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A moving boundary model for food isothermal drying and shrinkage: A shortcut numerical method for estimating the shrinkage factor

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ABSTRACT

We exploit prediction capabilities of the moving-boundary model for food isothermal drying proposed in Adrover et al. (2019). We apply the model to two different sets of literature experimental data resulting from the air-drying process of eggplant cylinders (two-dimensional problem) and potatoes slices (three-dimensional problem). These two food materials, both exhibiting non-ideal shrinkage, are characterized by very different "calibration curves", i.e. different behaviours of volume reduction V/V_0 as a function of the rescaled moisture content X/X_0. The purpose is twofold: to validate the model for different food materials and different sample geometries and to propose a simpler numerical approach for estimating the shrinkage factor, thus bypassing too lengthy analytical calculations and developing a general method that can be easily applied to any sample geometry and any food material characterized by a non-linear calibration curve.

1. Introduction

Drying is a very common process for food preservation and storage and mathematical modeling is a very useful task in order to provide information about process evolution when operating parameters are varied.

A practical obstacle to a simple and effective modeling is represented by food shrinkage. In point of fact, it is very common that water transport in food materials occurs together with deep structural changes and volume reduction (shrinkage) which strongly influence food quality as well as the drying process evolution (Brasiello et al., 2011). The intrinsic connection between volume reduction and water content evolution is supported by a wealth of literature experimental works (Mayor and Sereno, 2004). Therefore, the main goal of a theoretical approach should be to develop a mathematical model able to capture the evolution of both water content and volume reduction, by describing the intrinsic two-way coupling between the two phenomena.

In Aprajeeta et al. (2015) and Hassini et al. (2007), volume reduction is linked to time. However, this is a very simple approach that does not capture the physics of the process since the volume reduction is not described in terms of the water content evolution.

In Brasiello et al. (2013, 2017), Ortiz-Garcìa-Carrasco et al. (2015), López-Méndez et al. (2018), a diffusion coefficient varying with the water content is introduced. However, none of these models can predict sample volume reduction and surface deformation in time.

A very computationally expensive model is proposed by Curcio and Aversa (2014) where the overall volume reduction is derived from the evolution of the stress tensor evolving with the local values of water content.

In Adrover et al. (2019) we proposed a moving-boundary model for the description of food drying with shrinkage, which determines the sample volume reduction and surface deformation on the basis of the spatio-temporal evolution of the water content. This model has the great advantage of capturing all the essential features of the process with a quite simple formulation and can be applied to any sample geometry (discoidal, cylindrical, cubic, parallelepiped). The core of the model is the adoption of a pointwise shrinkage velocity, that, by enforcing the analogy between polymer swelling and food drying (Papanu et al. (1989); Adrover and Nobili (2015)), is equal and opposite in sign to the water diffusive flux, times a shrinkage factor depending on the pointwise water volume fraction. The shrinkage factor can be assumed *a priori* or can be directly derived from experimental "calibration curves" representing the behaviour of the rescaled volume V/V_0 vs the rescaled moisture content X/X_0 (hencefore referred to as moisture ratio). The introduction of the shrinkage factor gives to the model more flexibility in the description of drying processes of different food materials characterized by very different calibration curves.

In Adrover et al. (2019) we adopted the moving boundary model for

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the description of the water content evolution and sample shrinkage and deformation for potato slices (data from Ortiz-Garcìa-Carrasco et al. (2015)) thus proposing a fully analytical approach to determine the optimal shrinkage factor. The analytical approach has been fully developed for 2-d square samples but it can be generalized to other two and three dimensional geometries.

In the present paper, we apply the moving boundary model to two different sets of literature experimental data resulting from the air-drying process of eggplant cylinders (two-dimensional problem, data from Adiletta et al. (2014)) and potatoes slices (parallelepipeds, three-dimensional problem, data from Hassini et al. (2007)). These two food materials, both exhibiting non-ideal shrinkage, are characterized by very different calibration curves. The model provides very good results in terms of prediction of volume reduction, surface deformation, water content time evolution and water content spatial profiles (compared with NRM data) for both food materials analyzed. Beyond the objective of testing the model prediction capabilities for different food materials and different sample geometries, the main goal of the paper is to propose a simple numerical approach, alternative to the analytical method, for estimating the shrinkage factor from experimental calibration curves, thus bypassing too lengthy analytical calculations and developing a general method that can be easily applied to any sample geometry and any food material characterized by ideal or non-ideal shrinkage.

2. Mathematical model

In this section, we preliminary review the model equations derived in Adrover et al. (2019).

