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Finite element analysis and modeling of water absorption by date pits during a soaking process

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Abstract: Date pits for feed preparation or oil extraction are soaked in water to soften before milling or extrusion. Knowledge of water absorption by the date pits helps in better managing the soaking duration. In this research, the process of water absorption by date pits was modeled and analyzed using Fick's second law of diffusion, finite element approach, and Peleg model. The moisture content of the pits reached to its saturation level of 41.5% (wet basis) after 10 d. The estimated coefficient of diffusion was 9.89×10^{-12} m²/s. The finite element model with a proposed ellipsoid geometry for a single date pit and the analytical model fitted better to the experimental data with R^2 of 0.98. The former model slightly overestimated the moisture content of the pits during the initial stages of the soaking and the latter model generally underestimated this variable through the entire stages of soaking process.

Key words: Date pits, Soaking, Water absorption, Modeling doi:10.1631/jzus.B0910641 Document code: A

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1 Introduction

The date tree (*Phoenix dactylifera* L.) is an important staple food and a strategic plant in many arid regions of the world. The worldwide production of date fruits exceeded 6×10^6 t in 2007 (FAO, 2009). Date fruits are an important food item, with plenty vitamins and minerals. They are eaten fresh or are dried and stored for later consumption. Individual date fruits contain a pit which, depending on the variety, accounts for about 10% to 18% weight of the fruits (Salem *et al.*, 1989).

A major portion of annually produced date fruits is used by confectionaries and beverage production industries. Date pits are the main by-products in these processing plants. On average, the pits from different varieties contain about 9.5% moisture, 6.0% protein, 10.5% fat, and 70% carbohydrates (Hamada *et al.*, 2002). The pits are generally used as complementary feed materials (Vandepopuliere *et al.*, 1995) or as a conventional soil fertilizer. Portions of the pits are also used for extracting oil for cosmetic and pharmaceutical purposes (Devshony *et al.*, 1992).

For either feeding or extracting oil, the date pits are initially soaked in water and then they are ground. Soaking is necessary for softening the hard pit to facilitate grinding. Soaking of date pits like soaking of many other agricultural seeds is a time-consuming process. For instance, corn kernels are soaked for up to 72 h before milling (Ji *et al.*, 2004).

The amount of water absorbed by seeds during soaking is affected by different factors such as the initial moisture content, variety of the seeds, soaking duration, and temperature and acidity level of the water (Hsu *et al.*, 1983; Karapantsios *et al.*, 2002; Laria *et al.*, 2005). On the other hand, the agricultural seeds are not uniform and consist of three major parts, namely, seed coat, endosperm, and embryo. Since in most seeds the endosperm occupies the major part of the seed, a seed is usually considered as a uniform

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entity in many moisture transfer studies (Gaston *et al.*, 2004; Bakalis *et al.*, 2009).

Modeling the process of water absorption by agricultural seeds helps in understanding the dynamic and kinetic of this process and this knowledge is valuable for proper management of their soaking processes. Mathematical modeling of the agricultural seeds has been approached by three general methods: (1) empirical approach wherein a suggested model is fitted to experimental data (Hung et al., 1993; Turhan et al., 2002; Badau and Jideani, 2005; Noorbakhsh et al., 2006); (2) theoretical methods which are generally based on principles of moisture diffusion, sometimes coupled with heat or mass transfer equations (Vizcarra Mendoza et al., 2003; Gaston et al., 2004; Gely and Giner, 2007); and (3) semi-theoretical approaches which are generally a modified form of theoretical models (Misra and Brooker, 1980).

The conventional models for describing the moisture transfer phenomenon by a seed, generally predict the total amount of moisture absorbed or desorbed and they cannot estimate the temporal moisture distribution within a seed.

The numerical modeling methods such as finite element and finite difference offer an alternative tool for conventional approaches to analyze various processes (Inc, 2005). Using these methods, the temporal moisture distribution within a seed is estimated by a suitable discrete model composed of piecewise continuous functions defined over a finite number of internal elements. Examples are found in Igathinathane and Chattopadhyay (1999), Gaston *et al.* (2004), and Bakalis *et al.* (2009) who successfully applied the finite element modeling method for water diffusivity in wheat kernels, rice hydration, and drying of parboiled paddy components, respectively.

