Finite elements analysis of mass transfer and mechanical processes in ceramic ware at convective drying

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Abstract. Mathematical models of the coupled moisture diffusion and mechanical processes in ceramic ware at industrial drying are composed. They allow taking into account the impact of the drying regime on the plastic deformation and shrinkage of the articles. The models are validated and applied for numerical investigations of the transient fields of the moisture content, stresses and strains in building bricks in continuous dryers. Ways for their application for improving of the energy efficiency of drying installations are discussed.

1. Introduction
The reduction of energy consumption and subsequent carbon footprint at the industrial systems is an actual problem that provokes many research efforts [1]. The computational modelling and simulation are preferable approaches for analysis of technologies, aggregates and their performance [2]. They allow obtaining detailed information about different multi-physics problems at all stages of the manufacturing. The drying is a widespread technological process in the mining and processing industries. At the same time it is difficult for modelling due to the complex conjugate heat and mass transfer in the dryers and thermo-structural-diffusion processes in the dried materials. The non-uniform shrinkage and plastic deformation of the ceramic mass at the first period of drying can cause defects in the dried body not only during the drying, but also at the next firing [3]. These coupled processes are subject of a number of theoretical and experimental studies. Their prediction and proper organization are particularly important for faultless manufacturing in the ceramic industry. Investigations about the heat, mass transfer and mechanical behaviour in dried samples at laboratory conditions are known from the literature [4, 5 and 6]. But complex studies of coupled thermo-structural- mechanical behaviour in ceramic articles at drying in industrial conditions have not published to now. The investigations, presented in this paper aim developing of an algorithm for modelling and finite element analysis of the coupled mass transfer and mechanical processes in ceramic ware at industrial convective drying, suitable for analysis and improvement of the efficiency of the process.

2. Mathematical modelling and conceptions for numerical simulations

2.1. Kinetics of convective drying
The convective drying of the ceramic material can be examined in three main periods [3]: preheating period, constant drying rate period (CDRP) and falling drying rate period (FDRP). During the preheating period the material with an initial temperature is heated up/down to the wet bulb temperature of the drying media. The change of the moisture content is insignificant and that relatively short period can be examined as a part of the next one.
The CDRP begins at surface temperature of the material, equal to the wet bulb temperature, which remains constant during that period. A film of free water is available at the evaporating surface. The moisture migrates from the inside of the porous material to the surface by diffusion. The drying rate remains constant as long as the moisture transport rate from the interior of the material to the exchanging surface is equal to the evaporation rate. The moisture content at the end of the CDRP is known as critical moisture content \(W_c\). The evaporation rate starts to decrease at that point because of the disconnection of the liquid meniscus from the surface. This decreasing trend continues at FDRP until all liquid meniscuses are disconnected. The internal moisture transport rate specifies the drying rate of the FDRP. The temperature of material increases to the drying media temperature. The drying process stops when the equilibrium moisture content is reached \(W_{eq}\).

Several types of strains are expected to exist during the drying of wet bodies: shrinkage, provoked by the mass transfer, plastic deformation due to the gravity and temperature strains. The shrinkage is one of the most important factors effecting on drying behaviour of highly shrinkable porous media such as clay-like materials. It occurs during CDRP period and stops at the critical moisture content. The non-uniform shrinkage at that process results in stresses that may cause cracking in the dried products or even make them useless. If drying is performed sufficiently slowly, the shrinkage would be closer to uniform and the drying induced stresses are not dangerous for the material. By other hand the increasing of the drying time results in higher embodied energy and lower dryer productivity. For economic reasons the industrial drying processes are usually performed faster - that results in non-uniform shrinkage and subsequent high tensile stresses in the dried bodies.

It is important to choose suitable condition of drying for the specific products to prevent failures of the dried articles and to save energy. The time durations of the CDRP and FDRP are between the most important factors determining the efficiency of drying. They depend on the potential of drying, expressed by the difference between the dry and wet bulb temperatures of the drying media. As smaller is it as longer is the drying time. To prevent failure of the production due to non-uniform shrinkage, the CDRP is maintain at a relatively small drying power and during that period. The boundary conditions of the models below allow taking into account the influence of these fluid flow parameters on the coupled mass transfer and mechanical processes in the dried solid domain.

