Modeling and Simulation of Hydration Operation of Date Palm Fruits Using COMSOL®Multiphysics

A. Lakoud*[1], S. Curet[2], M. Hassouna[1]
[1] Ecole Supérieure des Industries Alimentaires de Tunis, Tunisie,
[2] L'UNAM Université, ONIRIS, CNRS, GEPEA, UMR 6144, Nantes, France
*Corresponding author: 58 Alain Savary, 1003 Tunis El Khadra, Tunisie, lakoudatef@yahoo.fr

Abstract: Hydration is the key unit operation in the thermal process of dates. This study focuses on modeling and simulation of this unit operation in order to improve the quality of final product and reducing processing time. The work is divided into two parts: an experimental investigation and a modeling approach with COMSOL® MultiPhysics release 5.1. In the first part, dry Tunisian Deglet Nour dates were hydrated experimentally at a laboratory scale by using saturated air. In the second part of the work, a 2D axisymmetric model was developed in COMSOL®Multiphysics by taking into account only mass transfer phenomena. This model considers the real shape of dates and the variation of density as a function of moisture content. Both moisture diffusivity and convective mass transfer coefficient at the surface were estimated by using an optimization algorithm based on least-square approach from experimental and numerical mean moisture contents. Results showed a good agreement between experimental values of average moisture contents and those numerically computed using estimated moisture diffusivity and convective mass transfer coefficient for various operating conditions. Such a methodology can be employed as a predictive tool to simulate the hydration of dates in order to optimize this unit operation.

Keywords: Dates hydration, modeling, moisture diffusivity, mass transfer coefficient of convection, simulation.

1. Introduction

In Tunisia, date palm (*Pheoenix dactylifera* L.), especially the Deglet Nour Cultivar, constitutes an important food and financial source. The chemical composition, in particular moisture content, of Deglet Nour date palm fruits can vary depending on agronomic practices, climatic conditions as well as ripening stage [1]. During last years, there has been an increase in the proportion of dry dates in annual crops. These dry dates are processed in the industry in order to obtain softer fruits with appearance and texture characteristics similar to those of Extra category dates. Hydration represents the main unit operation of this process. Hence, the control of this operation is of paramount importance especially when excessive times of hydration could reduce the shelf stability of dates and induce a waste of energy whereas insufficient hydration durations lead to non acceptable final product quality which is slightly different from that of the raw material.

2. Experiments

The Date palm fruits (Deglet Nour variety) used in this study were harvested in 2014 and stored at 4°C and 65% of relative humidity.
Hydration experiments were undertaken at laboratory scale approaching industrial conditions by putting dates in a closed environment at atmospheric pressure and where air reaches relative humidity of 100% and inner temperatures between 50 and 65°C. To realize this, a metallic enclosure was filled with water and heated with a temperature controlled hot plate. Dates were placed in the head space of the enclosure without any contact with the water. The cover of the enclosure was left without insulation in order to avoid overpressure and keep the saturated air at atmospheric pressure. The level of heating was set in such a way that temperatures of surrounding air medium, which are recorded by thermocouples placed near the dates, remain in the range of desired temperatures during each experiment. The experimental system designed is presented in figure 1.
Date fruits were weighted at regular intervals during hydration. Average moisture contents of dates flesh were determined following a method modified from Singh et al.(2013) [2] which consists of drying 3 g of dates in an oven at 105°C for at least 18h.

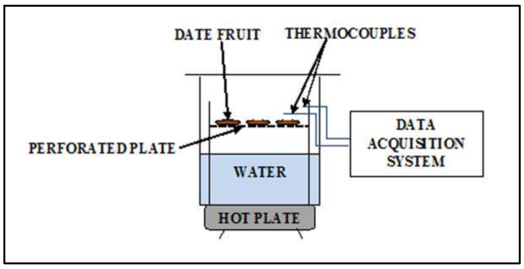

Figure 1. Experimental set-up

3. Use of COMSOL Multiphysics

3.1 Geometry and meshing

Since that the transport phenomena are symmetric, a 2D axisymmetric domain was considered to represent date flesh as shown in figure 2.

