Application of a Diffusion Model to Predict Drying Kinetics Changes Under Variable Conditions: Experimental and Simulation Study

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Abstract: This study focuses on the interplay between drying kinetics (encountered in typical industrial processes and particularly in the context of solar drying) and the possible variation of external (e.g., environmental) conditions. Theoretical models of these behaviours are introduced. Experimental results confirmed by simulation are also presented. Variation of the thermo physical properties of air is taken into account in terms of variation of viscosity, density and coefficient of diffusion. In particular, this coefficient is calculated from experimental data and expressed as a function of the wet bulb air temperature. When external conditions are modified and, as a natural consequence, also the drying kinetics undergo some change, in general, products exhibit a time of response. This response (the principal object of the present study) changes from the kernel of the product to its surface. Two kinds of conditions are simulated in the present work to model such behaviour: a constant flux and a convective flux. It is found that the convective flux is more affected by external conditions than the constant flux. A comparison between sudden and progressive changes of drying conditions is also considered for possible optimisation of the considered processes.

Keywords: Brick, Period of constant drying rate (PCDR), coefficient of diffusion, kinetic deformation, constant flux, convective flux

1 Introduction

Among the industrial processes, drying is one of the most common operations. Ceramics are dried with the objective to avoid cracks or deformations before baking them. Foods are dried with respect to preserve organoleptic characteristics and

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nutritional quality. Also, the good quality of pastes after drying is important for commercialization. In this context, the knowledge of moisture changing in time is indispensable.

The curves of drying kinetics allow calculating the necessary time to dry and to identify the behaviour of the dried product.

As the dried products are different and their behaviour, during this process, changes from one to another, a method to classify them is necessary. Van Brakel (1980) presented a classification of solids. He divided the products into capillary porous, hygroscopic porous and nonporous media. After that, he discussed some common drying kinetics that a product can exhibit during drying.

Generally, drying is obtained in laboratory under constant air conditions (temperature, humidity and velocity). However, industrialists need to control the process in order to gain time and energy. This control is based on the change of the air conditions likewise solar drying, where the external conditions change during the overall time duration of the process. A natural question in such a context is: *what are the limits of validity of the known model kinetics, when the local air characteristics change throughout time*?

A relevant mathematical model and a related simulation code were developed by Ratti and Mujumdar (1997) to predict the batch drying performance subjected to time varying air conditions (solar drying). The model based on mass and energy balances applied to the gas and solid phases. The results were compared with experimental ones, presented by Jayaraman (1992) and the comparison was favorable. Shrinkage of the material was taken into account.

Fohr, Arnaud, Ali Mohamed and Benmoussa (1990) also carried out experimental studies to assess the limits of validity of drying kinetics. These works were applied to two materials representing the most widespread classes of products; with a constant drying rate period (bricks) and without (clay pellet). Then, a simulation based on Whitaker's model with some simplifications, was presented. A good agreement, between modelling and experimental results, was observed.

Bennamoun and Belhamri (2006, 2004) simulated the behaviour of drying kinetics of agro-alimentary products with application to solar drying. At the change of temperature and velocity of the heated air the kinetics answered by changing their behaviour with a non-immediate response. Kooli, Fadhel, Farhat and Belghith (2007) have reported the same observations during their experimental work of open sun and green house drying of red pepper.

A theoretical analysis based on a simple diffusion model, (confirmed by an experimental one) is presented in this paper to study the interplay between drying kinetics and drying conditions during application of a constant flux and a convective flux.

2 Materials and method

The tested material is a sample of a brick, which has the following dimensions (in mm) $205 \times 100 \times 36$. This material presents a long period of constant drying rate (P.C.D.R.) that can be explained by its special porosity. This was moreover confirmed by some measurements of the surface humidity and some photos taken continuously during drying by Belhamri and Fohr (1996) and Belhamri (1992).

The material has the following physical characteristics:

Porosity: 0.6, volumetric mass: 1250 kg/m^3 (measured in laboratory). Indeed, it is important to note that the sample may be subjected to an imbibing procedure in order to have initial moisture around 0.4 (kg/kg dry basis).

The drying loop is represented in Fig. 1.



Figure 1: Sketch of the drying loop

Thermocouples allow the measurement of the temperature of the air at a location before the sample emplacement.

The fan allows air circulation in the drying loop. Air is heated using a heating resistance. It crosses the tranquilizing room before going to the sample emplacement.

The air velocity is measured using pressure difference across the two sides of the diaphragm.