The transport equations describing the space-time evolution of the water volume fraction ϕ and of the sample domain are

$$\frac{\partial \phi}{\partial t} = -\nabla\cdot(-D\nabla\phi + \mathbf{v}\phi) = \nabla\cdot(D\nabla\phi\,(1-\alpha\phi)), \quad \mathbf{x}\in V(t) \tag{1}$$

$$-D\nabla\phi\cdot\mathbf{n}|_{\mathbf{x}_b} = h_m K_p(\rho_{air}/\rho_s)\big(\phi|_{\mathbf{x}_b} - \phi_{eq}\big), \quad \mathbf{x}_b\in S(t) \tag{2}$$

$$\frac{d\mathbf{x}_b}{dt} = \mathbf{v}_S = \alpha D\nabla\phi|_{\mathbf{x}_b}, \quad \mathbf{x}_b\in S(t) \tag{3}$$

where $\mathbf{n}$ is the outward-pointing normal unit vector, h_m is a mass transfer coefficient [m/s], ρ_{air} is the air density on dry basis [kg dry air/m^3], ρ_s is the solid (pulp) density [kg pulp/m^3 product] and K_p is the water partition ratio between the gas and the solid phases $Y = K_p c/\rho_s = K_p(\rho_w/\rho_s)\phi$, Y being the air moisture content [kg water/kg dry air] and ρ_w the water density [kg water/m^3]. The subscript eq stands for equilibrium values.The pointwise shrinkage velocity

$$\mathbf{v} = -\alpha(\phi)\mathbf{J} = \alpha(\phi)\,D\nabla\phi \tag{4}$$

is proportional to the water concentration gradient times a proportionality function $\alpha(\phi)$ tuning, at each point of the system, the relationship between water flux $\mathbf{J}$ and volume reduction. The shrinkage velocity $\mathbf{v}_S = \mathbf{v}|_{\mathbf{x}_b}$ evaluated at each point $\mathbf{x}_b$ on the boundary of the physical domain, Eq. (3), controls the boundary shrinkage. The water diffusivity D is assumed constant in space and time.

By introducing the dimensionless space and time variables $\tau = tD/L_r^2$, $\tilde{\mathbf{x}} = \mathbf{x}/L_r$, $\tilde{V} = V/L_r^3$, $\tilde{S} = S/L_r^2$ and the dimensionless differential operators $\tilde{\nabla} = \nabla/L_r$, $\tilde{\nabla}\cdot = \frac{\nabla}{L_r}\cdot$, L_r being a characteristic reference length, the moving boundary model equations for the normalized water volume fraction $\psi = \phi/\phi_0$ attain the form:

$$\frac{\partial \psi}{\partial \tau} = \tilde{\nabla}\cdot(\tilde{\nabla}\psi\,(1-\alpha\phi_0\psi)), \quad \tilde{\mathbf{x}}\in\tilde{V}(\tau) \tag{5}$$

$$-\tilde{\nabla}\psi\cdot\mathbf{n}|_{\tilde{\mathbf{x}}_b} = Bi_m\big(\psi|_{\tilde{\mathbf{x}}_b} - \psi_{eq}\big), \quad \tilde{\mathbf{x}}_b\in\tilde{S}(t) \tag{6}$$

$$\frac{d\tilde{\mathbf{x}}_b}{d\tau} = \alpha\,\phi_0\tilde{\nabla}\psi|_{\tilde{\mathbf{x}}_b}, \quad \tilde{\mathbf{x}}_b\in\tilde{S}(\tau) \tag{7}$$

where Bi_m is the mass transfer Biot number $Bi_m = \frac{h_m L_r}{D}K_p\frac{\rho_{air}}{\rho_s}$. Initial conditions are $\tilde{V}(0) = \tilde{V}_0$, $\tilde{S}(0) = \tilde{S}_0$ and $\psi(\tilde{\mathbf{x}}, 0) = 1$ assuming initial uniform water distribution.

For the 2-d axial symmetric cylindrical problem analyzed in section 3, the initial sample domain is a cylinder $(r, z)\in[0, R_0]\times[-L_z/2, L_z/2]$, with $L_z > R_0$. We choose R_0 as the reference length $L_r = R_0$, and introduce the dimensionless space variables $(\rho, \zeta) = (r/R_0, z/R_0)$ and the dimensionless operators

$$\tilde{\nabla}f = \frac{\partial f}{\partial\rho}\mathbf{e}_\rho + \frac{\partial f}{\partial\zeta}\mathbf{e}_\zeta, \quad \tilde{\nabla}\cdot\mathbf{f} = \frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\,\mathbf{f}_\rho) + \frac{\partial\mathbf{f}_\zeta}{\partial\zeta} \tag{8}$$

The dimensionless initial domain is $(\rho, \zeta)\in[0,1]\times[-a_r/2, a_r/2]$, $a_r = L_z/R_0$ being the cylinder aspect ratio.

