

Study of the Bread Baking Process — II. Mathematical Modelling[†]

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ABSTRACT

A mathematical model of baking was set up and validated experimentally. The model describes heat and mass transport phenomena during baking of a cylindrical bread sample. The model was solved by finite difference numerical method. The model is based on the hypothesis described in a previous work (Zanoni, B., Peri, C. & Pierucci, S. (1993). J. Food Eng., 19, 383–98), that the variation in temperature and moisture of bread during baking is determined by the formation of an evaporation front at 100°C. The progressive advancing of the evaporation front towards the inside of the product determines different conditions of heat and mass transport in a crust and crumb portion. The validation shows that the model correctly simulates heat and mass transfer during baking.

NOTATION

a_w	Water activity, as relative pressure of water in product or air
C_p	Specific heat (J/kg K)
D	Mass diffusion coefficient (m ² /s)
dr	Infinitesimal radial interval (m)
dt	Infinitesimal time interval (s)
dx	Infinitesimal height interval (m)
h	Convective heat transfer coefficient (W/m ² K)

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h_m	Convective mass transfer coefficient (kg/s/m ² /Pa)
h_{tot}	Overall heat transfer coefficient (W/m ² K)
I	Node of the grid system } position of the grid system
J	
P	Vapour pressure (Pa)
P'	Vapour pressure under saturation conditions (Pa)
R	Sample radius (m)
r	Radial position (m)
t	Time (s)
T	Temperature (K)
x	Axial position (m)
X	Sample height (m)
W	Absolute moisture (kg water/kg dry matter)
ΔH	Latent heat of evaporation (J/kg)
ρ	Apparent density (kg/m ³)
λ	Thermal conductivity (W/m K)

Subscripts

d	With respect to dry matter
ext	With respect to environment of the sample, i.e. the inside of the oven
I, J	Position on the grid system
o	Conditions at time $t=0$
ss	With respect to surface
w	With respect to water
[...]	Bracketed terms indicate 'as a function of...'

INTRODUCTION

The setting up of mathematical models of the bread baking process is essential to control and optimize this process. There have been few published works in this area (Kaiser, 1974; Standing, 1974; Kriems & Reinhold, 1980; Hayakawa & Hwang, 1981; De Cindio *et al.*, 1986; De Vries *et al.*, 1989; Savoye *et al.*, 1992). One of the first studies published on this subject was that of Kaiser (1974) who proposed a phenomenological model, where cracker and biscuit baking is assimilated to a drying operation. It is a qualitative, non-mathematical model. Kaiser's hypothesis is, therefore, difficult to verify.

Standing (1974) proposed a mathematical model of biscuit baking in an indirect fired band oven by setting an energy balance between supplied

heat and heat absorbed by the product to increase temperature and evaporate water. The main limitations of this model are: (a) only the average temperature of the product can be predicted, (b) mass transport is not considered, and (c) thermophysical properties are considered to be constant during baking.

Kriems and Reinhold (1980) proposed a mathematical model of bread baking in an indirect fired band oven with vapour injection. In this case, too, mass transport is not considered and thermophysical properties are considered to be constant during baking. In the evaluation of the heat transfer rate these authors consider that the resistance to the internal diffusion of heat greatly exceeds external resistance to convective heating of the bread surface (Biot number $\gg 1$). This assumption is rather arbitrary.

Hayakawa and Hwang (1981) proposed an energy balance model and a mass balance model with reference to the baking process of cracker-like products in an indirect fired band oven. In this case, too, the models, despite the attempt to relate mass transport to heat transfer, appear to be limited because only average moisture and temperature values are evaluated and the product's thermophysical properties are considered to be constant throughout the process.

De Cindio *et al.* (1986) presented a mathematical model of heat transfer during bread baking by solving Fourier's equation for an infinite slab and Biot number $\gg 1$. A model was also set up for the volume increase of the product during baking. The above model is mainly limited by the hypotheses on heating conditions. Also, thermophysical properties are considered to be constant, and mass transport effects are completely neglected.

