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Improved finite element modeling of heat and mass transfers in single corn kernels during drying

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Abstract: Modeling of agricultural (biological) materials is very often used for describing physical processes. Our Institute at the West Hungarian University is dealing with modeling of heat physical treatments in agricultural (biological) materials. The essential key in order to gain accurate results is to know the driving forces during heat and mass transfers. In case of mass transfer processes the application of moisture gradient as driving force gives false results. Therefore, we use water potential gradients as the driving force. However, this needs exact physical measurements: the water potential curves of the materials have to be determined. The lower section of the water potential curves can be calculated from the sorption isotherms. Determination of water potential above saturation of corn kernel particles (starch, germ and pericarp) is difficult due to its perishable nature as a biological living material. This measurements were carried out at the Institute of Hydrology Slovak Academy of Sciences in Bratislava by using a so called "pressure plate extractor" method adapted from soil science for measurements of pF values6 (soil water potential). For modeling the COMSOL Multiphysics 4.1 software is used for the calculation the coupled heat and mass transfer in corn kernels. This is an improved model of an earlier COSMOS and later FEMLAB application (Kovacs et al., 2008). Modifications were carried out on geometry: extra plant anatomical structure namely the hilar layer was added. The input constants were also refined (specific heats, diffusion coefficients, etc.). The results give more realistic temperature and moisture migration within the grain. The main result is that the moisture content of different particles inside the kernel never equalize (in contrast to the misleading case where the driving force is the moisture gradient). The results were verified in real drying conditions by thermography (by using a FLIR PM675 type thermo-camera) and magnetic resonance imaging (at the BRUKER Microimaging Application Group, Karlsruhe, Germany).

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Keywords: heat and mass transfer, finite element modeling, drying.

1. Introduction

The characteristics of the heat and mass transfers in the bodies are determined first of all by the structure of the material. The living or once lived (e.g. agricultural commodities) materials are anisotropic, inhomogeneous and complex. In biological materials structural and dimension changes happen during environmental change or artificial external effect. These changes result hysteretic type functions (e.g. sorption isotherms). Moreover, most of the time chemical processes are initiated (e.g. denaturation) during unfavorable condition changes; and giving energy to the system causes endothermic or exothermic reactions. All of the above mentioned facts can be basically also true for non-living materials, however in biological materials phenomena appear together. In order to get better acquainted with these processes we have to enhance the mathematical models describing the heat and mass transfer processes first of all physical correctness point-of-views. In the past authors basically dealt with the modeling of heat and mass transfer in cereal grains, and therefore have literature experiences first of all in this area. The simplifications were the followings: (i) the materials were considered to be homogenous and isotropic, therefore density (moisture concentration) gradient was used as the driving force of the mass transfer; (ii) some parameters (first of all the transfer coefficients) were considered to be constants; (iii) complex geometries were simplified to squares or spares. As the result of these simplifications the models could follow only in certain accuracy the integral moisture content changes or the average temperature changes.

Exact physical measurements are needed as input parameters for the models. Knowing the driving potentials (forces) during heat and mass transfers are necessary for an accurate model. Water potential gradients as the driving force are used in contrast with the practice (where moisture gradients were used) for modeling of mass transfer in maize hybrids. For this the water potential curves of the materials are have to be determined. Desorption isotherms were measured on 40 and 50 °C of maize hybrids and their constituents (pericarp, scutellum, endosperm.).

Water potential curves can be either directly calculated from the sorption equations. On the other hand sorption isotherm measurements of agricultural materials have been carried out for decades [3]. Several papers were published for wheat and maize grains' isotherms [4, 5, 6, 7]. Most of the cases different salt solutions were used to set the relative humidity of the measuring chamber and the kernels were set until equilibrium weight. The method is time consuming and the kernels can deteriorate especially over 80% RH [4]. The literature data of the sorption isotherms of maize constituents are in controversy [1, 2]. First of all data of the high moisture content region is differ. Other difficulties are the great number of empirical equation that present in literature [8, 9]. A general equation has not been developed so far. Special measurement technique is required to determine the higher sections of the water sorption isotherms. Direct measurements for water potential were initiated using a „pressure plate extractor" (PPS) developed at the University of Saskatchewan, Canada for measuring soil samples [10]. The PPS consist of a calibrated ceramic plate and a pressurized chamber. This method was adapted from soil science where measurements of pF values (soil water potential) are well known. In this way a water content of the sample is determined in such way that the mass of the sample and the equipment are measured together.