For the 3-d Cartesian problem analyzed in section 4, the initial sample domain is a rectangle-shaped slice (parallelepiped) $(x, y, z)\in[-L_x/2, L_x/2]\times[-L_y/2, L_y/2]\times[0, L_z]$. Since $L_z < L_y < L_x$ we choose L_z (initial slice thickness) as the reference length $L_r = L_z$, and introduce the dimensionless space variables $(\tilde{x}, \tilde{y}, \tilde{z}) = (x/L_z, y/L_z, z/L_z)$ and the dimensionless operators

$$\tilde{\nabla}f = \frac{\partial f}{\partial\tilde{x}}\mathbf{e}_{\tilde{x}} + \frac{\partial f}{\partial\tilde{y}}\mathbf{e}_{\tilde{y}} + \frac{\partial f}{\partial\tilde{z}}\mathbf{e}_{\tilde{z}}, \quad \tilde{\nabla}\cdot\mathbf{f} = \frac{\partial\mathbf{f}_{\tilde{\mathbf{x}}}}{\partial\tilde{\mathbf{x}}} + \frac{\partial\mathbf{f}_{\tilde{\mathbf{y}}}}{\partial\tilde{\mathbf{y}}} + \frac{\partial\mathbf{f}_{\tilde{\mathbf{z}}}}{\partial\tilde{\mathbf{z}}} \tag{9}$$

The dimensionless initial domain is $(\tilde{x}, \tilde{y}, \tilde{z})\in[-L_x/(2L_z), L_x/(2L_z)]\times[-L_y/(2L_z), L_y/(2L_z)]\times[0,1]$.

Since drying experiments on parallelepipeds are performed after covering the bottom surface $\tilde{z} = 0$ with a thin aluminum film in order to make the surface waterproof, Eqs. (6) and (7) at $\tilde{z} = 0$ must be replaced with

$$\left.\frac{d\tilde{\mathbf{x}}_b}{d\tau}\cdot\mathbf{n}\right|_{\tilde{z}=0} = 0, \quad \tilde{\nabla}\psi\cdot\mathbf{n}|_{\tilde{z}=0} = 0 \tag{10}$$

thus implying that there is no water flux and no vertical movement at the bottom surface of the parallelepiped.

The 2-d and 3-d moving boundary problems have been numerically solved using finite elements method (FEM) in Comsol Multiphysics 3.5. The convection-diffusion package (conservative form) has been coupled with ALE (Arbitrary Lagrangian Eulerian) moving mesh, allowing re-meshing during the time evolution of the physical domain. Free displacement induced by boundary velocity conditions has been set. Lagrangian quadratic elements have been chosen. The linear solver adopted is UMFPACK, with relative tolerance 10^{-3} and absolute tolerance 10^{-6}. The number of finite elements was $2\times10^5 - 5\times10^5$ for 2-d simulations and $8\times10^5 - 10\times10^5$ for 3-d simulations with a non-uniform mesh. Smaller elements have been located close to the moving boundaries in order to accurately compute concentration gradients controlling the velocity of the moving fronts.

The shrinkage factor $\alpha(\psi)$ can be assumed *a priori* or estimated, for a specific food material, from the experimental calibration curve represented by experimental data for the rescaled sample volume V/V_0 vs the moisture ratio X/X_0 evaluated at the same time instants during the drying process.

In point of fact, from the macroscopic balance equation we obtain

$$\frac{d(X/X_0)}{dt} \simeq \frac{1}{\phi_0\alpha(\psi_b)}\frac{d(V/V_0)}{dt} \to \alpha(\psi_b) \simeq \frac{1}{\phi_0}\frac{d(V/V_0)}{d(X/X_0)} \tag{11}$$

where ψ_b is the normalized water volume fraction evaluated in one or more suitable points, called probe points, lying on the sample surface. In the following, the choice of probe points as points characterized by the maximum displacement (i.e. the maximum shrinkage) is adopted for ψ_b. We will further discuss in more details such a choice for different geometries and dimensions of the sample.Only in the case of $\alpha(\psi) = C =$ constant, Eq. (11) is an exact equation and can be further integrated over time, thus obtaining:

$$1 - V/V_0 = C\,\phi_0\,(1 - X/X_0) = C\,V_{rw}/V_0 \tag{12}$$