is the dryer temperature. The water flow to the sample surface equals
First of all, a number of calculations were performed for different temperatures of the drying apparatus, which ranged from 50 °C to 100 °C, a number of calculations were performed for different temperatures of the drying apparatus.

Figure 1 shows the dependencies of temperature (a) and moisture content (b) on time in the center of the spherical sample for $T_0 = 20$ °C, $U_0 = 0.4$, $\varphi_a = 7.2\%$, and for different temperatures of the drying apparatus. Black squares denote the experimental data obtained in the work [8].

$$ q_U = \frac{k_0 M_U}{R_0} \left( \frac{\varphi_s P_{w,sat}(T_s)}{T_s} - \frac{\varphi_m P_{v,sat}(T_m)}{T_m} \right), \quad (10) $$

where $k_0$ is the water vapor transfer coefficient ($k_0 = h_i/\rho c$), $M_u$ is the molecular weight of water, $R_0$ is the universal gas constant, $\varphi_s$ and $\varphi_m$ are the relative humidity of the surface of the clay and the drying apparatus correspondingly, $P_{v,sat}(T)$ is the saturated vapor pressure. In this model $\varphi_s$ defined as [8]:

$$ \varphi_s = \begin{cases} 1, & \text{for } U \geq U_{cr} \\ 1 - (1 - \varphi_m) \frac{U_{cr} - U}{U_{cr} - U_{eq}}, & \text{for } U_{cr} \geq U \geq U_{eq}, \end{cases} \quad (11) $$

where $U_{cr} = 0.135$ kg/kg, $U_{eq} = 0.05$ kg/kg are critical and final equilibrium moisture content in the dried sample [8].

3. Results

In the calculations, a spherically isotropic clay sample was analyzed. Unless otherwise stated, the radius of the sample is $R = 2.7$ cm, and its initial mass is $m_0 = 0.176$ kg. The initial temperature and the initial humidity were set constant throughout the volume $T(r, t_0) = T_0$, $U(r, t_0) = U_0$. All experiments were set in such a way that the clay of the initial temperature $T_0$ and humidity $U_0$ was placed in an environment with a temperature $T_m$, and then the evolution of the moisture and temperature distributions throughout the sample, or at various points, was observed. The relative humidity of the environment $\varphi_s$ was set as a parameter and was equal to $\varphi_a = 7.2\%$ in this paper.

As a result of the calculations, the time dependencies of the radial distributions $T(r, t)$ and $U(r, t)$ are obtained. At each moment in time, the boundary values of these distributions were self-consistently adjusted in accordance with external heat flux $q_T$ and moisture flux $q_u$ at the sample boundary according to equations (9) and (10).

First of all, a numerical experiment simulating the clay drying is conducted. Figure 1 shows the experimentally obtained temperature and moisture content as a function of time, measured at the center of the sample. This graph is a logical continuation of the results obtained in [11]. However, in this case, for relative ambient humidity $\varphi_a = 7.2\%$ and for uniform initial conditions $T_0 = 20$ °C, $U_0 = 0.4$, a number of calculations were performed for different temperatures of the drying apparatus $T_m$, which ranged from 50°C to 100°C.
As in [11], the obtained dependences are divided into four intervals, defined by [6]: preheating period (PP), constant drying rate period (CDRP), transition period (TP), and falling drying rate period (FDRP). The qualitative characteristics of each of these heating periods were described in detail in [11], and therefore only the main points will be considered below.

According to the data obtained, with an increase in the temperature of the external apparatus, several trends can be established. First, with increasing temperature, the lifetime of each of the heating periods decreases. The duration of each of these periods can be described by a simple approximation $t_p \sim T_m^{-B_p}$, where $p$ is period type designation. The $B_p$ coefficient for different periods varies from 0.9 to 1.4. Secondly, as the temperature of the dryer increases, the temperature of the constant drying rate period is also increasing. For example, for $T_m = 50^\circ C$, $T_{cdrp} = 32.73^\circ C$, and for $T_m = 100^\circ C$, $T_{cdrp} = 57.17^\circ C$. The dependence of the temperature of the constant drying rate period on the ambient temperature turned out to be linear, with a coefficient close to 0.5.