2. Governing Equations

The basic governing differential equation system for the drying processes was given by Luikov [11]. It was simplified by Husain et al. [12] in the following form:

$$\frac{\partial X}{\partial \tau} = \nabla(D\nabla X) \qquad (1)$$

$$\rho\frac{\partial T}{\partial \tau} = \nabla k\nabla T + L\rho\frac{\partial X}{\partial \tau} \qquad (2)$$

where: X is the moisture content d.b. [kg/kg]; D is the diffusion coefficient [m^2/s]; ρ is the density [kg/m^3]; c is specific heat [J/kgK]; T is the temperature [K]; τ is the time [s]; k is the thermal conductivity [W/mK]; L is the latent heat of vaporization of water [J/kg].

The previously mentioned simplifications were realized by other scientist and they try to consider the problem by e.g. taking account the different physical properties of the different constituents [13, 14]. Other way was to give the coefficients as functions instead of constants [15].

The above equation systems proved that inside moisture distribution in e.g. a single maize kernel and the calculated distribution does not agree [16]. The authors try to enhance the model accuracy by taking account the non-permeability of the epithelium layer between the scutellum and germ [17]. The biggest problem with the so-far used modeling is that the model intents to equalize the moisture concentration that is not correct since the moisture content of the constituents are different in equilibrium state (Fig. 1.).

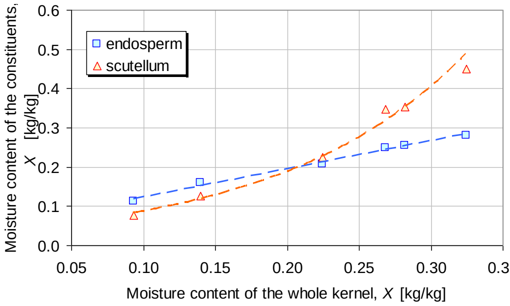


Figure 1. Moisture content of the particles vs. whole maize kernels.

Based on the above mentioned facts it is clear that the using moisture gradient as the driving force is not correct. Luikov [11] took the water potential (mass transfer potential) the same way as the heat transfer potential (temperature). He proposed cellulose as the standard body. The authors give the following equation for mass transfer potential based on the chemical potential of ideal gases and considering that the material is a capillary-porous body:

$$[\Psi]_X = \frac{R_U \cdot T}{m_V} \ln \varphi \quad (3)$$

where: φ is the relative humidity of the air (decimal); R_U is the universal gas constant; m_v is the molecular weight of vapor.

The sorption isotherm equations ψ(X,T) can be determined [6] based on the function (Fig. 2.):

$$X_{equilibrium} = f(T, \varphi) \quad (4)$$

In this case the Eq. 1. can be redrawn [8]:

$$\frac{\partial X}{\partial \Psi}\frac{\partial \Psi}{\partial \tau} = \frac{\partial}{\partial x}\left[D\frac{\partial X}{\partial \Psi}\cdot\frac{\partial \Psi}{\partial x}\right] + \frac{\partial}{\partial y}\left[D\frac{\partial X}{\partial \Psi}\cdot\frac{\partial \Psi}{\partial y}\right] + \frac{\partial}{\partial z}\left[D\frac{\partial X}{\partial \Psi}\cdot\frac{\partial \Psi}{\partial z}\right] \quad (5)$$

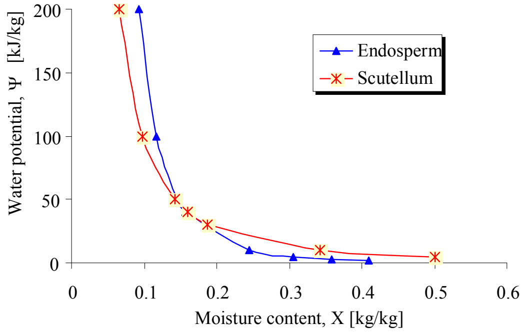


Figure 2. Water potential curves of maize particles as a function of moisture content (d.b).