Date pits are hard, and the process of water uptake by them takes an extended period of time. In this research, for efficient control of the soaking process, the water absorption by date pits was studied and modeled by three modeling approaches: (1) analytical approach using Fick's second law of diffusion; (2) finite element approach based on Fick's law; and (3) Peleg (1988) model. In this investigation, the date pits were assumed to have a uniform material with uniform initial moisture content. The goodness of fit of each model was evaluated by calculating the coefficient of determination (R^2) and root mean square error (RMSE) between the experimental moisture data and the values obtained in the models.

2 Materials and methods

2.1 Material preparation and soaking process

Date pits dedicated for the experiments were derived from Mozafati cultivar fruits harvested in summer of 2008 from a date palm grove in Bam City, Kerman, Iran. The pits were cleaned, washed, and spread on a tray at laboratory conditions for a period of two weeks to allow the pits to reach uniform moisture content. Prior to soaking, the moisture content of the pits was determined by oven method at 103 °C for 36 h (ASAE, 1997). The dimensions of the kernels including length, width, and thickness were measured by a digital caliper. From these measured values the sphericity and geometric mean diameter (GMD) of the seed were determined (Jain and Bal, 1997).

For conducting the experiments, 250 g of the pits were placed in a mesh fabric bag and the bag was immersed in 25 °C distilled water. At predetermined time intervals, the pits were removed from water and superficially dried by a paper towel and immediately weighed using an electronic balance with 0.01 g accuracy. This procedure continued until there were no appreciable changes in the mass of the soaked pits. The experiments were performed in three replicates and their averages were used for modeling and analyses.

2.2 Analytical approach

During a diffusion process at constant temperature, it is assumed that the process follows Fick's second law of diffusion. For an axisymmetric diffusion, Fick's three-dimensional (3D) equation is given by:

$$\frac{\partial M}{\partial t} = D\left(\frac{\partial^2 M}{\partial x^2} + \frac{\partial^2 M}{\partial y^2} + \frac{\partial^2 M}{\partial z^2}\right), \qquad (1)$$

where M is the instantaneous moisture content at a specified time t and D is the diffusion coefficient. A solution for the above equation for an object with a sphere shape of radius r was presented by Crank (1975), as

MR =
$$\frac{M - M_i}{M_e - M_i} = 1 - (\frac{6}{\pi^2}) \sum_{i=1}^{\infty} (\frac{1}{i^2}) \exp(-Di^2 \pi^2 \frac{t}{r^2}),$$
 (2)

where MR is the moisture ratio, and M_i and M_e are, respectively, the initial and the equilibrium moisture contents of the object during a moisture transformation process. In most cases, only a finite number of Eq. (2) is used for estimating MR values. In fact, most researchers use only the first two terms of this equation.

In this research, the experimental MR values at specific time intervals were calculated and used as input to the curve fitting tool box of MATLAB (R2006a) software and the diffusion coefficient of the date pits, *D*, was estimated. The typical shapes for side and cross section views of a date pit are presented in Fig. 1.



Fig. 1 Schematic geometry of a date pit (a) Side view; (b) Cross sectional view along the width

Since the general shape of a typical pit is closer to an ellipsoid than to a sphere, the coefficient of diffusion should be adjusted in Eq. (1). Gaston *et al.* (2004) presented a procedure to estimate the coefficient of diffusion for an ellipsoid (D_e) using the following equation:

$$D_{\rm e} = f_{\rm e}^2 \times D, \tag{3}$$

where f_e is the sphericity factor of ellipsoid (Gaston *et al.*, 2002). Then, the coefficient of diffusion *D* in Eq. (2) should be replaced by the calculated D_e .

2.3 Finite element approach

In a finite element approach, an estimated value for D is supplied to the Eq. (1) and the MR values are numerically determined for specified locations at given time intervals. In applying this approach the following assumptions were made for the individual date pits: 1. The diffusion coefficient is independent of moisture concentration.

