MODELING VOLUME CHANGES IN FOOD DRYING AND HYDRATION

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Abstract—Many processes in food technology involve water migration from or into the processed product. Modeling of food water migration knowledge could result speeding up the processes, improving the quality of final products, and reducing energy costs. A mathematical formulation for mass transfer during drying and hydration of a porous solid sphere with volume change was developed in terms of the diffusion equation. The present model also provides an analytical expression for the activation of water diffusivity with moisture content based on a simple relationship between the activation energy for diffusion and sorption energy. The nonlinear diffusion equation was solved numerically, moisture profiles, the kinetics curves for drying and hydration and the moisture concentration dependence of diffusivity coefficient were calculated. Marked differences were observed in the moisture profiles for drying and hydration. The kinetic curves of both processes are strongly dependent on the range of moisture tested. Moisture diffusivity falls drastically at low moisture contents.

Keywords—shrinking, hydration, swelling, drying, moisture diffusivity.

I. INTRODUCTION

Although drying and rewetting cause shrink and swelling of the processed samples respectively, the usual mathematical treatment of the experimental results involves the assumption that the drying process is controlled by internal diffusion in a homogeneous and isotropic solid which does not change its size. Based on these assumptions, the diffusive process is usually described in terms of Fick’s second law of diffusion for which analytical solutions for the three conventional geometries (infinite slab, cylinder and sphere) are available in the literature (Crank, 1979).

One of the first investigations focused to solve the diffusion problem in swelling or shrinking bodies is due to Crank (1979). That author proposed the use of a reference frame fixed to one of the components of the system that remains unchanged, to solve the Fick’s diffusion equation. Such procedure was used by Gekas and Lamberg (1991) to determine the diffusion coefficient in systems with volume change. The differential equation that describes diffusion in an infinite slab, with unidirectional shrinkage, was derived by Viollaz and Suarez (1985) and integrated by means of Von Karman’s method. To account for the effect of shrinkage on food dehydration, a usual procedure is to solve Fick’s second law for diffusion by numerical procedure, assuming that the instantaneous thickness of the solid is proportional to the amount of evaporated water (Simal et al., 1996). An alternative procedure which supposes that the phenomenon of shrinkage is equivalent to a convective flow was employed by Hawlander et al. (1999) to simulate the drying of a solid slab, assuming linear and quadratic variations with moisture content for the shrinkage velocity. More recently, Bialobrzewski (2006) proposed the use of Lagrange-Eulerian method to solve mass transfer equation when the shrinkage phenomenon is present.

The exact evaluation of water diffusivity, and particularly its dependence on moisture concentration, is usually a quite difficult task. Solutions for different functionalities of diffusivity with moisture concentration were reported by Crank (1979). Particularly, for the drying of food materials, Schoeber and Thijssen (1977) developed a method to determine the concentration-dependent diffusion coefficient for systems in that the water diffusivity diminishes when decreasing the moisture concentration.

The purpose of the present work was the following:
1. To derive an analytical expression for moisture migration in a solid that undergoes change of volume during drying or hydration processes.
2. To solve the resulting diffusion equation by numerical procedure, taking into consideration the variability of the diffusion coefficient with moisture content. The present model will be used to simulate moisture migration in a solid sphere that undergoes swelling or shrinkage during the respective process of hydration or drying.

II. METHODS

A. Model Development

Is an experimental fact that food materials usually undergo swelling on water uptake. Swelling occurs as a result of the creation of a transient capillary structure (Stamm and Millet, 1941). Water migration in a porous solid that suffer dimensional changes is regarded as a diffusive process in a binary system formed by a solid B whose mass remains constant and a diffusant A, migrating in liquid phase. Fick’s equation is applied to de-
scribe the movement of moisture in a spherical porous solid. To facilitate the calculation procedure following assumptions are performed:

- Dimensional changes are only due to moisture migration, taking place in the direction of diffusion
- Water migration processes are assumed to occur under isothermic conditions (Liu and Bruin, 1982; Sun and Meunier, 1997; Tolaba et al., 1997; Efremov and Kudra, 2004.)
- Volume additivity for diffusant and dry solid. (Haw-lader et al., 1999; Krokida and Philippopoulos, 2005.)

