Modelling of Drying Kinetics During Non–isothermal Convective Drying of Passion Fruit Seeds

Henry VAQUIRO1†, Óscar RODRÍGUEZ2, Susana SIMAL2, José F. SOLANILLA–DUQUE1, Javier TELIS–ROMERO3

1Facultad de Ingeniería Agronómica, Universidad del Tolima, Barrio Santa Helena, A.A. 546, Ibagüé, Tolima, Colombia.
2Departamento de Química, Universidad de las Islas Baleares, Ctra. Valldemossa km 7.5, 07122 Palma de Mallorca, Spain
3Departamento de Engenharia e Tecnologia de Alimentos, Universidade Estadual Paulista, A.A 136, São José do Rio Preto, São Paulo, 15054–000, Brazil

A model to identify the effective diffusivity and to predict the drying kinetics during non–isothermal convective drying of yellow passion fruit (Passiflora edulis Sims f. flavicarpa Degener) seeds was formulated and validated. The governing equations for coupled mass and heat transfer phenomena were expressed in a generalized coordinate system in order to obtain a one-dimensional model suitable for the non–regular geometry of the seeds. Solid shrinkage, moisture and temperature–dependent transport properties, convection heat and mass transfer at the seed surface and symmetrical distribution of moisture content and temperature inside the material were considered. To identify the moisture effective diffusivity, model estimations were fitted to data from drying experiments carried out at air temperatures of 40, 50, and 60 °C and at air velocities of 0.6 and 1.4 m·s−1. The air velocity promoted a lower effect than the air temperature on drying rate, suggesting the internal resistance to mass transfer controlled the water diffusion. The proposed model could contribute to understand the diffusion mechanisms in the material, offering an alternative approach to study the convective drying of non–regular particles due to it requires a simpler solving process and a shorter calculation time than some multidimensional approaches.

Keywords: Mass and heat transport, shrinkage, generalized coordinates, effective diffusivity

1. Introduction

The yellow passion fruit (Passiflora edulis Sims f. flavicarpa Degener) is an important raw material for juice production in Brazil due to its higher yield in comparison with other varieties [1].

The juice processing of yellow passion fruit at industrial scale generates a large quantity of by–products that can lead up to 70% of the initial weight of the fresh fruits [2]. About 34% of these by–products correspond to the seeds, which are used as source of oil, fiber and protein [3–5].

As other agricultural products, passion fruit seeds need to be dried to achieve proper moisture levels for a safe storage and prior to oil and protein extraction. Drying models based on mass and heat transport mechanisms would contribute to understand the physical behavior of this by–product as well as to design and optimize drying operation or equipment used [6].

The transformation between coordinate systems have been used as a technique to formulate one–dimensional models which are less complex and time consuming than multi–dimensional ones [7,8]. However, the cited studies are only suitable for spheroid geometries and do not consider the coupled mass and heat transfer mechanisms, the diffusivity in terms of local moisture and temperature and the solid shrinkage.

The irregular geometry of the passion fruit seeds and the shrinkage they exhibit during drying may make necessary to take into account some considerations in the formulation of drying models based on physical principles. In this work, a one–dimensional approach was proposed for modelling the coupled mass and heat transport during the convective drying of yellow passion fruit seeds. The model was used to determine the effective diffusivity of the material, as well as to simulate the drying kinetics and moisture profiles.
2. Materials and methods

2.1 Sample preparation

Seeds of yellow passion fruits (P. edulis Sims f. flavicarpa Degener) were separated from the pulp, washed and stored at 17°C for 24 h prior to drying experiments.

2.2 Drying experiments

Samples (around 500 g of seeds) were dried in a convective tray dryer at controlled conditions of both air temperature and velocity. The experiments were carried out in duplicate at air temperatures of 40, 50, and 60°C at air velocities of 0.6 and 1.4 m·s⁻¹. For each sample, weight was measured every 2 min up to a constant weight was reached. Initial moisture content of the samples was determined according to AOAC official method 934.06 [9].