De Vries *et al.* (1989) set up a mathematical model of simultaneous heat and mass transfer in dough and bread crumb during baking. This model simulates temperature and moisture profiles both inside the dough and inside the crumb during baking, but cannot be applied to bread crust. This model is based on a phenomenological hypothesis, which stresses the effect of air bubbles, contained both in the dough and in the crumb, on heat and mass transfer. According to this phenomenological hypothesis, heat transfer includes the following two different mechanisms: conduction in the so-called liquid phase (i.e. the continuous phase consisting of starch, water, proteins, etc.) and evaporation–condensation in the gas phase (i.e. evaporation, diffusion of water in the gas phase, condensation). Mass transfer is only determined by the evaporation–condensation mechanism.

Savoye *et al.* (1992) have presented a heat and mass transfer model of a gas indirect fired biscuit baking tunnel-oven. This model simulates the

heating of the product in the oven by conductive, convective and radiating heat flow and simultaneously models the product's weight loss.

It is based on the phenomenological hypothesis that the limiting heat and mass transfer phenomena occur at the biscuit's surface (Biot number $\gg 1$). The product's surface is heated by conduction, convection and radiation, and the temperature of the whole product is instantaneously raised to the surface temperature. The product's surface is simultaneously subjected to the following three sequences of mass transport: condensation, drying and boiling. The surface moisture initially increases by condensation, which occurs until the vapour pressure of water in the air is higher than that in the biscuit. When the vapour pressure of water in the air is lower than that in the biscuit, the surface dries. When the same vapour pressure is observed in the oven air and in the biscuit, dehydration by boiling occurs. The moisture inside the product instantaneously becomes the same as the surface moisture.

Concerning this model, it may be observed that the hypothesis of negligible internal resistance to heat and mass transfer may be accepted for thin-layered products, such as biscuits, but not for soft-baked products, such as bread.

The aim of the present work is to set up a mathematical model as versatile and as close as being 'real' as possible. It is based on the phenomenological model of baking reported in a previous work (Zanoni *et al.*, 1993). According to this model, the variation in temperature and moisture of bread during baking is determined by the formation of an evaporation front at 100°C. The progressive advancing of the evaporation front toward the inside of the product results in the formation of two separate regions: the crust, where moisture is very low and temperature asymptotically tends to the oven temperature; and the crumb, where moisture is constant and temperature asymptotically tends to 100°C.

THEORY AND METHODS

Material and equipment

The dough (210 g flour (14.5% moisture, 13% proteins, 0.5% ash, pH 5.7–6.1), 126 g water, 8.4 g baking powder and 4.2 g salt) was placed into a cylindrical steel mould (11.0 cm diameter, 9.7 cm height). Baking was carried out in a forced-convection electric oven, suitably adapted from a GC Carlo Erba oven.

In order to minimize the heat supply by radiation, the oven walls were cooled by an air space circulation system; a glass holder was used to

support the mould over the oven's floor in order to avoid heat supply by conduction. Air speed in the oven was about 1.4 m/s, air temperature was kept at $203 \pm 1^\circ\text{C}$ and the baking time was 30 min.

Further details are reported in Part I of this paper (Zanoni *et al.*, 1993).

Measurement of temperature

Air and bread sample temperatures during baking were measured by thermocouples connected to a data acquisition and recording system (DATASCAN 7220 — Measurement Systems Limited, Newbury, UK) interfaced by RS 232 to a PC.

Measurement of weight loss

The total weight loss of the sample was measured in triplicate during baking (at 5, 10, 15, 20, 25, 30 min) by weighing the dough both before baking and immediately after extraction. The same measurement was performed on a dough sample placed in a mould having the same shape and size as the original mould but consisting of a stainless steel close-mesh net.

Mathematical model

Based on the above experimental conditions and the phenomenological model described in Part I the baking process can be represented as follows. The bread sample, placed in a mould, is modelled as a finite cylinder of radius R and height X (Fig. 1). The changes of volume with baking time are evaluated according to the relationship reported in Table 1 (Zanoni *et al.*, 1993). The rectangular cross-section of the finite cylinder is divided into a grid system whose nodes, I and J, show the sequence of vertical and radial volume elements, respectively.