The diffusion equation for a spherical porous solid is,

\[
\frac{\partial \rho_A}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \rho_A}{\partial r} \right).
\]

In Eq. 1, \( \rho_A \) is the volumetric concentration of diffusant, \( D \) represents the effective diffusivity (function of diffusant concentration), \( r \) is the radial coordinate and \( t \) the time. For a solid that undergoes a volume change it is necessary to evaluate the total derivative of \( \rho_A \) as follows,

\[
\frac{d \rho_A}{dt} = \frac{\partial \rho_A}{\partial t} + \frac{\partial \rho_A}{\partial r} \frac{dr}{dt}.
\]

Introducing Eq. (1) into Eq (2) it results,

\[
\frac{d \rho_A}{dt} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 D \frac{\partial \rho_A}{\partial r} \right) + \frac{\partial \rho_A}{\partial t} \frac{dr}{dt}.
\]

To solve Eq. (3) uniform initial concentration, the following boundary conditions are assumed,

For \( t = 0 \), \( \rho_A = \rho_{A_0} \),

For \( t > 0 \) at \( r = R \), \( \rho_A = \rho_{A_i} \),

For \( t > 0 \) at \( r = 0 \), \( \frac{\partial \rho_A}{\partial r} = 0 \),

where \( R \) is the instantaneous radius of the sphere.

Equations (3) to (6) cannot be solved analytically due to the movement of the solid boundary with respect to the fixed coordinate. To overcome this difficulty, the following transformation is used here (Landau, 1950),

\[
z = \frac{r}{R}
\]

which varies between zero and unity.

If Eq. (3) is now expressed in terms of the variable \( z \) it results,

\[
\frac{d \rho_A}{dt} = \frac{1}{(z \cdot R)^2} \frac{\partial}{\partial z} \left( z^2 D \frac{\partial \rho_A}{\partial z} \right) + \frac{1}{R^2} \frac{\partial \rho_A}{\partial z} \cdot \frac{dR}{dt}.
\]

As Eq. (8) is undetermined at the center of the solid, \( z = 0 \), L'Hopital rule can be applied to obtain,

\[
\frac{\partial \rho_A}{\partial t} = \frac{3}{R^2} \frac{\partial^2 \rho_A}{\partial z^2}.
\]

To solve Eq. (8) together with Eq. (9), it is necessary to have an expression for the movement of the interface, \( dR/dt \).

The instantaneous radius \( R \) can be easily calculated as a function of the solid mean concentration, \( \bar{\rho}_B \), due to the mass of solid is constant, by,

\[
R = R_0 \left( \frac{\rho_{B_0}}{\rho_B} \right)^{1/3}
\]

where \( R_0 \) is the initial radius of the sphere and \( \rho_{B_0} \) the initial solid concentration.

The surface flux of water is:

\[
-D \frac{\partial \rho_A}{\partial r} \bigg|_{r=R} = -\frac{1}{R} \frac{d \rho_A}{dz} \bigg|_{z=1}
\]

which can also be expressed as a function of the instantaneous radius \( R \) as,

\[
\rho_w \frac{dV}{A} \frac{dt}{dt} = \rho_w \frac{dR}{dt} \frac{R}{R_0}
\]

where \( \rho_w \) is the density of water and \( A \) and \( V \) are, respectively, the surface area and volume of the sphere. Then, from Eq. (11) and Eq. (12), it results

\[
\frac{dR}{dt} = -\frac{D}{\rho_w R} \frac{d \rho_A}{dz} \bigg|_{z=1}.
\]

B. Moisture Dependence Diffusivity

The dependence of the diffusivity with moisture content is introduced in the Arrhenius equation using the simple relationship, proposed by de Boer (1968), between the activation energy for the diffusive process, \( E_D \), and the adsorption energy, \( E_A \), as,

\[
E_D = a \cdot E_S.
\]

Based on data available in the literature for \( E_D \) and \( E_S \) for various food products Aguerre et al. (1989) found that \( a = 0.5 \). Introducing this relationship in the Arrhenius equation, it results,

\[
D = D_0 \exp \left( -\frac{E_S}{2RT} \right).
\]

It is convenient to express \( E_S \) in terms of the isosteric heat of sorption in order to have an explicit function between moisture diffusivity and moisture concentration,

\[
E_S = Q_S(u) + \lambda(T).
\]

where \( Q_S(u) \) is the isosteric heat of sorption, generally correlated with the local moisture content in dry basis, \( u \), and \( \lambda(T) \) is the heat of water vaporization at the temperature \( T \) of the process.