2. The pits are isothermal and heat transfer during soaking is neglected.

3. The pits are homogeneous and isotropic.

4. Throughout the soaking process, the surface of a pit maintains saturation moisture content, M_e (the boundary condition).

5. The initial moisture content of the pits is constant and it is uniformly distributed within a pit, M_i (initial condition).

The geometry of a date pit was considered to be an ellipsoid. For modeling a date pit, one quarter of an ellipse was used in a time-dependent axisymmetric two-dimensional (2D) analysis (Fig. 2). The grids for date pit consisted of 243 triangular elements with a total of 546 nodes. The commercial finite element analysis software ANSYS (Rel. 10.0, 2005) was used to evaluate instantaneous moisture distribution at the nodes. The coefficient of diffusion estimated by fitting Eq. (2) to the experimental data was provided to the software and the moisture content of each node was calculated at one-second time steps. The overall moisture content for a date pit was also calculated at every 30 min by averaging the moisture contents of the nodes.



Fig. 2 Finite element grid for a single date kernel

2.4 Peleg model

One of the most frequently used empirical models for estimating the overall moisture content M as a function of time t during a moisture absorption process is the Peleg model defined as:

$$M = M_{i} + \frac{t}{k_{1} + k_{2}t},$$
(4)

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where M_i is initial moisture content (decimal, dry basis), k_1 and k_2 are two constants known as the Peleg rate constant (h·%⁻¹) and the Peleg capacity constant (%⁻¹), respectively. These two constants must be determined for a particular product under certain moisture absorption processes. We used the Peleg model to estimate the overall moisture content of the date pits during the soaking process. The data for overall moisture contents at specified time intervals were used as input to curve fitting tool box of MATLAB commercial software and the two constants of the Peleg model were determined.

2.5 Comparison and evaluation of the models

The goodness of fits for the finite element model, analytical solution, and Peleg model was evaluated by calculating the coefficient of determination (R^2) and root mean square error (RMSE) by the following formulae:

$$R^{2} = \frac{\left(\sum MR_{e}MR_{p}\right)^{2}}{\sum MR_{e}^{2}\sum MR_{p}^{2}},$$
(5)

$$RMSE = \sqrt{\frac{\sum (MR_p - MR_e)^2}{n}},$$
 (6)

where MR_e and MR_p are the experimental and the predicted moisture ratios, respectively. A model having a high value of R^2 (close to 1) and a low value of RMSE (close to 0) is considered to be a well-fitted model.

3 Results and discussion

The measured physical characteristics of the date pits before and after soaking are presented in Table 1. From the dimensions, the date pit geometry is very close to an ellipsoid and it retains its general shape after soaking. However, due to a relative increase in the thickness and width of the pits as a result of moisture gain, the sphericity of the pits increases and changes from 0.41 to 0.49. The increase in the dimensions is due to the migration of water between and within the cells of the pits which causes an overall swelling of the pits. A detailed discussion on changes of dimensions during soaking is given by Ahromrit *et al.* (2006).

 Table 1 Some physical characteristics of the experimental date pits

	Length	Width	Thickness	Sphericity	GMD
	(mm)	(mm)	(mm)	(mm)	(mm)
Before soaking	23.77±3.61	6.6±1.91	5.38±1.87	0.41±0.03	9.44±1.77
After soaking	24.61±3.82	8.1±1.23	6.51±1.51	0.49±0.11	9.88±2.02
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Data are expressed as mean±SD. GMD: geometric mean diameter

The moisture percentages, both on wet and dry bases, absorbed by the pits are presented in Fig. 3. During the first 2 h of soaking, the moisture content increased rapidly from 12% to near 30% on the dry basis. Then, the rate of water absorption gradually decreased until the saturation moisture content, 71% on the dry basis, was reached after 240 h. Thus, under normal environmental conditions, it takes about 10 d for the date pits to reach their saturation moisture level.



Fig. 3 Changes in the moisture content of the date pits during the soaking process

The sphericity factor (f_e) for an average date pit was calculated to be equal to 0.78. Using Eqs. (2) and (3), the coefficient of diffusion D_e was calculated to be equal to 9.89×10^{-12} m²/s. The same procedure was used by Gaston *et al.* (2002) and they calculated the coefficient of diffusion for wheat kernels within a range of 1.35×10^{-11} to 6.88×10^{-11} m²/s. Bakalis *et al.* (2009) estimated this coefficient for rice equal to 7×10^{-10} m²/s. The lower D_e calculated for date pits indicates that the date pits absorb water at a slower rate than wheat and rice kernels.