2.3 Mathematical model

Considering that the process is not isothermal, the material is homogeneous and isotropic, the transport properties are not constant, and the main internal transport mechanisms are liquid and thermal diffusion, mass and heat governing equations in Cartesian coordinates can be written as Eqs. (1) and (2).

\[
\frac{\partial W}{\partial t} = \frac{\partial}{\partial x} \left( D \frac{\partial W}{\partial x} \right) + \frac{\partial}{\partial y} \left( D \frac{\partial W}{\partial y} \right) + \frac{\partial}{\partial z} \left( D \frac{\partial W}{\partial z} \right) \tag{1}
\]

\[
\frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( \rho c_p \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho c_p \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( \rho c_p \frac{\partial T}{\partial z} \right) \tag{2}
\]

With the aim to solve the governing equations in an appropriately geometry for passion fruit seeds, a transformation from the Cartesian coordinate system \((x, y, z)\) was carried by using conversion functions (Eqs. 3–5) of a deformed–spherical coordinate system \((r, \theta, \phi)\) [10].

\[
x = (1 - \delta_x z) \delta_x r \sin(\theta) \cos(\phi) \tag{3}
\]

\[
y = \delta_x r \sin(\theta) \sin(\phi) \tag{4}
\]

\[
z = r \cos(\theta) \tag{5}
\]

The governing equations in the new coordinate system (Eqs. 6–7) in terms of the scale factors \((\gamma_1, \gamma_2, \gamma_3)\) (Eqs. 8–10) and the Jacobian determinant \((J)\) (Eq. 11) were analytically calculated by the symbolic computation tools of Matlab® R2013b (The MathWorks Inc., Natick, MA, USA).

\[
\frac{\partial W}{\partial t} = J \left[ \frac{\partial}{\partial r} \left( \gamma_1 \frac{\partial W}{\partial r} \right), \frac{\partial}{\partial \theta} \left( \gamma_2 \frac{\partial W}{\partial \theta} \right), \frac{\partial}{\partial \phi} \left( \gamma_3 \frac{\partial W}{\partial \phi} \right) \right] \tag{6}
\]

\[
\frac{\partial T}{\partial t} = J \left[ \frac{\partial}{\partial r} \left( \frac{\gamma_1 c_p}{\rho} \frac{\partial T}{\partial r} \right), \frac{\partial}{\partial \theta} \left( \frac{\gamma_2 c_p}{\rho} \frac{\partial T}{\partial \theta} \right), \frac{\partial}{\partial \phi} \left( \frac{\gamma_3 c_p}{\rho} \frac{\partial T}{\partial \phi} \right) \right] \tag{7}
\]

As drying–air properties are considered uniform on the seed surface, both moisture and temperature profiles inside the seed were assumed to be symmetric around the \(r\)-axis. Thus, the governing equations (6–7) can be simplified to one dimensional expressions (Eqs. 12–13), by dropping the derivatives of moisture and temperature with respect to \(\theta\) and \(\phi\), and by appropriately selecting \(\theta = \pi/2\) and \(\phi = 0\) [6].

\[
\frac{\partial W}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r^2 \frac{\partial W}{\partial r} \right) \tag{12}
\]

\[
\frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r^2 \frac{\partial T}{\partial r} \right) \tag{13}
\]

The moisture effective diffusivity \((D)\) was calculated in terms of both local temperature and local moisture content according to Eq. (14) [11].

\[
D = \alpha_1 \exp \left[ \frac{\alpha_2}{\gamma(T + 273.15)} + \alpha_3 \left( \frac{W}{W_0} \right) \right] \tag{14}
\]

To solve the governing equation, as initial and boundary conditions the moisture and temperature distributions inside the solid were considered uniform at the beginning (Eq. 15), the moisture and temperature gradients at the symmetry point were assumed zero (Eq. 16), and the mass and heat external resistances were considered not negligible [12] (Eqs. 17–18).