The local moisture content, \( u \), and local volumetric concentration, \( \rho_A \), are related by the equation,
\[ u = \frac{\rho_A}{\rho_B} \] (17)

where \( \rho_B \) is the local volumetric concentration of solid.

Aguerre et al. (1986) derived a rather simple analytical expression that correlates the isosteric heat with moisture content, which form is,

\[ Q_S (u) = R_g K_1 K_2 u^{u/u_m} \] (18)

where \( K_1 \) and \( K_2 \) are constants calculated from the desorption isotherms of the product, \( u_m \) is the monolayer moisture content and \( R_g \) the universal gas constant. Introducing Eq. (18) and Eq. (17) into Eq. (16) we finally obtain the desired expression,

\[ D = D_0 \exp \left( -\frac{R_g K_1 K_2 u^{u/u_m} + \lambda (T)}{2R_g T} \right) \] (19)

C. Numerical Solution

Equations (8) and (9) together with the initial and boundary conditions (4, 5, 6) and Eq. (19) that gives the variation of the diffusivity with moisture content, were solved numerically by the three-level implicit method (Lees, 1959).

Once performed the numerical integration for each time interval, the moisture profile in terms of local concentration, \( \rho_A \), was obtained. The mean moisture concentration, \( \bar{\rho}_A \), was then calculated by integration of moisture profile by means of Simpson’s rule. The new mean value of solid concentration, \( \bar{\rho}_B \), was also calculated from the law of volume additively,

\[ \frac{\bar{\rho}_A + \bar{\rho}_B}{\rho_w} = 1 \] (20)

where \( \rho_w \) represents the bone density of the solid. Finally, the instantaneous radius of the sphere was calculated replacing \( \bar{\rho}_B \) from Eq. (20) into Eq. (10).

The input parameters for the simulation are the number of concentric shells into which the sphere was subdivided, the initial moisture concentration at all nodal points, the sphere dimension and the parameters values listed in Table 1.

<table>
<thead>
<tr>
<th>Table 1. Physical properties used for simulations</th>
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<tbody>
<tr>
<td><strong>D_0</strong>: 3.44 × 10^{-4} m² s^{-1}</td>
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<tr>
<td><strong>K_1</strong>: 9.03 K</td>
</tr>
<tr>
<td><strong>K_2</strong>: 0.274</td>
</tr>
<tr>
<td><strong>u_m</strong>: 0.072 kg water kg(^{-1}) dry solid</td>
</tr>
<tr>
<td><strong>\rho_w</strong>: 1530 kg m(^{-3})</td>
</tr>
<tr>
<td><strong>\rho_s</strong>: 1000 kg m(^{-3})</td>
</tr>
<tr>
<td><strong>T</strong>: 60 °C (drying temperature)</td>
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<tr>
<td><strong>\lambda(T)</strong>: 3423.8 + 5.237T + 9.86 × 10^{-2}T^2 + 1.13 × 10^{-4}T^3</td>
</tr>
</tbody>
</table>

† Rovedo, 1994; † Wexler, 1976

D. Results and Discussion

Plots showing moisture profiles evolving with time for drying and hydration are shown, respectively, in Fig. 1 and Fig. 2 in terms of moisture content \((u)\), for a range between 4.0 and 0.1 kg water/kg dry solid.

Moisture profiles were also calculated in terms of local moisture concentration per unit of volume \((\rho_A)\), making use of the following relationship,

\[ \rho_A = \frac{\rho_w \rho_s u}{\rho_w + \rho_s u} \] (21)

These are represented in Fig. 3 and Fig. 4 for the respective processes of drying and hydration for a range of moisture concentration from 137.93 and 864.86 kg water m\(^{-3}\).

Figure 1. Moisture profiles for drying of a sphere of initial moisture content \(u_0=4.0\) kg water per kg dry solid and initial radius \(R_0=3.588\) mm.

Figure 2. Moisture profiles for hydration of a sphere of \(u_0=0.1\) kg water per kg dry solid and \(R_0=1.991\) mm.