2.2. Modeling of mass transfer and mechanical processes in the dried bodies
System of equations
The transient fields of the moisture content and subsequent mechanical behaviour of the materials are obtained by coupled numerical solution of diffusion equation (1) and stress-strain relationship (2) for 3-dimensional finite element mesh, approximating the geometry of the ceramic body [7]:

\[
\frac{\partial C}{\partial \tau} = [D_{ef}] \nabla^2 C
\] (1)

where: \(C\) = water concentration, kg m\(^{-3}\); \(D_{ef}\) - effective diffusion coefficient, m\(^2\)s\(^{-1}\); \(\tau\) - time, s.

\[\{\sigma\} = [D]\{\epsilon\}\] (2)

where: \{\sigma\} - stress vector; \{\epsilon\} - elastic strain vector; \([D]\) - elastic stiffness matrix, formed by module of elasticity \(E\) and Poisson ratio \(v\).

In a coupled structural –diffusion analysis the total strain is formed of elastic \(\{\epsilon^{el}\}\) and diffusion \(\{\epsilon^d\}\) parts, respectively:

\[\{\epsilon\} = \{\epsilon^{el}\} + \{\epsilon^d\} = [D]^{-1}\{\sigma\} + \{\beta\} \Delta C\] (3)

where: \{\beta\} = vector of coefficient of diffusion expansion, m\(^3\)kg\(^{-1}\); \(\Delta C\) = concentration change according reference value \(C_{ref}\):

\[\Delta C = C - C_{ref}\] (4)
The modulus of elasticity $E$, Poisson ratio, coefficient of diffusion expansion $\beta$ and $D_{ef}$ can be obtained experimentally and used in the models as function of moisture content in the dried material [7].

**Boundary conditions**

The mass transfer from the boundaries $S$ of the ceramic body to the drying gas can be computed by mass flux, depending on the thermodynamically and fluid flow conditions in the dryer [3 and 8]:

$$D_{ef} \frac{\partial C}{\partial n} |_S = \dot{q}_m$$

(5)

The intensity of drying in CDRP is expressed by:

$$\dot{q}_{ml} = \frac{h_{ml}}{R_w T} (p_s - p_w)$$

(6)

where: $\dot{q}_{ml}$ - mass flux of evaporated water by unit surface, kg m$^{-2}$s$^{-1}$; $h_{ml}$ - mass transfer coefficient in CDRP, m$^{-1}$s; $T$ - temperature of the drying media, K; $R_w$ - specific gas constant for water vapour: $R_w = 462$ J kg$^{-1}$K$^{-1}$; $p_w$ and $p_s$ are partial pressures of unsaturated and saturated water vapor respectively, Pa.

The coefficient $h_{ml}$ depend on the fluid velocity, relative humidity and temperature field in the drier and can be determined by Nusselt number at the mass transfer:

$$Nu_{ml} = \frac{h_{ml} l}{D_{d,m}}$$

(7)

where: $l$ - length of the ceramic body on the drying gas way; $D_{d,g}$ - diffusion coefficient of the wet drying gas, m$^2$s$^{-1}$.

At isobaric process it is function of the temperature of the drying media $t$, °C:

$$D_{d,m} = 22.63.10^{-6} \left( \frac{t + 273}{273} \right)^{1.64}$$

(8)

The Nusselt number is given in the common form in the literature [3]:

$$Nu_{ml} = 2 + A_1 Pr_m^{0.33} Re^{m_1} Gu^{m_1}$$

(9)

where: $A_1$, $m_1$ and $n_1$ depend on Reynolds number (Re). They are known for large limits of Re and can be calibrated on the base of operating conditions in the dryer. Re, Prandtl number at mass transfer and Guhman number, used as non-dimensional drying potential, correspondently are:

$$Re = \frac{wl}{v}; Pr_m = \frac{v}{\nu_{d,m}}; Gu = \frac{T - T_w}{T}$$

(10)

where: $w$ - average velocity, m$s^{-1}$; $v$ - kinematic viscosity of the drying gas, m$^2$s$^{-1}$; $T_w$ - wet bulb temperature, K.

The mass flux, evaporated from ceramic ware at FDRP can be obtained according a hypothesis for linear decreasing of the drying rate [3]:

$$\dot{q}_{ml} = \frac{\dot{q}_{ml}}{C_c - C_{eq}} (C - C_{eq}) = h_{ml} (C - C_{eq})$$

(11)

where: $C_c$ - water concentration at the critical moisture content, kgm$^{-3}$; $C_{eq}$ - equilibrium water concentration, kgm$^{-3}$; $h_{ml}$ - mass transfer coefficient in FDRP, m$^{-1}$s$^{-1}$.