\[
W|_{t=0} = W_a; \quad T|_{t=0} = T_0 \tag{15}
\]

\[
\frac{\partial W}{\partial r}|_{r=a} = 0; \quad \frac{\partial T}{\partial r}|_{r=a} = 0 \tag{16}
\]

\[
-\frac{\rho \alpha D W}{\partial r}_{r=a} = h_a \left( \frac{Y_r}{Y_v} - \frac{Y_u}{Y_v} \right) \tag{17}
\]

\[
-k \frac{\partial T}{\partial r}|_{r=a} = h(T|_{r=a} - T_0) + D \frac{\partial W}{\partial r}|_{r=a} \tag{18}
\]

According to Ferreira de Souza et al. [13], the volume of passion fruit seeds significantly reduced during the dry-
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The formulation of the mathematical model was completed using relationships to estimate the thermal properties \( (k, c, \rho) \), the equilibrium moisture content \( (W_e) \) and the sorption isosteric heat \( (Q) \) of yellow passion fruit seeds [13].

The mass \( (h_m) \) and heat \( (h) \) transfer coefficients for forced convection were estimated by using empirical relationships for spheres immersed in fluids [14] and assuming the characteristic length as the square root of the seed surface area.

The average moisture content for each time was calculated by integrating the local moisture content over the volume and dividing by the volume of the seed (Eq. 20).

\[
\bar{W} = \frac{3}{4\pi\delta_0 R^3} \int_0^{2\pi} \int_0^{\pi/2} \int_0^{\pi/2} W J d\phi d\theta dr \tag{20}
\]

2.4 Identification and validation of model parameters

Experimental drying curves were used for the identification of effective diffusivity parameters \( (\alpha_1, \alpha_2, \alpha_3) \) by minimizing the mean relative error (MRE) between experimental and estimated data. The statistical significance of the estimated parameters was evaluated through their 95% confidence intervals (CI).

The goodness of model fit was quantified by the determination coefficient \( (R^2) \) and the model adequacy was assessed by a residual analysis.

The algorithm used for identification procedure were implemented in Matlab® and included the functions \texttt{pdepe} and \texttt{fminsearch} for the numerical solving of the partial differential equation system, and for the nonlinear regression, respectively.

3. Results and discussion

Regarding the drying curves of passion fruits seeds at both air velocities; an important increment of water loss with the increase of the temperature can be observed (Fig. 1). However, the drying curves showed slight differences between 0.6 m·s\(^{-1}\) (Fig. 1a) and 1.4 m·s\(^{-1}\) (Fig. 1b), being indicative of a water diffusion mainly controlled by the internal resistance to mass transfer.

The identified values for the parameters in Eq. (14) were 2.496 m\(^2\)·s\(^{-1}\) (CI: -1.227 to 6.219), -58.86 kJ·mol\(^{-1}\) (CI: -54.83 to -62.89) and -2.540 (CI: -3.565 to -1.515) for \( \alpha_1, \alpha_2 \) and \( \alpha_3 \), respectively.

Considering the identified parameters, satisfactory simulations of the drying curves were obtained (Fig. 1) in terms of both MRE and \( R^2 \). Thus, the model could represent 98.8% of the variation of all experimental data with estimates deviated on average 14.7% from the real values. However, confidence intervals showed the pre-exponential factor \( (\alpha_1) \) did not was significant, thereby it suggests that other functions could be tested for the moisture effective diffusivity.

The difference between the experimental and estimated average moisture contents (residuals) versus the experimental ones are shown in Fig. 2. As it can be seen the residuals appeared scattered randomly around zero with absolute values less than 0.053 kg·kg\(^{-1}\) (d.b.), 84.1%...
of which were below 0.026 kg·kg\(^{-1}\) (d.b.). Thus, corroborating the suitability of the proposed model to accurately predict the drying kinetics of passion fruit seeds.