The obtained coefficient of diffusion was supplied to Eq. (1) and this equation was solved by finite element approach to estimate the moisture distribution within the pits at various time intervals.

The MR values calculated from the moisture absorption experimental data and their different fitted models are presented in Fig. 4. The predicted MR values calculated by finite element method were close to those of both measured and analytical solutions. As illustrated in Fig. 4, the finite element model provided a good prediction of the MR values at the end of the soaking process, while during the initial and intermediate stages it slightly overestimated the MR values. The analytical model generally underestimated the MR values.



Fig. 4 Comparison of moisture ratios determined by the experimental data and three modeling approaches

The visualization of finite element predictions for the moisture content is presented in Fig. 5 at 1, 17, 41, and 240 h after the commencement of the soaking. Fig. 5 shows a gradual migration of the water from the surface to the center of a pit. Theoretically, the finite element model, as shown in Fig. 5, indicates that even at the end of the soaking process the moisture content throughout the pit is not quite uniform. In a practical sense, as shown in Fig. 6, the average moisture content reached its saturation level, 71.0% on dry basis, after 240 h. Fig. 6 indicates that the moisture gradient within a pit is large during the initial stages of soaking and the gradient decreases with the progress of soaking, and after 240 h the moisture content is practically uniform and reaches a saturation level at all the nodes. The shortcoming of the finite element model, with respect to the analytical model, is that the former relies on a coefficient of diffusion developed by other sources, i.e., analytical modeling or experimental values.



Fig. 5 Typical distribution of moisture in a date pit during soaking as determined by finite element analysis (a) 1 h; (b) 17 h; (c) 41 h; (d) 240 h. The bar below each shape represents the level of moisture content (%) within a pit region at a given time



Fig. 6 Moisture contents at various points along the cross section from the surface to the center

Using the experimental data for moisture contents of date pits at different time intervals and the curve fitting tool box of MATLAB commercial software, the following model was obtained based on the Peleg formula:

$$M=0.12+t/(37.68+1.685t), R^2=0.94.$$
 (7)

The Peleg model, as shown in Fig. 4, underestimated the MR values at the initial and the final stages of the soaking process. Comparing the R^2 value of the three developed models, the Peleg model is inferior to analytical and finite element models for predicting the water absorption by date pits.

The R^2 and RMSE values calculated for the finite element model, analytical solution, and Peleg model are shown in Table 2. The R^2 values were 0.98 for finite element and analytical solution. The RMSE value for finite element model is very close to, but slightly lower than, that for the analytical solution. Thus, both analytical and finite element approaches are well suited for modeling this water absorption process. However, the finite element model slightly overestimated the MR values of the pits at the initial and intermediate stages while the analytical approach generally underestimated these values (Fig. 4). The superiority of the finite element model is due to its power to predict the moisture content changes at specified nodes within a date pit rather than estimating an overall moisture transfer for a pit.

Table 2 Estimated coefficients of determination (R^2) and root mean square errors (RMSE) for the three models

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Model	R^2	RMSE
Finite element	0.98	0.0724
Analytical solution	0.98	0.0788
Peleg	0.94	0.1097

4 Conclusions

The process of water absorption by date pits was investigated and the process was modeled by three different approaches. The rate of water diffusion was high during the first 2 h of soaking and then it gradually decreased. The date pits reached their equilibrium moisture content of 41.5% on the wet basis after 240 h of soaking in distilled water. The analytical approach based on Fick's second law of diffusion and the finite element approach based on Fick's law fit well to the experimental data. However, the RMSE value calculated for the finite element model was slightly lower than that for the analytical model. The finite element model is able to predict the moisture distribution at any given point within the pit as a function of time while the analytical model gives an overall moisture content of the pit at a specified time. The Peleg model is inferior to the analytical and finite element models, and predicts overall moisture content for the pit as a function of time.

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