Along the drying process, an electronic balance (0.1g accuracy) is linked to a microcomputer. It continuously weighs the sample and treats data whereby drying curves are obtained.

2.1 Mathematical model and simulation

Van Brakel (1980) highlighted that Sherwood's diffusion model, based on Fick's law, can detect the mass transfer inside all the drying media. He presented experimental results for many products with and without a first constant drying rate period. Belhamri (1992) and Pel, Landman and Kaasschieter (2002) proved in their studies that a diffusion model can predict well the drying process of a brick. It can detect the changes that occur to the product, with very good agreement with experimental results. Therefore, a diffusion model is chosen for this study.

The product is considered as a one dimensional plane sheet, with symmetrical form. Accordingly, the equation of diffusion is written in the following form:

$$\frac{\partial C}{\partial t} = D_i \frac{\partial^2 C}{\partial y^2} \tag{1}$$

i can take the value 1 or 2: i = 1: represents the first drying rate period (P.C.D.R.), i = 2: represents the second drying rate period.

The initial boundary condition is given as:

$$t = 0: \quad C = C_0 \tag{2}$$

The symmetry condition is expressed by:

$$\frac{\partial C}{\partial y}\Big)_{y=0} = 0 \tag{3}$$

At the surface the following condition holds:

$$-\rho_s D_i \frac{\partial C}{\partial y} \bigg|_{y=ep} = F \tag{4}$$

Fig. 2 presents a sketch of the studied problem.

Two types of heated air flow are studied: a constant and a convective flux. Crank (1975) gives analytical solutions of the posed problems as follows:

Case 1: application of a constant flux

$$\frac{(C-C_0) \rho_s D_i}{F.ep} = \frac{D_{i.t}}{ep^2} + \frac{3y^2 - ep^2}{6ep^2} - \frac{2}{\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \exp\left(\frac{-D_i n^2 \pi^2 t}{ep^2}\right) \cos\left(\frac{yn\pi}{ep}\right)$$
(5)



Figure 2: Sketch of the problem

Case 2: application of a convective flux, which can be written:

$$\frac{F}{\rho_s} = h\left(C - C_{eq}\right) \tag{6}$$

The solution is:

$$\frac{C-C_0}{C_{eq}-C_0} = 1 - \sum_{n=1}^{\infty} \frac{2L\cos\left(\frac{\beta_n y}{ep}\right)\exp\left(\frac{-\beta_n^2 D_i t}{ep^2}\right)}{(\beta_n^2 + L^2 + L)\cos\left(\beta_n\right)}$$
(7)

 β_n are the positive roots of the equation:

$$L = \beta \tan(\beta) \tag{8}$$

And:
$$L = \frac{eph}{D_i}$$
 (9)

The used formulas to calculate the moist air characteristics are presented in Appendix A.

The equation of diffusion, the boundary and initial conditions are rewritten in dimensionless form then discretized using a finite difference method, leading to a system of equations written in matrix form. It is resolved using the iterative Gauss-Seidel method, which have a sufficient condition for convergence. When the coefficient matrix is sparse (has many zeros), an iterative method may be more rapid and more economical in memory requirement of a computer (Gerald and Wheatly, 1989). A calculus code using FORTRAN has been developed to simulate the drying of the product. The calculus has been performed to a relative error of about 0.01%.

2.2 Determination of the coefficient of diffusion

The bottleneck related to the use of a diffusion model is the determination of the coefficient of diffusion. In this study, the coefficient is determined via a comparison between the experimental drying kinetics and the analytical solutions proposed by Crank (1975). Some of the obtained results are illustrated in Tab. 1.

Dry bulb	Relative	$D_1 \cdot 10^8$	$D_2 \cdot 10^9$
temperature	humidity	(m ² /s)	(m ² /s)
(°C)	(%)		
27.5	51	1.200	7.16
40	27	1.817	9.76
50	28	1.875	7.82
50	31	1.917	8.20
50	16	1.868	10.70

Table 1: Variation of the coefficient of diffusion with air temperature and relative humidity

These results allow writing the coefficient of diffusion as a function of the wet bulb temperature:

For the first drying rate period (P.C.D.R.):

$$D_1 = \left(-0.021T_{wb}^2 + 1.098T_{wb} - 12.185\right) 10^{-8}$$
⁽¹⁰⁾

For the second drying rate period:

$$D_2 = \left(-0.003T_{wb}^2 + 0.197T_{wb} - 2.024\right) \ 10^{-8} \tag{11}$$

 T_{wb} is measured in °C.

The results show that diffusion during the P.C.D.R. is more important than during the second drying rate period and these results are in agreement with those presented by Chirife (1983).