The sample, at uniform temperature (T_o) and moisture (W_o), is placed into the oven at a temperature T_{ext} and water activity $a_{w,\text{ext}}$.

The sample upper surface, directly exposed to air, is heated by convective heat transfer, and the sides and lower surface, in contact with the mould, are heated by combined convective and conductive heat transfer. The heating of the surface resulted in a conductive heat flux toward the inside of the sample.

At the upper surface, convective mass transport between the sample surface and the air is controlled by the difference between the respective vapour pressures. The upper surface temperature is determined by a

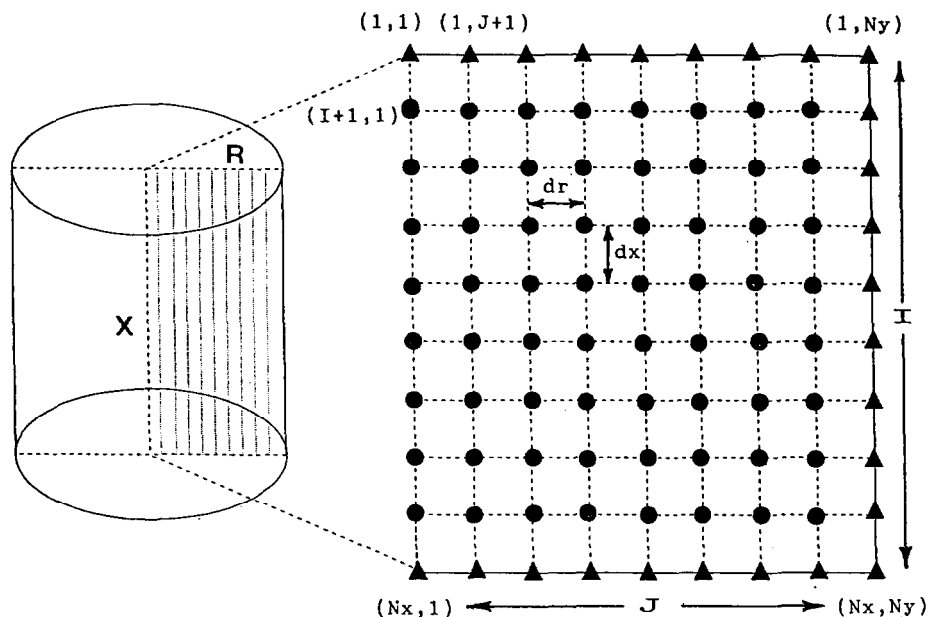


Fig. 1. Subdivision of a rectangular cross-section of the sample for numerical solution of heat and mass transfer equations by finite differences. Internal nodes (•), surface nodes (▲).

combination of the heat supply by convection, the conductive heat transfer toward the inside of the sample and the convective mass transport toward the outside:

$$\frac{dT_{ss}}{dt} = \left(\frac{h(T_{ext} - T_{ss}(I, J))}{dx} + \frac{d^2 T}{dx^2} + \frac{\lambda d^2 T}{dr^2} + \frac{\lambda dT}{dr} \frac{1}{r} \right) \frac{1}{\rho_d C_p} - \frac{h_m}{\rho_d C_p dx} (P_{ss}[T, W] - P_{ext}[T, W]) \Delta H[T, W] \quad (1)$$

where dT is the infinitesimal temperature variation associated with conductive heat transfer with respect to the cylinder height and radius, respectively:

$$dT = (T(I+1, J) - T_{ss}(I, J)) \quad (2)$$

$$dT = (T(I, J+1) - T_{ss}(I, J))$$

TABLE 1
Process Variables and Input Equations for Solving the Model

Dough sample initial weight (g)	341
Sample radius (cm)	5.5
Sample initial height (cm)	4.6
Sample height variation with baking time:	
$\frac{H_t}{H_0} = 1.07 + 9.2 \times 10^{-4}t \quad t \leq 1140 \text{ s}$	
$\frac{H_t}{H_0} = 2.61 - 4.5 \times 10^{-4}t \quad t > 1140$	
Thickness of lateral mould wall (mm)	0.25
Thickness of mould bottom (mm)	0.50
Sample initial temperature (°C)	26
Sample initial moisture (%)	44
Raw sample density (kg/m ³)	950
Oven air temperature (°C)	203
Relative air moisture (%)	70
Baking time (min)	30
Convective heat transfer coefficient at the upper surface (W/m ² °C)	50
Overall heat transfer coefficient at the lateral and lower surface (W/m ² °C)	38
Convective mass transfer coefficient at the upper surface (kg/s/m ² /Pa)	6.0×10^{-9}
Mould thermal conductivity (W/m °C)	45

The upper surface moisture of the sample is determined by the combination of the convective mass transport toward the outside and the water diffusion from inside the sample:

$$\frac{dW_{ss}}{dt} = \frac{D d^2 W}{dx^2} + \frac{D d^2 W}{dr^2} + \frac{D dW}{dr} \frac{1}{r} - \frac{h_m}{\rho_d dx} (P_{ss}[T, W] - P_{ext}[T, W]) \quad (3)$$

where dW is the infinitesimal absolute moisture variation associated with water diffusion with respect to the cylinder height or radius. This variation may be described by similar equations to dT .

The lateral and lower surface temperatures and moistures of the sample are determined from similar equations to the upper surface with the convective mass transport term omitted and a resistance term for heat transfer through both mould walls and a thin layer of still air between the sample and the internal mould wall included.

When the sample surface is at 100°C, dehydration by evaporation at constant temperature is observed, resulting in the formation of an evaporation front. The heat of evaporation is obtained by the difference between the heat supplied to the surface and the heat removed by conduction toward the inside of the sample. The temperature equation is as follows:

$$\frac{dT_{ss}}{dt} = 0 \quad (4)$$

Considering the effect of dehydration by evaporation and water diffusion from inside the sample, the moisture equation for the upper surface is as follows:

$$\frac{dW_{ss}}{dt} = \left\{ \frac{Dd^2W}{dx^2} + \frac{Dd^2W}{dr^2} + \frac{DdW}{dr} \frac{1}{r} - \left[\frac{\left(\frac{h(T_{ext} - T_{ss}(I,J))}{dx} + \frac{\lambda d^2T}{dx^2} + \frac{\lambda d^2T}{dr^2} + \frac{\lambda dT}{dr} \frac{1}{r} \right)}{\rho_d \Delta H[T, W]} \right] \right\} \quad (5)$$

Equation (5) is also applied to the lateral and lower surface.

The temperature of the dried surface increases asymptotically up to the oven temperature, and the evaporation front moves toward the inside. In this case, temperature and moisture equations for the upper surface are as follows:

$$\frac{dT_{ss}}{dt} = \left[\frac{\left(\frac{h(T_{ext} - T_{ss}(I,J))}{dx} + \frac{\lambda d^2T}{dx^2} + \frac{\lambda d^2T}{dr^2} + \frac{\lambda dT}{dr} \frac{1}{r} \right)}{\rho_d C_p} \right] \quad (6)$$

$$\frac{dW_{ss}}{dt} = \frac{Dd^2W}{dx^2} + \frac{Dd^2W}{dr^2} + \frac{DdW}{dr} \frac{1}{r} \quad (7)$$

The same equations are applied to the lateral and lower surface.

The progressive heating and drying of the sample surface results in heat and mass transfer inside the sample.