According to Eq. (14), the computed values for the effective diffusivity would change with both the local temperature and the local moisture content: between \(2.995 \times 10^{-11}\) and \(3.779 \times 10^{-10}\) m\(^2\)·s\(^{-1}\) at 0.509 and 0.001 kg·kg\(^{-1}\) (d.b.), respectively, for 40\(^\circ\)C; and between \(1.164 \times 10^{-10}\) and \(1.468 \times 10^{-9}\) m\(^2\)·s\(^{-1}\) at 0.509 and 0.001 kg·kg\(^{-1}\) (d.b.), respectively, for 60\(^\circ\)C. These figures of \(D\) were between 1.2% and 22.1% lower than those reported by Váquiro et al. [10] for a comparable model which did not consider solid shrinkage and convection mass transfer at the seed surface. Likewise, estimated \(D\) figures were within the range of those obtained for parboiled polished rice and lentil dried at 50\(^\circ\)C and 60\(^\circ\)C [7,15].

The proposed model allowed to estimate the moisture content distribution as well as to represent the shrinkage effect during the drying process (Fig. 3). It could contribute to understand the diffusion mechanisms in non-regular geometries and it offers an alternative approach to study the process from its physical principles which facilitates the adoption of further considerations as well as the process optimization.

### 4. Conclusions

A mathematical model for a tear-drop shape was developed considering the external and internal resistances to mass and heat transfer, local moisture and temperature dependence on moisture effective diffusivity and material shrinkage. The model was fitted to predict kinetics during the drying of passion fruit seeds at different air temperatures and velocities. Satisfactory estimations were obtained for all the experimental data, which supported the considerations admitted to formulate the model.

The proposed model could be useful for the study of transport phenomena in other particulate materials of non-regular geometry. In addition, this approach could allow an easier solving and a shorter calculation time than multidimensional ones, enabling its use in optimization problems.

### Nomenclature

- \(c\) : heat capacity, kJ·kg\(^{-1}\)·K\(^{-1}\)
- \(D\) : effective diffusivity, m\(^2\)·s\(^{-1}\)
- \(h\) : heat transfer coefficient for forced convection, kW·m\(^{-2}\)·K\(^{-1}\)
- \(h_m\) : mass transfer coefficient for forced convection, m·s\(^{-1}\)
- \(J\) : Jacobian determinant
- \(k\) : thermal conductivity, kW·m\(^{-1}\)·K\(^{-1}\)
- \(Q\) : sorption isosteric heat, kJ·kg\(^{-1}\)
- \(r\) : deformed-spherical coordinate, m
- \(R\) : characteristic dimension, m
- \(\mathcal{R}\) : ideal gas constant, kJ·kmol\(^{-1}\)·K\(^{-1}\)
- \(T\) : temperature, \(^\circ\)C
- \(t\) : time, s
- \(v\) : specific volume of air (dry basis), m\(^3\)·kg\(^{-1}\)
- \(V\) : seed volume, m\(^3\)
- \(W\) : local moisture content of solid (dry basis), kg·kg\(^{-1}\)
- \(\bar{W}\) : average moisture content of solid (dry basis), kg·kg\(^{-1}\)
- \(x\) : Cartesian co-ordinate, m
- \(y\) : Cartesian co-ordinate, m
- \(Y\) : moisture content of air (dry basis), kg·kg\(^{-1}\)
- \(z\) : Cartesian co-ordinate, m
- \(\alpha_1\) : effective diffusivity parameter, m\(^2\)·s\(^{-1}\)

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\( \alpha_2 \): effective diffusivity parameter, kJ·kmol\(^{-1}\)
\( \alpha_3 \): effective diffusivity parameter
\( \gamma \): scale factors
\( \delta \): shape factors
\( \phi \): deformed-spherical coordinate, rad
\( \rho \): density, kg·m\(^{-3}\)
\( \theta \): deformed-spherical coordinate, rad

**Subscripts**

\( \infty \): drying air
\( \text{dm} \): dry material
\( 0 \): initial
\( e \): equilibrium

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