Numerical modelling of heat and moisture transfer in a clay-like porous material

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Abstract. A new model for the convective drying of a kaolin spherical sample is presented. The model is based on the self-consistent solution of the heat and the moisture transfer equations with the effective thermal conductivity and water diffusion coefficients for wet porous clay-like medium. The radial distributions of the temperature and the moisture content were calculated for different boundary conditions for heat and moisture fluxes on the surface of the kaolin sample. To test the model, the drying kinetics of the kaolin sample heated up to 60°C and 100°C were calculated. The results show a good agreement with the experimental and numerical data of the other authors. In the process of the sample cooling, the effect of the overcooling to the temperatures lower than the ambient temperature was found.

1. Introduction
Industrial drying is an essential step in manufacturing of many products such as building materials, clay/ceramic products and food [1]. Though the high power density applied to the product can significantly decrease the drying time and operation cost, it can also lead to a strong deformation (shrinkage) of the material, modify its surface properties and even damage the product [2-6]. In many manufacturing processes the cracking of the material is fatal. However, it can be used for disintegration of the fine gold particles from the wet clay material by applying the extreme ambient conditions. To control the drying processes, the drying kinetics model is useful to construct.

The real behavior of the clay materials is very complex and depends strongly on moisture content, temperature and time. The drying phenomenon can be considered as a process of simultaneous energy and mass transfer occurring both inside and outside the material. In common case, the drying is characterized by several internal transport mechanisms, such as moisture diffusion due to concentration gradients, thermo diffusion, Knudsen diffusion, capillary flow, evaporation and condensation. However, moisture diffusivity is the most important mass transport mechanism of matter and a Fick's law for water diffusion can be used. The heat conduction in the porous clay-like material can be considered as a Fourier's law with an effective heat conduction coefficient.

The aim of the paper is to develop a mathematical model describing the drying of kaolin clay. Simulations will predict the time evolutions of the moisture content and the temperature radial distributions during the drying process. The calculations will be made for different drying ambient conditions in order to test the model. The stresses induced by the variation of the temperature and moisture content in space in time will not be considered at this step. A comparison between the numerical results and the results of the other authors will be made and discussed.
2. Model
To simplify the problem, the following assumptions are made in the model. We consider homogeneous and isotropic porous clay-like material. The porous medium of the sample is saturated, and only the solid and liquid phases of the drying kinetics are retained. These phases are both incompressible and present in a local thermodynamic equilibrium (one-temperature approximation). The gravity and all other external forces as well as the conservative inertial effects are neglected. During the drying process, water evaporation occurs only at the surface of the sample. Energy dissipation is also neglected.

To demonstrate the convective drying behavior of the porous clay-like material, the system of equations analogous to Fourier's law for heat conduction, and Fick's law for water diffusion is considered:

\[ \rho c \frac{\partial T}{\partial t} = \text{div}[\lambda_{\text{eff}} \cdot \text{grad} T], \quad (1) \]

\[ \frac{\partial U}{\partial t} = \text{div}[D_{\text{eff}} \cdot \text{grad} U], \quad (2) \]

where \( \rho \) and \( c \) are the material density and specific heat capacity, correspondingly, and \( \lambda_{\text{eff}} \) and \( D_{\text{eff}} \) are the effective heat conduction and water diffusion coefficients, correspondingly. The heat conduction equation (1) and moisture transfer equation (2) are strongly coupled through the dependencies of parameters \( \rho(U,T), c(U,T), \lambda_{\text{eff}}(U,T), D_{\text{eff}}(U,T) \) on variables \( U \) and \( T \). \( U \) is the local moisture content measured in the units of kg/kg, i.e. the mass of water per unit mass of solid fraction of dry sample. \( T \) is the local temperature.