The above mentioned equation system was solved with the COMSOL Multiphysics software [17]. Fig 3. shows the mesh window of a maize kernel that was based on an actual image of a grain.

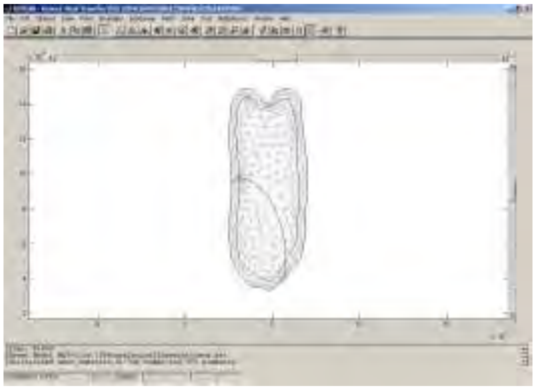


Figure 3. Finite element mesh of a maize kernel

3. Results and Discussion

The results are more accurate because they follow the physical theories. The theory and practical applications of the models can be extended to other processes occurring in living materials (e.g. water movements), not only in drying application of agricultural commodities. The results of this model followed well the measurements of sorption isotherms and nuclear magnetic resonance imaging (MRI), unlike the models based on the moisture gradients as the driving force (Figs. 4 and 5).

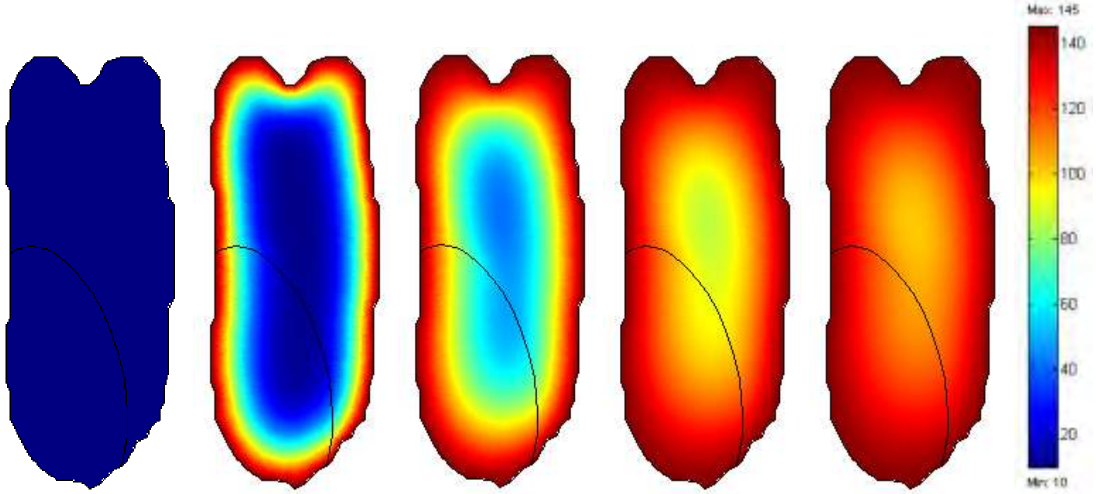
Fig. 4. shows that the water potential moves one equilibrium state ($\Psi_{\text{Before drying}}$) to an other equilibrium state (Ψ_n), where the potentials are not the same but they are homogeny. The inhomogeneous moisture distribution before drying remains inhomogeneous after drying that is seen on Fig. 5.

The evaluation the model - e.g. by magnetic resonance imaging (Fig. 6.) - proved that the mass transfer equation with water potential gradient was correct [18]. The magnetic resonance imaging (MRI) is a non-destructive and non-invasive technique that enables the moisture distribution inside intact kernels to be determined.