The boundary conditions for the structural analysis include zero normal displacements at the contact surface between the transport and the dried body and the symmetry boundaries (if there exists any). The gravity is taken into account.
Analogy between the heat and mass transfer

The advanced software for numerical simulation [9] allows structural-diffusion analysis at limited opportunities for definitions of boundary conditions and material properties for solution of equations (1) and (2). The modelling of the mass flux \( \dot{q}_m \), mechanical properties and coefficient of mass diffusion as function of the concentration is not possible. An alternative approach is to implement the structural-diffusion simulation using the analogies between the mass and heat transfer and between the diffusion and thermal stresses.

The effective diffusion coefficient in equation (1) can be expressed by:

\[
D_{ef} = \frac{K_{art}}{\rho_d c}
\]

where: \( K_{art} \) = artificial thermal conductivity, Wm\(^{-1}\)K\(^{-1}\); \( \rho \) - density of the dry mass, kdm\(^{-3}\); \( c \) - specific heat capacity, J kg\(^{-1}\)K\(^{-1}\).

The concentration can be referred to the dry mass of the material:

\[
C = u \rho_d = \frac{W}{100} \rho_d
\]

where: \( u \) - moisture content of the wet mass, kg water/kg dry material; \( W \) - moisture content, %.

Then equation (1) is transformed to:

\[
\rho_d c \frac{\partial W}{\partial t} = [K_{art}] \nabla ^2 W
\]

and the boundary conditions (5) for its solution can be expressed by artificial heat flux \( q_{art} \):

\[
\frac{K_{art} \partial W}{100 c \partial n} \bigg|_S = \dot{q}_m \quad \text{or} \quad K_{art} \frac{\partial W}{\partial n} \bigg|_S = 100 c \dot{q}_m = \dot{q}_{art}
\]

If \( W \) is replaced by \( T \) in equations (14) and (15), they are transformed respectively to Fourier equation for heat transfer and the second kind of boundary conditions for its solution, respectively.

Taking into account equations (11) and (15) the mass flux, used as boundary condition to model the mass transfer between the ceramic ware and the dried media can be written in common form:

\[
\dot{q}_{art} = \begin{cases} 
-100c\dot{q}_{ml} = \text{constant (average value) at } W \geq W_c & \text{(CDRP)} \\
100c\dot{q}_{ml} \frac{(W_{eq} - W)}{W_c - W_{eq}} & \text{at } W < W_c & \text{(FDRP)}
\end{cases}
\]

The diffusion strain can be expressed as thermal strain in equation (2):

\[
\varepsilon^d = \beta(C - C_{ref}) \rightarrow \varepsilon^{th} = \alpha(T - T_{ref})
\]

where \( \alpha \) = instantaneous coefficient of thermal expansion, K\(^{-1}\). It is accepted equal to \( \beta \):

\[
\beta = \frac{\Delta l}{l(W_{in} - W_c)}
\]

where \( W_{in} \) is the initial moisture content, %.

### 3. Finite element analysis of structural-diffusion processes in row building bricks in an industrial dryer

The proposed models are used to investigate the structural-diffusion behaviour of building bricks in industrial continuously working dryer. Detail information about the operating conditions in the dryer is not possible due to confidential rules.

The drying gas (air-flue gases mixture with predominant air fraction) and the wet ceramic articles are moved in counter flow through the drying tunnel. The change of the fluid flow temperature, relative humidity and velocity are obtained by in situ measurements, mass and thermal balances. The figures below illustrate the change of the Re number and the drying potential \( \varepsilon \) of the drying media with the time:

\[
\varepsilon = T - T_w
\]
The wet raw mass is a mixture of clay and combustible supplements. Standard geometry samples made by the wet material after the extruder in the plant are dried to different moisture content in a laboratory installation. They are tested at series of experiments to obtain the critical moisture, relative deformations at the shrinkage, modulus of elasticity, Poisson ratio and effective diffusion coefficients as function of the water content [7]. These physical properties variations with the moisture content are used in the numerical analyses below. The change of the compressive and flexure strength (modulus of rupture) of the material with \( W \) are also determined experimentally to be used as criteria for failure.

Three dimensional geometrical model, representing the real shape of a wet article after the forming by the extruder, is created. It is discretised by a finite element mesh in ANSYS Mechanical APDL using elements, suitable for coupled thermal –structural analysis (figures 4 and 5).

Series of numerical solutions are implemented in order to achieve agreement between the numerical results and the real behaviour of the body during the drying process. Final average moisture content, shrinkage mode during the process (measured by retractometers in the plant) and final dimensions are accepted as criteria to be reached at the simulations.