The heat flux density \( F_T \) and the moisture flux density \( F_U \) are:

\[ F_T = -\lambda_{\text{eff}} \cdot \text{grad} T, \quad (3) \]

\[ F_U = -D_{\text{eff}} \cdot \text{grad} U. \quad (4) \]

At the surface of the sample, the heat flux is determined by the convection term \( F_c \) and by the heat flux \( F_\nu \) due to evaporation/condensation of water from/to the sample surface:

\[ F_T = h_c (T_s - T_a) + h_\nu F_U, \quad (5) \]

where \( F_U \) is the rate of evaporation at the surface (kg/m²/s), \( h_c = 2500 \text{ kJ/kg} \) is the latent heat of water evaporation/condensation, \( h_c = 40 \text{ W/m²/K} \) is the convection heat transfer coefficient, \( T_s \) is the sample surface temperature, and \( T_a \) is the ambient drying temperature. The water flux at the exchange surface is expressed as:

\[ F_U = \frac{k_\nu M_\nu}{R_0} \left( \varphi_s \frac{P_{\nu,\text{sat}}(T_s)}{T_s} - \varphi_a \frac{P_{\nu,\text{sat}}(T_a)}{T_a} \right), \quad (6) \]

where \( k_\nu \) is the water vapor transfer coefficient \( (k_\nu = h_c/\rho/c), M_\nu \) is the water molecular weight, \( R_0 \) is the universal gas constant, \( \varphi_s \) and \( \varphi_a \) are the relative air humidity at the surface of the sample and in the ambient drying boundary, correspondingly, \( P_{\nu,\text{sat}}(T) \) is the saturated vapor pressure temperature dependence taken in the form of well-known Buck formula. We assume the following form of the air relative humidity at the sample surface [5]:

\[ \varphi_s = \begin{cases} 1, & \text{for } U \geq U_{eq} \\ 1 - (1 - \varphi_s) \frac{U_{eq} - U}{U_{eq} - U_{eq}} & \text{for } U_{eq} \geq U \geq U_{eq} \end{cases}, \quad (7) \]
where \( U_c \) and \( U_{eq} \) denote the critical and the final equilibrium moisture contents in dried sample. These parameters determined experimentally and were taken from [5], i.e. \( U_c = 0.135 \) kg/kg, \( U_{eq} = 0.05 \) kg/kg.

The common specific heat \( c \) of the wet porous material is expressed through the specific heat of the solid phase (kaolin) \( C_{p,s} = 1.1 \) kJ/kg/K and the liquid phase (water) \( C_{p,l} = 4.22 \) kJ/kg/K:

\[
c = \frac{C_{p,s} + UC_{p,l}}{1 + U}.
\] (8)

The sample density \( \rho \) 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 \( U_0 \):

\[
\rho = \frac{m_0(1 + U)}{V(1 + U_0)}.
\] (9)

The effective heat conduction coefficient \( \lambda_{eff} \) is the function of the porosity of the sample \( \phi = U \rho_s/(\rho_l + U \rho_s) \), where \( \rho_s = 2600 \) kg/m\(^3\) is the solid phase density, and \( \rho_l = 1000 \) kg/m\(^3\) is the liquid phase density, \( \lambda_s = 1.178 \) W/m/K is the solid thermal conductivity, and \( \lambda_l = 0.597 \) W/m/K is the liquid thermal conductivity.

The effective diffusion coefficient \( D_{eff} \) (m\(^2\)/s) is the function of both temperature and moisture content, and is taken in the form [5, 7]:

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

3. Results

To test the model, we took into consideration a kaolin sample having spherical form with radius \( R \). Equations (1, 2) were considered in a spherical system of coordinates, and all parameters depend on radial coordinate \( r \) and time \( t \). Initially \((t = t_0 = 0)\), the temperature and the moisture content were uniformly distributed in the sample medium, i.e. \( T(r, t_0) = T_0 \) and \( U(r, t_0) = U_0 \). Different drying parameters were used as boundary conditions for heat and moisture fluxes in equations (5,6), i.e. the ambient temperature \( T_a \) and the relative humidity of the ambient air \( \varphi_a \). As the result of the numerical solution, the time dependencies of radial distributions \( T(r, t) \) and \( U(r, t) \) were calculated. At any time step \( t \), the boundary parameters \( T(r=R, t) \) and \( U(r=R, t) \) are determined in a self-consistent way by the exchange of heat \( F_T \) and moisture \( F_U \) between the spherical kaolin sample and ambient air.