Figure 3. Moisture profiles in terms of moisture concentration per unit of volume, vs. radius, \(z\), for drying of a sphere of initial moisture content \(u_0=4.0\) kg water per kg dry solid and \(R_0=3.588\) mm.
It is observed certain differences between moisture profiles calculated in terms of $\rho_A$ and $u$, which are due to the non-linear relationship between both magnitudes as well as moisture and solid concentrations are not uniform distributed within the sphere, i.e., for drying solid concentration is higher at the surface than in the centre of the sphere. On the other hand, independently of the variable used to calculate moisture concentration, the plots also show marked differences in the shape of the moisture profiles for drying and hydration. Moisture profiles for drying looks similar to that of the classical Fickian diffusion, even though they contain something different due to the fact that diffusivity used in the present calculation is not constant but greatly varies with the moisture content.

As it can be seen in Fig. 1 and Fig. 3 moisture content profiles have parabolic shape before flattering at the end of drying. The moisture profiles for hydration in Fig. 2 and Fig. 4 show that unlike the concave profiles in the case of Fickian analytical solution, convex moisture profiles are formed in the region near to the surface. It is also observed that moisture content evolution for small times conducts to a kind of frontier that moves into the sphere at an almost constant rate. This can be seen by observing the position where the curves intercept the horizontal axis markers. For longer times, the moisture content is almost uniform across the solid. The rapid increase of moisture concentration near the interface can be attributed to the variation of the diffusivity with moisture content. The increase of the diffusivity with moisture content tends to accelerate the rate of water absorption, with the sudden increase in the moisture content near the surface, giving rise to the appearance of the mentioned frontier. Moisture profiles similar to that shown in Fig. 2 and Fig. 4 were observed by Stapley et al. (1998) by means of NMR techniques during water adsorption of wheat grains.

In Figs. 5 and 6 are represented in semilogarithmic coordinates the kinetics curves for drying and hydration, respectively, in terms of the dimensionless mean moisture content $u^* = \frac{(u_i - u_f)}{(u_i - u)}$ vs. time for different ranges of moisture content, where $u_i$ and $u_f$ are the initial and equilibrium moisture content, and $d^* = \frac{\rho_A}{\rho_B}$.

The curves show, in general, a nonlinear shape which is usually attributed to a variable moisture diffusivity. Such as can be seen in Figs. 5 and 6, the curves show a slight change of curvature during the first stages of the process (particularly observable in the hydration curves). Another point to be mentioned is the influence of the range of moisture contents on the kinetic curves of both processes. It can be observed in Fig. 5 that a solid containing an initial moisture content of 1.0 kg water/kg dry solid, dries slower than another with an initial moisture of 4.0 kg water/kg dry solid. This fact has practical consequences and would contribute, at least in part, to explain the differences in the diffusivity values found in the literature for a given food product.

As it is usual in food dehydration, the slope method derived from the series solution to the Fickian equation provides a simple means to obtain the diffusivity coefficient. However, marked differences in the diffusivity values must be expected if the slope method is not applied to samples with similar initial moisture values.

According to the results shown in Fig. 5, samples with different initial moisture content will present different drying curves and therefore different diffusivity values.
III. CONCLUSIONS

A mathematical model describing mass transfer process in a solid sphere that undergoes volume change is proposed and used to simulate the characteristics of drying and hydration in solid foods.

To account for the effect of shrinkage, a simple mathematical procedure was used that transforms the problem of diffusion with moving boundaries into one with fixed domain of integration. The resulting diffusion equation was integrated numerically together with an analytical expression of the variation of diffusion equation with moisture content.

Drying and hydration processes were simulated and moisture profiles and mean moisture contents variation with time were calculated for a moisture range between 4.0 and 0.1 kg water/kg dry matter.

It was found that the shape of moisture profiles depends on the variable adopted to express moisture concentration. Marked differences exist between moisture profiles when they are represented in terms of moisture concentration by unit volume and dry basis moisture content.

It was also observed that the initial moisture content has a marked effect on the drying and hydration characteristics of the solid. This fact is of practical importance in drying process, where the slope of drying curve for drying times long enough is used to estimate the diffusion coefficient of the sample.

ACKNOWLEDGMENTS

The authors acknowledge the financial support of Agencia Nacional de Promoción Científica y Tecnológica, Universidad de Buenos Aires, Universidad Nacional de Lujan and CONICET.

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Received: October 22, 2007.
Accepted: February 12, 2008.
Recommended by Subject Editor: Walter Ambrosini