The sample is heated by conductive heat transfer according to Fourier's equation:

$$\frac{dT}{dt} = \frac{\lambda}{\rho_d C_p} \left(\frac{1}{r} \frac{dT}{dr} + \frac{d^2 T}{dr^2} + \frac{d^2 T}{dx^2} \right) \quad (8)$$

Moisture is controlled by diffusion according to Fick's equation:

$$\frac{dW}{dt} = D \left(\frac{1}{r} \frac{dW}{dr} + \frac{d^2 W}{dr^2} + \frac{d^2 W}{dx^2} \right) \quad (9)$$

When the temperature reaches 100°C, dehydration by evaporation at a constant temperature takes place. The heat of evaporation is obtained from the difference between the supplied heat and the heat transferred toward the core by conduction, and the temperature equation is:

$$\frac{dT}{dt} = 0 \quad (10)$$

The moisture equation is:

$$\frac{dW}{dt} = D \left(\frac{1}{r} \frac{dW}{dr} + \frac{d^2 W}{dr^2} + \frac{d^2 W}{dx^2} \right) - \frac{\lambda}{\rho_d \Delta H[T, W]} \left(\frac{1}{r} \frac{dT}{dr} + \frac{d^2 T}{dr^2} + \frac{d^2 T}{dx^2} \right) \quad (11)$$

When, at the evaporation front, the water has entirely evaporated, the front moves toward the inside, and the temperature and moisture of the dried layer vary according to eqns (8) and (9). Consequently, a difference in bread structure is found: a dried layer, the crust, the thickness increases with baking, and a wet core, the crumb, which remains at constant moisture.

The crust temperature tends asymptotically toward the oven temperature, and the crumb temperature tends asymptotically toward 100°C, i.e. the evaporation front temperature.

Solving the mathematical model

An original numerical computer model in FORTRAN programming language was set up and a Digital VAX 2000 computer (Digital, Milan, Italy) was used to solve the mathematical model.

The symmetric heating of the sample, which has been verified in Part I of this paper, facilitates solving the mathematical model in the same way for any rectangular cross-section of the finite cylinder.

Each cross-section is divided into a grid system whose nodes represent the calculated points of temperature and moisture of the product (Fig. 1). Nodes are marked with I and J to show the sequence of vertical and radial volume elements, respectively.

The above-mentioned equations were solved by the numerical explicit solution by finite differences, i.e. derivatives were replaced with relevant incremental ratios. These equations represent the core of the numerical computer model that permits the determination of moisture and temperature of each node at given time intervals.

Boundary conditions are:

$$\begin{aligned}
 \text{at } t=0 \quad T &= T_0 & \text{for } 0 \leq r \leq R \text{ and } 0 \leq x \leq H \\
 W &= W_0 & \text{for } 0 \leq r \leq R \text{ and } 0 \leq x \leq H \\
 \\
 \text{at } t > 0 \quad T &= T_{ss} & \text{for } r = R \text{ and } 0 \leq x \leq H \\
 T &= T_{ss} & \text{for } x = 0 \text{ and } r \leq x \leq R \\
 T &= T_{ss} & \text{for } x = H \text{ and } r \leq x \leq R \\
 dT/dr &= 0 & \text{for } r = 0
 \end{aligned}$$

A flow diagram describing the computer model is shown in Fig. 2.