The results shown on Figures 1 present the typical drying curves of the porous materials. The drying process can be divided on four consequent periods [3]: preheating period (PP), constant drying rate period (CDRP), transition period (TP), and falling drying rate period (FDRP). In the preheating period (part A-B in figures 1(c, d)), the temperature of the material increases from its initial rate period (CDRP), transition period (TP), and falling drying rate period (FDRP). In the preheating period, the total heat flux on the surface of the sample (equation 5) is equal to zero due to the equality of the heat conduction to/from the ambient air and latent heat gain/loss in condensation/evaporation processes. In the CDRP, a film of free water is always available at the evaporating surface. The moisture migrates inside the porous material to the surface by diffusion [7]. The drying rate remains constant as long as the moisture transport rate from the interior of the material to the exchange surface can withstand the evaporation rate from the exchange surface. The evaporation rate in the CDRP is supplied by the capillary flow from the material depth to the evaporation surface in porous clay-like material. The moisture content at the end of the CDRP is called the critical moisture content \( U_{cr} \) (point C). In the transition period (part C-D), the evaporation rate starts to decrease because of the disconnection of the liquid meniscus from the surface and this decreasing trend continues until all the liquid meniscuses are disconnected. Detachment of the last liquid...
meniscus from the surface marks the onset of the FDRP (point D). The internal moisture transport rate specifies the drying rate of the FDRP. During the transition period and the FDRP the temperature of material surpasses the wet bulb temperature and grows up to the drying air temperature \( T_a \) (D-E). Finally, the drying process stops when the equilibrium moisture content \( U_{eq} \) achieved.

Figure 1 presents the drying curves time dependencies for spherical kaolin sample with radius \( R = 2.7 \) cm, initial temperature \( T_0 = 20 \) °C, initial moisture content \( U_0 = 0.4 \) kg/kg, initial mass of the sample \( m_0 = 0.176 \) kg. Two different drying regimes were calculated. In the first regime, the ambient temperature is \( T_{a,1} = 60 \) °C and the ambient relative humidity is \( \phi_{a,1} = 7.2\% \) (figures 1(a) and 1(c)), and in the second regime \( T_{a,2} = 100 \) °C, \( \phi_{a,2} = 4\% \) (figures 1(b) and 1(d)).

In the first case, the preheated period (A-B) takes approximately \( t_{pp} \approx 4500 \) seconds. The sample reaches the wet bulb temperature \( T_{m,1} \approx 38\) °C. The constant drying rate period (B-C) takes place until the moisture on the sample surface reaches the critical value \( U(r=R,t_{cr,1}) = U_{cr} = 0.135 \) kg/kg. Further drying process leads to the decrease of the drying rate and to the increase of the sample temperature. The time necessary for achieving the critical point is approximately equal to \( t_{cr,1} = 18 \) 440 s.

In the second case, the preheated period takes approximately \( t_{pp} \approx 3500 \) s. The sample achieves the wet bulb temperature \( T_{m,2} \approx 54.3\) °C. The critical time is approximately equal to \( t_{cr,2} = 8 \) 890 s. It should be noted, that the corresponding numerical calculations shown on figure 1 were made in order to compare the results with the obtained previously numerical and experimental data [5]. In the paper [5], the data was obtained for the cylindrical kaolin sample with the mass of dry sample \( m_s = 150 \) g, initial moisture content \( U_0 = 0.4 \) kg/kg, and initial sample temperature \( T_0 = 20\) °C. The ambient conditions in the drying processes were taken for two cases \( T_{a,1} = 60\) °C, \( \phi_{a,1} = 7.2\% \), \( T_{a,2} = 100\) °C, \( \phi_{a,2} = 4\% \). Thus, excepting spherical (present paper) and cylindrical [5] geometry of the sample, the parameters of the drying processes were the same. However, the results of the present paper show a good correlation with the results [5], i.e. \( t_{cr,1,k} = 19 \) 200 s, \( T_{m,k} = 37\) °C in the first case of drying conditions, and