3 Results and discussion

P.C.D.R. is the most important phase in drying, because this period is affected by external drying conditions. In this section, the study is concentrated on this part of the process.

We present, in a first time, the obtained results at the application of a constant flux "F", which equals to $3.4 \times 10^{-4} \text{ kg/(m^2 s)}$

The distribution of the moisture, inside the product is represented in Fig. 3, with the following drying conditions: $V_{ach} = 4.6$ m/s, $T_{ach} = 50$ °C and $\phi = 14\%$. The moisture content decreases with time increasing result of the evaporation of water, with a clear P.C.D.R., for all the parts of the product. However, drying is occuring in a non-homogeneous manner. It can be seen in fact that, it is easier to evaporate surface water, which is at the contact of the heated air, than its kernel. As a result, the surface reaches the critical point at the end of the P.C.D.R. more rapidly (after 9000 seconds) than the kernel (18000 seconds) with a considerable difference in time. It is important to note that the obtained results are in perfect concordance with experimental results obtained by Belhamri (1992).



Figure 3: Distribution of the moisture content inside the product during the P.C.D.R. and using simulation

The existence of the P.C.D.R. for a brick is in concordance with experimental works done by Belhamri (2003), Belhamri (1992), Ali Mohamed (1992), Chen and Pei (1989), Fohr, Arnaud, Ali Mohamed and Benmoussa (1990) and Belhamri and Fohr (1992).

It is evident that the curves of the figure can be expressed mathematically as a linear function of time. In this way, the obtained drying rate derived from the moisture content is constant (confirming existence of the P.C.D.R.). This is also confirmed by the experimental results shown in Fig. 4, and the existence of the constant parts in curves (a) and (b).

Now, we proceed, as illustrated in Fig. 4, to a sudden augmentation of the heated air temperature from 40° C (curve a) to 54° C (curve b).



Figure 4: Experimental results of the influence of the temperature variation on the drying kinetic behaviour

The kinetic answers, to this augmentation, by modifying its behaviour, as seen in the figure (curve c). However, this variation is imposed at the middle of the P.C.D.R., and the result of the experiment shows that the new conditions are attained at the critical point at the end of the P.C.D.R. and the beginning of the second drying period. A non-immediate answer is then observed and a time of response is registered.

Fig. 5 comes, using the simulation, to confirm the obtained experimental results. The augmentation of the air temperature, from $Ta = 40^{\circ}C$ to $Tb = 54^{\circ}C$, is applied at the middle of the P.C.D.R. (after 10800 seconds of drying time), and as it is seen in the figure, the kinetic changes its behaviour and goes to the kinetic of the new applied conditions. However, this is attained at the end of the P.C.D.R. (at t = 18000 seconds). The time of reaction of the product to the new application of the new drying conditions can be calculated. It is around 7200 seconds (2 hours). A similar trend for the kinetics was registered in the experimental work done by Fohr, Arnaud, Ali Mohamed and Benmoussa (1990), Ali Mohamed (1992), and using simulation, by Bennamoun and Belhamri (2006). For all the works, the kinetic presents a non-immediate reaction and a time of response can be calculated.



Figure 5: Kinetics of the product kernel as a function of air temperature

Convective drying has a particular importance in drying studies. It depends entirely on the external conditions. Along these lines, this part, presents the simulation results obtained by application of a convective flux.

As indicated before, the equation of diffusion and the boundary and initial conditions are rewritten in dimensionless form. Whereby, Eq. 1, 2, 3 and 6 can be rewritten respectively:

$$\frac{\partial C^*}{\partial t^*} = \frac{\partial^2 C^*}{\partial y^{*2}} \tag{12}$$

For
$$t^* = 0$$
: $C^* = 1$ (13)

$$\frac{\partial C^*}{\partial y^*} \bigg|_{y=0} = 0 \tag{14}$$

$$\frac{\partial C^*}{\partial y^*}\Big)_{y^*=1} = Sh(C^*) \tag{15}$$

Sherwood Number "*Sh*" is known to be a function of the velocity, the viscosity, and the density of the air and the physical properties of the drying media. The following formula is proposed (Belhamri (2003)) for a flat plane:

$$Sh = 0.332Re^{0.5}Sc^{0.33} \tag{16}$$

Thus, the characteristics of the wet air need to be calculated (see Appendix A for the characteristics of the wet drying air).

Fig. 6 and 7 show the behaviour of the kinetic according to the temperature change for, respectively, the kernel and the surface of the product.