The first numerical simulation was done at the assumption that the time duration of the CDRP is 50\% of the full time duration, corresponding to the maintained small drying potential in the dryer (Figure 1). The exponent of \( Re \) and \( Gu \) in equation (8) were calibrated to obtain the mass transfer
coefficient and mass flux in equation (5) correspondent to the evaporated amount of water per article at the change of the moisture content from the initial to the critical value according to factory data. So obtained mass flux was used in (15) to compute the boundary conditions.

The simulation was implemented at discretised model using elements Solid 226 – hexaeder with intermediate nodes on each side (total 20 nodes). That allows performing the analyses at a relatively coarse mesh (figure 2) with enough nodes to estimate the gradients in the body. The computation procedure was performed at a relatively long CPU time (19 days at workstation with 128 RAM Memory and processor Intel Xeon E5 2603).

Transient 3D fields of the moisture content, stresses and strains are obtained [8]. Validations of the models were implemented comparing the computed and the maintained in the factory final sizes and moisture content at the dried body. The differences between the computed and real final sizes of the deformed body are less than 2 %. That is a proof for the adequacy of the models of mechanical processes. But the computed final average moisture content was three times higher than the real one. That results in difference of 10 % between the computed and the maintained evaporated amount of water.

Figure 5. Finite element mesh at elements Solid 5.

Studies were undertaken in several directions to improve adequacy and the efficiency of the models:

1) Finite element mesh with elements Solid 5 (hexaeders with 8 modes) is used. That allows faster computation procedures due to the lower nodes number in comparison to finite element mesh with Solid 226.

2) Numerical analyses of the pressure and velocity fields of the drying media, surrounding the dried bodies were implemented in order to estimate possibilities for model inadequacy due to the assumption of equal mass flux of the mass exchanging surfaces. Such CFD analyses were done at the beginning, middle and end of the drying process (figures 6 and 7). Maximal difference of 10 % in the local velocities around the mass transferring surfaces and subsequent change of the mass flux of 4 % according to equation (8) were obtained. That gives reasons to continue the investigations with equal mass fluxes for all surfaces, contacting with the drying media.

3) Correction of the mass flux taking into account the reduction of the sizes of the mass exchanging surfaces. That computed mass flux, used in the boundary conditions is increased dividing the initial value by the square of the average relative linear deformation. As results closer average final moisture content to the real one is obtained. The difference between the computed and reached in the factory amount of evaporated water is reduced to 7 %, which is also unsatisfactory.
4) Subsequent increasing of the mass fluxes was done at the assumption that the real time duration of CDRP is shorter than the half of the drying process. Actually the moisture content field is non-uniform and the nodal critical moisture content is achieved at different moments of the drying. After several numerical simulations final average moisture content, enough close to the real one was obtained at a difference between the computed and real amount of evaporated water of 3%. Additional reduction of this difference may be sought through a non-linear dependence of the mass flux of the moisture in equations (11) and (16) at FDRP [3].

Figure 6. Velocity field in the start of the drying process, m s\(^{-1}\) (cross section).

Figure 7. Velocity field in the end of the drying process, m s\(^{-1}\) (cross section).

Figure 8. Moisture content at the beginning of the process, % (symmetry plane and insulated surfaces view).

Results about the investigated fields are shown on the Figures 8-12. The non-uniform moisture fields are obvious from the figures bellow. The domains around the insulated boundaries are dried with a smaller rate. That leads to non-uniform deformations, resulting in stresses. The maximal first principal tensile stresses are several times smaller than the modulus of rupture of the material at the correspondent moisture content. Also the maximal absolute values of the first principal compressive stresses don’t exceed the maximal permissible compressive stress of the material. So defects in the
articles due to non-uniform shrinkage and plastic deformations are not expected. That corresponds to the faultless drying in the factory at the maintained regime.

Figure 9. Moisture content at the final of the process, %.

Figure 10. Moisture content at the moment with the maximal stresses in the body, % (symmetry plane and insulated surfaces view).

Figure 11. First principal stress at the moment with the maximal stresses, Pa (symmetry plane and insulated surfaces view).
4. Conclusions
An algorithm for numerical investigation of the structural-diffusion processes in ceramic ware at drying in industrial conditions is composed, tested on a real object and validated. It will be used for investigation of the possibilities for improvements of the efficiency of the dryer installations by reduction of the time duration of the process. That is possible if the moment local stresses, obtained at the numerical simulations at different drying regimes don’t exceed the strength at the correspondent moisture content, reduced by a safety coefficient.

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