4. Conclusion

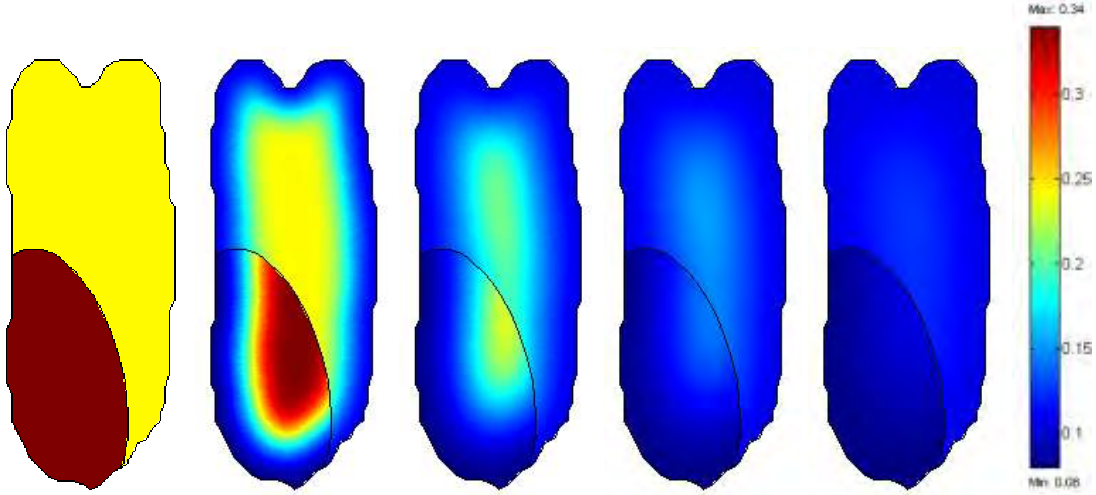
The description of the heat and mass transfer processes is very difficult, because the moisture movement depends on the number of features. In the majority of cases the researchers have to simplify the calculation methods, consequently a limited number of parameters have to be taken into consideration. By calculating the mass transfer the most characteristic method was the use of moisture concentration gradient as a driving force. However, from physical point-of-view in composites and inhomogeneous materials the correct way for modeling of heat and mass transfer is the use of mass transfer potential (G) gradient. This method is difficult to accomplish at the biological materials. The most suitable method to determine the moisture transfer potential is the use of the pF function of the different components [pF (water activity, temperature)]. The partial derivative of the moisture content with respect to the mass transfer potential is the specific isothermal mass capacity, which is according to our experiences constant in the most cases at the biological components. Considering these facts the solving of the partial differential equation systems will be simplified.

Finite element method is applied to solve the heat and mass transfer equations. The COMSOL Multiphysics software is used for the calculation of the composite biological materials (corn constituents, starch, vegetables - carrots).



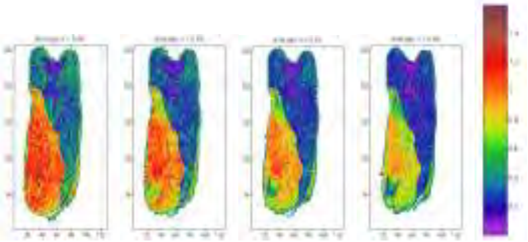
Before drying **60 min** **120 min** **180 min** **240 min of drying**

Figure 4. Moisture potential changes in a cross section of a maize hybrid kernel during (Ψ) drying calculated by COMSOL Multiphysics program (drying temperature: 40 °C).



Before drying **60 min** **120 min** **180 min** **240 min of drying**

Figure 5. Moisture content distribution during drying of a maize kernel calculated from the result of model where water potential was the drying force.



Before drying 30 min 60 min 90 min

Figure 6. Measurements of magnetic resonance imaging (MRI) of actual drying maize kernels for evaluating the finite element modeling of mass transfer

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