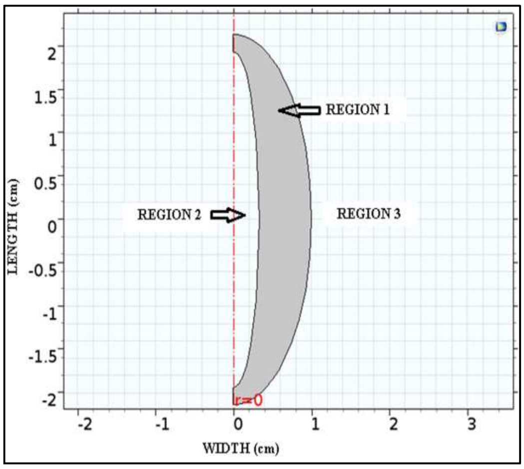

Figure 2. 2D-geometry

- The geometry consists of one domain corresponding to the region 1 representing the date flesh.
- Date pit corresponds to the region 2.
- The saturated air allowing the hydration of the date corresponds to the region 3.

The computational domain is meshed using triangular elements. User-controlled mesh with fine predefined size is selected in the mesh settings window. External boundary (in contact with air) was meshed using 5 elements within the boundary layer with an automatic size of the first element and a growth rate of 1.2 in order to avoid convergence problems due to curved edges and rounded corners. The meshed geometry is represented in figure 3.

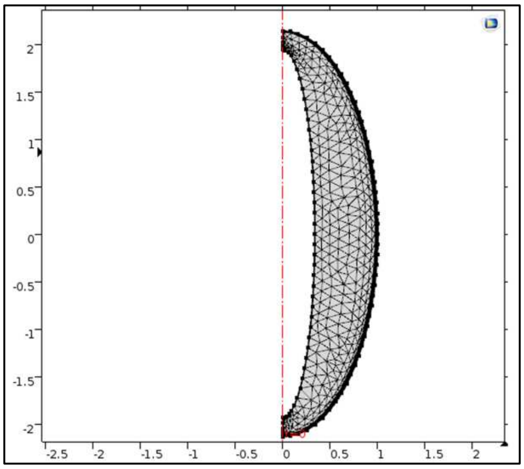

Figure 3. Meshed domain

3.2 Governing equations

Prior to modeling, monitoring of the temperatures within the dates flesh for the range of hydration times used for undertaking experiments showed that the temperature can be considered as homogenous. Therefore only mass transfer phenomena were considered. Diffusion in date flesh is described by the Fick's law according to Eq.(1).

$$\frac{\partial C}{\partial t} = \nabla.(D\nabla C) \qquad (1)$$

Where C and D are the molar concentration (mol/m^3) and the diffusivity (m^2/s) of moisture within the date flesh.

3.3 Modeling description

"Transport of diluted species" physic and "optimization module" of the software COMSOL® MultiPhysics release 5.1 were used to develop the 2D axisymmetric model. Date flesh moisture distribution is computed during hydration and the average moisture concentration is then calculated as a function of time with the average coupling operator.
By using the Levenberg-Marquardt optimization solver, both moisture diffusivity and convective mass transfer coefficient at the surface were

estimated by minimizing the least-square objective function calculated from experimental and numerical mean moisture contents. Experimental measured values were implemented in COMSOL® using Eq.(2).

$$C_t = \frac{X_t \rho_t}{M_w} \quad (2)$$

Where X_t , ρ_t and M_w are the average date flesh moisture content on humid basis (kg/kg), density of date flesh (kg/m^3) and the molecular weight of water (kg/mol). ρ_t is determined using Eq.(3).

$$\rho_t = \frac{m_t}{V} \quad (3)$$

Where m_t and V are the mass (kg) and the volume (m^3) of date flesh which is considered constant and equal to the arithmetic mean of initial and hydrated date.

3.4 Initial and Boundary conditions

The initial and boundary conditions are as follows:

1. Uniform initial moisture molar concentration C_0 which is calculated from Eq.(4) similarly to Eq.(2).

$$C_0 = \frac{X_0 \rho_0}{M_w} \quad (4)$$

Where X_0 and ρ_0 are the initial average date flesh moisture content on humid basis(kg/kg) , and initial density of date flesh (kg/m^3).
ρ_0 is determined using Eq.(5).

$$\rho_0 = \frac{m_0}{V} \quad (5)$$

Where m_0 is the initial mass (kg) of date flesh.