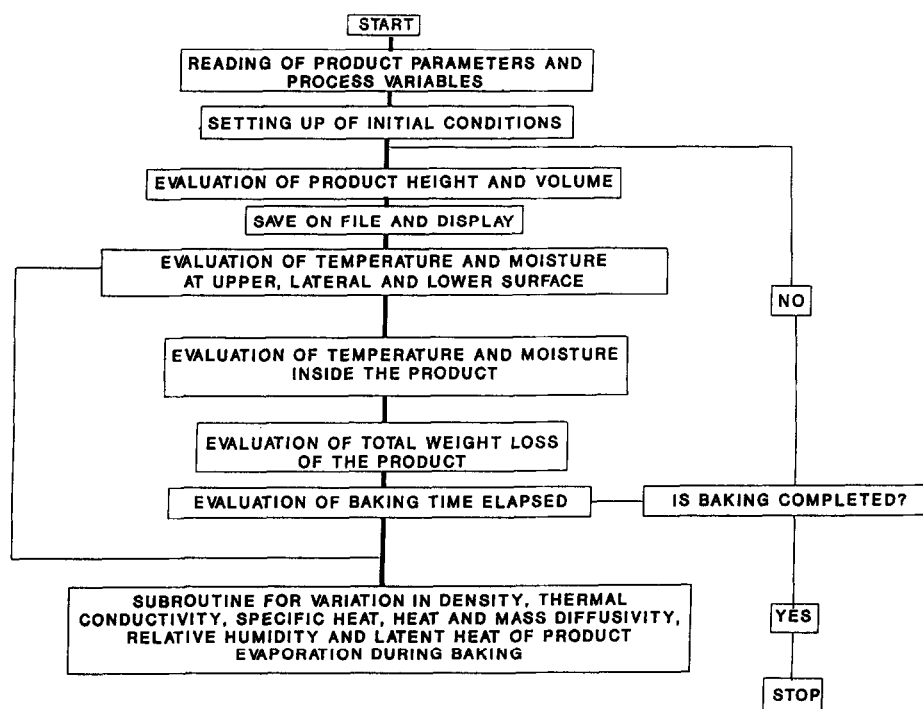


Fig. 2. Flow diagram describing computer program.

Input values and hypotheses for solving the model

Table 1 shows the equations and process variables that were applied to solve the model. Some hypotheses were also proposed to define some operating parameters. Considering the thermophysical properties of the sample, it was assumed that thermal conductivity (λ), density (ρ_d) and specific heat (Cp) vary during baking as follows.

The thermal conductivity varies as a function of moisture content according to the following equation:

$$\lambda = \lambda_d \frac{1}{(1 + W)} + \lambda_w \frac{W}{(1 + W)} \quad (12)$$

where:

$\lambda_d = 0.40 \text{ W/m K}$ (from Tadano, 1987);

$\lambda_w = 0.60 \text{ W/m K}$ (from Polak, 1984).

The density varies as a function of volume increase according to the following equation:

$$\rho_d = \frac{\rho}{(1 + W_o)} \left(\frac{dr_o}{dr} \right)^2 \frac{dx_o}{dx} \quad (13)$$

Since the sample is contained in a stainless steel mould, expansion cannot take place in the radial direction and therefore $(dr_o/dr) = 1$. The specific heat varies as a function of temperature and moisture according to the following equation:

$$Cp = Cp_d + WCp_w \quad (14)$$

where the specific heat of the dry matter (Cp_d) and the specific heat of the water (Cp_w) are calculated as a function of temperature according to the following equations (Zanoni & Petronio, 1991):

$$Cp_d = 5T + 25 \quad (15)$$

$$Cp_w = (5.207 - 73.17 \times 10^{-4}T + 1.35 \times 10^{-5}T^2)1000 \quad (16)$$

The vapour pressure of air in the oven is calculated by the following equation:

$$P_{\text{ext}} = a_{w,\text{ext}} P'_{\text{ext}} \quad (17)$$

where P'_{ext} is derived from Antoine's law (Perry & Green, 1984):

$$P'_{\text{ext}} = 133.3 \exp \left[A_{\text{ANT}} - \frac{B_{\text{ANT}}}{(T_{\text{ext}} + C_{\text{ANT}})} \right] \quad (18)$$

where:

$$A_{\text{ANT}} = 18.3036$$

$$B_{\text{ANT}} = 3816.44 \text{ K}$$

$$C_{\text{ANT}} = -46.13 \text{ K}$$

Similarly the vapour pressure of the surface P_{ss} is calculated by the following equation:

$$P_{\text{ss}} = a_{\text{w,ss}} P'_{\text{ss}} \quad (19)$$

The vapour pressure is calculated as a function of temperature and moisture of the sample. P'_{ss} is calculated as a function of temperature according to Antoine's law (Perry & Green, 1984):

$$P'_{\text{ss}} = 133.3 \exp \left(A_{\text{ANT}} - \frac{B_{\text{ANT}}}{(T_{\text{ss}}(I, J) + C_{\text{ANT}})} \right) \quad (20)$$