![Figure 1](image-url). Time dependencies of the moisture content (a,b) and the temperature (c,d): on the surface of the sample \( r = R \) (solid lines), at the center \( r = 0 \) (dashed lines), mean volume values (dotted lines). (a,c) \( T_{a,1} = 60\) °C, \( \phi_{a,1} = 7.2\% \), (b,d) \( T_{a,2} = 100\) °C, \( \phi_{a,2} = 4\% \). The experimental and calculated data [5] are shown by circles for mean moisture content and by squares for mean temperature.
t_{cr,1,k} = 9,300 \text{ s}, \ T_{m,k} = 52^\circ \text{C} \text{ in the second case. Some inconsistency of the present results and experimental and calculating data [5] can be described by different sample geometries.}

The numerical calculations were also performed for the cooling process of the spherical kaolin sample. The initial temperature of the sample was \( T_0 = 30^\circ \text{C} \), moisture content \( U_0 = 0.15 \text{ kg/kg} \), sample radius \( R = 5 \text{ cm} \). The ambient drying conditions were the following: \( T_a = 20^\circ \text{C} \), \( \varphi_a = 10\% \). The time dependences of the temperature and the moisture content are shown on figure 2a and 2b, correspondingly. Solid lines represent the parameters on the surface of the sample, and the dashed lines represent the parameters in the center of the spherical sample. It is seen that at the very beginning of the cooling process the temperature and the moisture content starts to evaluate at the surface of the sample, while the same characteristics at the center of the sample remain constant for some time. The effective heat conduction coefficient exceeds the effective moisture diffusion coefficient. Hence, the moisture content at the surface of the sample starts to evaluate a little bit later (2000 s) than the temperature of the sample center (500 seconds).

Figure 2c presents the time dependences of the heat flux terms of the equation (5) on the sample surface, i.e. the convection term \( F_c = h_r(T_s - T_a) \), the evaporation/condensation term \( F_u = h_r F_{Us} \), and the total heat flux \( F_T = F_c + F_u \). The positive sign of the fluxes means their positive direction along the radial coordinate \( r \) and, correspondingly, the heat losses by the sample. At the start of the cooling process, the evaporation and the heat conduction have the same positive sigh, i.e. the heat fluxes are outwarded from the sample. The temperature of the sample starts to decrease. At the moment \( t = 800 \text{ s} \), the sample surface temperature reaches the value of the ambient temperature \( T_a = 20^\circ \text{C} \), and the conduction heat flux changes direction towards the sample, and then becomes negative. However, the heat losses due to the evaporation of the water from the sample surface exceed the conduction flux, and the total heat flux is positive. At the time range \( t = 0.5-2 \times 10^4 \text{ s} \), the sample attain the wet bulb temperature \( T_w = 14^\circ \text{C} \) with zero total heat flux on the surface of the sample and a constant drying rate. After that, the temperature of the sample starts to increase till the equilibrium ambient temperature \( T_w = 20^\circ \text{C} \), and the moisture content decreases to its equilibrium value \( U_{eq} = 0.05 \text{ kg/kg} \).
4. Conclusions
A new model for the convective drying of a kaolin spherical sample was developed based on the self-consistent solution of the heat and the moisture transfer equations with the effective thermal conductivity and water diffusion coefficients for wet porous clay-like medium. The radial distributions of the temperature and the moisture content were calculated for different boundary conditions for heat and moisture fluxes on the surface of the kaolin sample. To test the model, the drying kinetics of the kaolin sample heated up to 60°C and 100°C were calculated. The results showed a good agreement with the experimental and numerical data of the other authors.

The process of the sample cooling from 30°C to 20°C was numerically simulated. The spatial and the time evolution of the temperature and the moisture content were calculated. The balance of heat fluxes on the surface of the spherical kaolin samples was analyzed. The effect of the overcooling to the temperature (14°C) lower than the ambient temperature (20°C) was found.

The stresses induced by space and time variations of the temperature and moisture content were not considered in the paper. The presented model was developed as an initial step for future investigations of heat and moisture evolution under extreme ambient conditions implemented for disintegration of fine gold particles from the wet porous clay-like material.

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