2. Null mass flux at the surface in contact with the date pit.

3. Natural mass convection at the outer surface in contact with the saturated air. The mass flux $N(mol.m^{-2}.s^{-1})$ of moisture inward date flesh is given by Eq. (6).

$$N = k_c(C_b - C_s) \quad (6)$$

Where k_c , C_b and C_S are convective mass transfer coefficient (m/s), bulk molar water vapor concentration (mol/m^3) and molar water vapor concentration in the air adjacent to the outer surface (mol/m^3).
C_b and C_S are determined using respectively Eq.(5) et Eq.(6).

$$C_b = \frac{P_{vs}}{RT} \quad (7)$$

$$C_s = \frac{P_{vs}}{RT} a_w \quad (8)$$

Where P_{vs} , R and a_w are saturated vapor pressure at the average absolute temperature T (K) of the air, gas constant $(8.314\,J.mol^{-1}.K^{-1})$ and water activity of date flesh. Neglecting sorption hysteresis phenomenon, a_w was defined using the GAB model, Eq.(9), proposed by Kechaou and Mâalej(1999;2000) [3,4].

$$X = \frac{X_m C k a_w}{(1-ka_w)(1-ka_w+Cka_w)} \quad (9)$$

Where X is the moisture content on dry basis(kg/kg). X_m , C and k are the constants of the model.
k_c is determined initially using the correlation for natural mass transfer coefficient around a sphere according to Eq.(10) [5].

$$\mathrm{Sh} = \frac{\mathrm{k_c D_{eq}}}{\mathrm{D_{w,a}}} = 2 + 0.6(\mathrm{Gr})^{\frac{1}{4}}(\mathrm{Sc})^{\frac{1}{3}} \quad (10)$$

Where Sh, Gr and Sc are Sherwood, Grashof and Schmidt numbers. D_{eq} is the surface-equivalent sphere diameter of the date (m). $D_{w,a}$ is the diffusivity of the water vapor in air (m^2/s) which is estimated using Eq.(11) [6].

$$\mathrm{D_{w,a}} = -2.775 \times 10^{-6} + 4.479 \times 10^{-8}\mathrm{T} + 1.656 \times 10^{-10}\,\mathrm{T}^2 \quad (11)$$

4. Results

Only results for one type of Deglet Nour dates which are slightly harder and drier than labeled Extra category dates are presented despite that experiments were conducted for several types of dates. As cited above, the molar moisture concentration distribution is computed

at times when average moisture contents were measured experimentally.
The mean water concentration is then computed. By using the optimization solver, the estimation of both moisture diffusivity and mass transfer coefficient was undertaken as follows:

1. Effective mass diffusivity is estimated initially by taking mass transfer coefficient determined from the Eq.(10).

2. By considering the value of mass diffusivity found from the first run, a second optimization is performed to estimate the mass transfer coefficient.

The table 1 shows the estimated diffusivities and convective mass transfer coefficients for two dates from the considered type.

Table 1: Estimated moisture diffusivities and mass transfer coefficients

Date Number	Date 1	Date 2
D(m^2/s)	5.54E-11	5.54E-11
kc **(m/s)**	0.00123	0.00126

The values of estimated convective mass transfer coefficient which depend on the dimensions of dates are close to the values found using the correlation for natural convection (Eq.10).

The figure 4 and figure 5 represent experimental (red markers) and calculated (blue curves) moisture molar concentration data as a function of time for the two considered dates using estimated moisture diffusivities and convective coefficients.