Similar trends can be seen on figure 1b, which shows the dependence of moisture content on time. Humidity curves experience a bend at the point where the transition period begins. The higher the temperature of the drying apparatus, the earlier this bend occurs.

The obtained data are in good agreement with the experimental results obtained in the paper [8]. All insignificant differences are explained by the difference in the geometry of the samples: while in this work the object of a study is a spherical isotropic sphere, in [8] the object of the study is an isotropic cylinder.

A reverse experiment was also conducted: cooling a clay sample of different initial temperatures. The time dependencies of temperature and moisture content in the center of the sample are shown in figures 2a and 2b, respectively.

A phenomenon of great interest is the appearance of a negative region in the temperature curve. As indicated in [11], its appearance is associated with heat loss due to evaporation of the liquid from the sample surface and with these losses being greater than heat obtained from the external environment. It is evident from the graph that, despite the different initial temperatures of the sample, the time during which the temperature is cooled first to a constant temperature of 14°C and then reaches the ambient temperature $T_m = 20^\circ C$ is the same for all calculation modes. The same applies to moisture content, where the curves almost completely coincide. This means that the time of the cooling process does not greatly depend on the initial temperature of the sample.

Figure 3 shows the evolutionary temperature and moisture content curves measured at the centers of samples of different radii. Four series of experiments with clay spheres of radii $r_0 = 5, 10, 20$ and 40...
cm were carried out. The data of the temporary abscissa were divided into ratios of the radii of these samples, in other words, the time was normalized. The normalization factor was chosen so that the data would be in a single temporal interval.

From the presented data it can be seen that, despite the convergence of data due to normalization, the match is not perfect. This contrasts sharply the results of [10], where, with normalization of the temporal abscissa to the ratio of the squares of the radii, the temporal dependencies of the temperatures ideally coincided with each other. With increasing sample radius, the following trend is observed: the region of constant temperatures shrinks. When the sample reaches a radius of 20 cm, it disappears altogether. This suggests that the sample has time to dry sufficiently before the temperature front reaches the center of the sphere. Such drying seems natural and would even occur if the temperature of the drying chamber was equal to the room temperature. In other words, for a fairly large sample, the constant drying rate does not exist.

The moisture content also differs qualitatively. The smaller the clay sample the faster it dries. This result seems natural due to the fact that the amount of water in the sample is proportional to the volume, and the rate of evaporation of moisture from its surface is proportional to the surface area of the clay sphere.

4. Conclusions
In this article, the evolution of temperature and moisture distributions inside an isotropic clay ball is investigated. An experiment was conducted to heat the sample for different temperatures of the drying chamber. Temperature dependencies demonstrate the appearance of four heating periods. The results obtained from the simulation of the heating process are in good agreement with the experimental data. It is established that, with an increase in the external temperature, the lifetime of each heating period decreases. This decrease can be approximated by power dependence. With an increase in the temperature of the external environment the value of the temperature of the constant drying rate period increases. The relationship between this temperature and the temperature of the drying apparatus is linear.

An experiment was conducted to cool the sample for different initial sample temperatures. It was determined that the initial temperature of the sample does not affect the time and the qualitative characteristics of the temperature dependence; all evolutionary curves reach the boundary values at the same time.

Figure 3 The dependencies of temperature (a) and moisture content (b) on time for the drying process ($T_m = 60^\circ C$, $T_0 = 20^\circ C$) for clay samples of different sizes. The abscissa axis is normalized to the ratio of the radii of various samples.
The process of heating clay spheres of different radii was simulated. It was determined that, taking into account changes in moisture content, temperature dependences are qualitatively different from each other and there is no normalization factor that would reduce the results to a single curve.

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