In the light of Fig. 6, it is evident that the temperature is an influent parameter; for a dry bulb temperature of 40°C around 14000 seconds are necessary to reach the critical point. Nevertheless, it takes around 9000 seconds for 54°C. An important gain in time can be obtained comparing to the application of a constant flux. Moreover, the relaxation is more difficult for the kernel of the product than its surface, as shown in the two figures. The kinetic of the surface has attained one of the new conditions at the end of the P.C.D.R., which is not the case of the kernel of the product.

Simulations of sudden and progressive augmentations of the air temperature are illustrated in Fig. 6.

In one hand, sudden augmentation is applied at t = 3600 seconds, it means that the temperature of the air is carried to 54°C at this time. The figure shows then a response time of the product of more than 5400 seconds. On the other hand and for progressive augmentation, the temperature of the air increases 3.5 degrees for each 1000 seconds. The temperature of 54°C is attained at t = 9000 seconds. Better results are obtained with this strategy of augmentation with a low time of reaction and gain in energy for the process.



Figure 6: Kernel drying kinetic behaviour according to the change of the heated air temperature (Convective flux case)



Figure 7: Surface drying kinetic behaviour according to the change of the heated air temperature (Convective flux case)

4 Conclusion

It has been shown that a simple diffusion model can predict the variations that occur to drying kinetics as a function of external conditions in considerable agreement with experimental data.

A variation of the heated air conditions is responsible for a non-immediate reaction; a time of response can be then registered and calculated. This time is higher for convective conditions than for constant drying conditions.

As drying is effectuated in a non homogenous manner; the kernel of the product takes a time longer than its surface to adapt its behaviour to the new drying conditions.

It has been also proven that the application of progressive change can give more satisfactory results than sudden variations (the time of reaction becomes shorter).

Appendix

The characteristics of the wet air are calculated using the following equations (the temperature is given in Kelvin):

Daguenet (1985) gives:

$$Dv = 2.26 \times 10^{-5} \frac{1}{p} \left(\frac{T_{ach}}{273}\right)^{1.81}$$
(17)

$$\rho_{as} = \frac{\rho_{ah}}{1+W} \tag{18}$$

$$W = 0.622 \frac{\phi P_{vsat}}{P_{ah} - \phi P_{vsat}} \tag{19}$$

P and P_{ah} are, generally, equal to the atmosphere

$$\rho_{vap} = \rho_{ah} - \rho_{as} \tag{20}$$

$$P_{vsat} = 10^{17.433} - \frac{2795}{T_{ach}} - 3.868 \log\left(T_{ach}\right) \tag{21}$$

The viscosity of the wet air is calculated using the following equations (Lampinen & Ojala, 1993)

$$\mu_{ah} = \frac{\mu_{as}\rho_{as} + \mu_{vap}\rho_{vap}}{\rho_{as} + \rho_{vap}} \tag{22}$$

$$\mu_{as} = \frac{1.448\sqrt{T_{ach}}}{1 + \frac{110.4}{T_{ach}}} 10^{-6} \tag{23}$$

$$\mu_{vap} = (0.0361T_{ach} - 1.02) \ 10^{-6} \tag{24}$$

Its density is calculated (Maake, Eckert and Cauchepin 1993):

$$\rho_{ah} = \frac{348.3}{T_{ach}} p_{ah} - \phi \ p_{vsat} \frac{131.6}{T_{ach}}$$
(25)

Here the pressure is in atmosphere.

Nomenclature

- *C* moisture content (kg/kg)
- C^* Dimensionless moisture ($C^* = \frac{C C_{cr}}{C_0 C_{cr}}$)
- D coefficient of diffusion (m²/s)
- Dv diffusion of vapour in the air (m²/s)
- *ep* overall product thickness (m)
- F flux (kg/s.m²)
- *h* mass transfer coefficient (m/s)
- *P* pressure (Pa)
- *T* temperature (°C or K)
- t time (s)
- t^* dimensionless time $(t^* = \frac{t.D}{ep^2})$
- *W* absolute humidity (kg/kg)
- y product thickness (m)
- y^* dimensionless thickness $(y = \frac{y^*}{ep})$

Greek symbols

- μ viscosity (kg/m.s)
- ϕ relative humidity
- ρ density (kg/m³)

Subscripts

ach	heated air
ah	wet air
as	dry air
cr	critical
eq	equilibrium
S	product
vap	vapour
vsat	saturated vapour
wb	wet bulb

Dimensionless numbers

Re	Reynolds number
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- Sc Schmidt number
- *Sh* Sherwood number

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