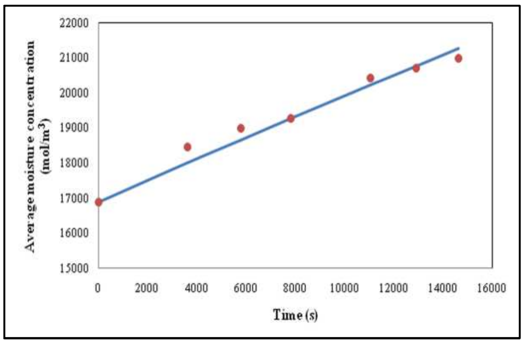

Figure 4. Experimental vs calculated average moisture concentration of Date 1

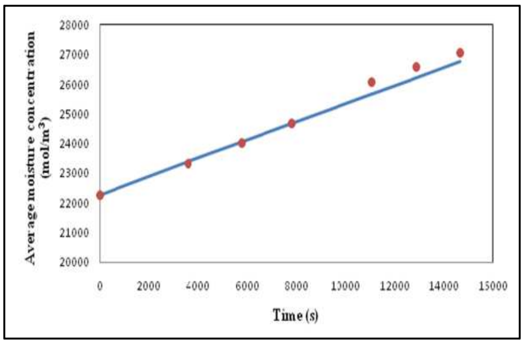

Figure 5. Experimental vs calculated average moisture concentration of Date 2

It is observed that the simulated curves fit well with the experimental data.
The root mean square difference (RMS) is also calculated using the method followed by Kechaou and Maâlej [4].

$$RMS = \sqrt{\frac{\sum_i \left(\frac{Cav_{i,exp} - Cav_{i,cal}}{Cav_{i,exp}}\right)^2}{n-1}}.100 \quad (12)$$

Where Cav_i is the average moisture molar concentration at the *i*-th experimental data.

The table 2 shows that the root mean square differences (RMS) do not exceed the value of 1.39% and therefore confirms the accuracy of the modeling.

Table 2 : Root mean square differences between experimental and calculated curves

Date Number	Date 1	Date 2
RMS (%)	1.39	0.97

From the curves, it is also remarked that there is no period of falling in moisture uptake rate. This could be explained by the relatively short times of hydration (in comparison to maximum processing times in industry).
The estimated moisture diffusivities and convective coefficients shown in Table 1, Figure 4 and Figure 5 indicate that these values do not vary greatly with the initial average moisture concentration. Therefore, this model can be used to simulate hydration operation and predict times necessary to reach desired final moisture contents taking into account the variability of raw material for this type of dates.
The figure 6 illustrates simulated molar moisture profile within the flesh of one date after 14640s

(≈ 4h) of hydration at the average temperature of the air.

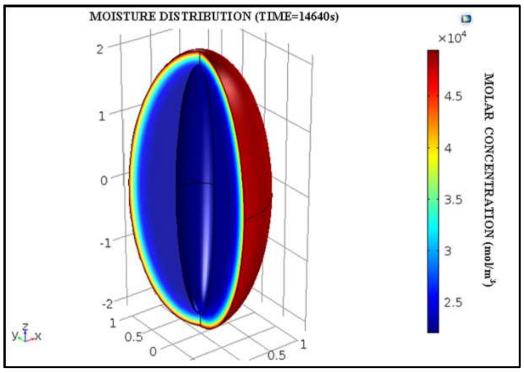

Figure 6. Moisture concentration distribution within date flesh after 4h

It is shown that the gradient of moisture concentration is at its highest values near the surface in contact with air and decreases up to zero towards the center where moisture concentration remains at its initial value. This indicates that diffusion is mainly occurring near the outer surface for the considered range of hydration durations.

5. CONCLUSION

The control of the hydration during the thermal process of dates is crucial in order to save energy and to obtain a good quality for the final product. However there are a scarce data about the capacity of moisture uptake during hydration. In this work, a theoretical model was developed to describe the mass transfer phenomena involved in this operation. The model allowed to estimate both moisture diffusivity and convective mass transfer coefficient by using a numerical investigation which was validated experimentally. This model can be used to optimize the hydration of dates by simulating this operation and predicting times necessary to reach desired water contents. In addition, the model could be used to optimize the maximum time of hydration. In fact, for current industrial applications, this operation often lasts during more than 4h. The proposed modelling approach may thus help for the optimization of this operation in order to enhance the mass transfer at the surface and to reduce the energy consumption during hydration.

6. REFERENCES

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