From data on adsorption isotherms reported by Lind and Rask (1991), it was assumed that the water in the sample is unbound, i.e. $a_{\text{w}} = 1$, as long as $W \geq 0.43$ and that any sample fraction is dried when it has reached $W = 0.005$, corresponding to a highly bound, non-evaporable water content. Below 0.43, the water activity is calculated as a function of moisture according to the GAB (Guggenheim-Andersson-De Boer) equation (Lind & Rask, 1991):

$$\frac{UR}{W} = \alpha UR^2 + \beta UR + \gamma \quad (21)$$

where:

$$\alpha = -17.19 + 9.83 \times 10^{-3} (T - 273);$$

$$\beta = 19.79 - 0.091 (T - 273);$$

$$\gamma = -1.69 + 0.095 (T - 273).$$

The latent heat of evaporation (ΔH) and the mass diffusion coefficient of water (D) vary as a function of the moisture content of the sample. As long as the sample contains unbound water ($W \geq 0.43$), the latent heat of evaporation is 2.3339 MJ/kg (ΔH_0). When the moisture content drops

below 0.43, the latent heat increases on decreasing moisture according to the Clausius–Clapeyron equation (Perry & Green, 1984) as follows:

$$\Delta H = \frac{k}{(100 W)} + \Delta H_o \quad (22)$$

where:

$k = 2.4948$ MJ/kg dry matter.

When the sample contains unbound water, the mass diffusion coefficient (D) is 1.0×10^{-9} m²/s (D_o). When the moisture content is below 0.43, the diffusion coefficient decreases linearly with moisture according to the following relationship:

$$D[W] = \frac{D_o}{0.43} W \quad (23)$$

$D[W]$ becomes equal to zero at 0.005 moisture.

RESULTS AND CONCLUSIONS

Validation of the mathematical model and conclusions

Calculated and experimental profiles of temperature versus time on the central axis of the sample at the upper surface, the lower surface, 2 cm from the upper surface and 3 cm from the lower surface are reported in Figs 3, 4, 5 and 6, respectively. It can be observed that the model satisfactorily simulates temperature profiles of both bread crust and crumb.

Figure 4, which is related to the sample lower surface in contact with the mould, shows an irregular curve with a constant temperature at 5–10 min. This constant temperature phase is derived from the hypothesis that the evaporation front temperature remains constant at 100°C as long as all the unbound water has evaporated. However, after that time interval, a good correlation between calculated and experimental data is obtained. At the upper surface, which is exposed to hot air, heat transfer is more rapid and the irregular trend less evident.

Concerning mass transport, calculated and experimental weight loss are shown in Fig. 7. Experimental weight loss, obtained by placing the sample into the stainless steel mould described in the 'Theory and Methods' section, is shown by the triangles. The square symbols refer to

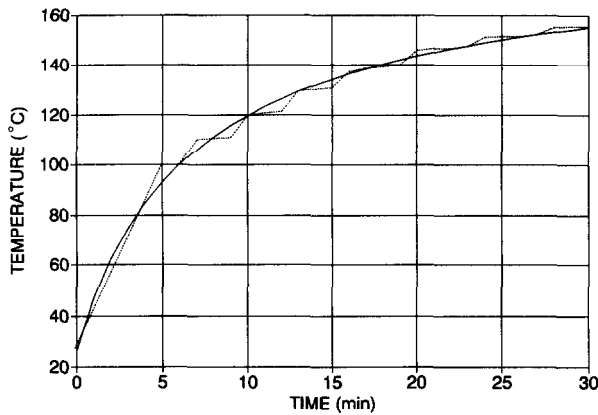


Fig. 3. Calculated (---) and experimental (—) temperature profiles of the sample upper surface at $r=0$.

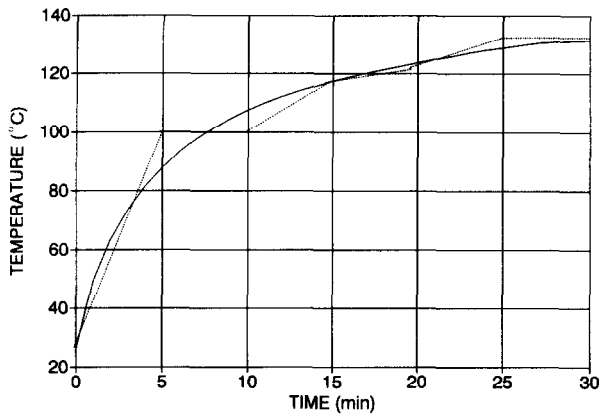


Fig. 4. Calculated (---) and experimental (—) temperature profiles of the sample lower surface at $r=0$.

weight loss obtained under the same experimental conditions as above, but placing the sample into a stainless steel net mould. This facilitates the evaporation of water from the sample surface, resulting in a more rapid weight loss. Calculated data (broken lines) are well correlated with the experimental values obtained using the net mould.

In conclusion, the comparison between experimental and calculated data shows that the phenomenological model, the mathematical model and the values for thermophysical constants proposed in this work satisfactorily represent the real trend of heat and mass transfer during baking.

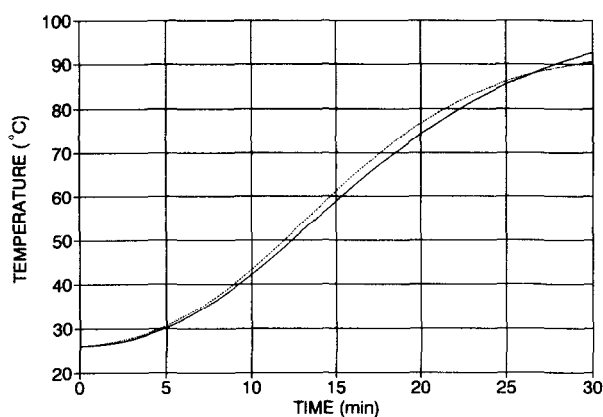


Fig. 5. Calculated (---) and experimental (—) temperature profiles in the crumb, at 2 cm from the sample upper surface and $r=0$.

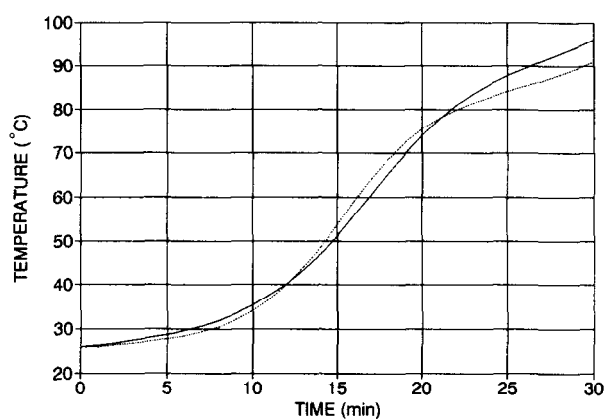


Fig. 6. Calculated (---) and experimental (—) temperature profiles in the crumb, at 3 cm from the sample lower surface and $r=0$.

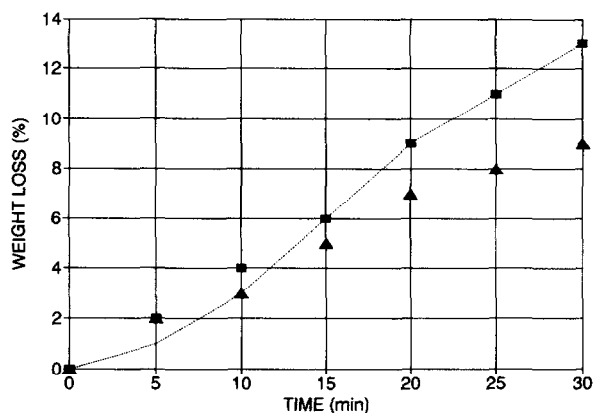


Fig. 7. Calculated and experimental weight loss of the bread sample during baking: ---, calculated; \blacktriangle , experimental (the bread sample is placed in a stainless steel mould); \blacksquare , experimental (the bread sample is placed in a stainless steel net mould).

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