Modeling Heat and Mass Transfer in Bread during Baking

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Abstract: In this paper, we present a first model carried out with Comsol Multiphysics® to model bread baking, considering heat and mass transfer coupled with the phenomenon of swelling. This model predicts the pressures, temperatures and water contents evolutions in the dough for different energy requests. First results obtained are analyzed according to various physical parameters in order to better apprehend interactions between the various mechanisms in the porous matrix.

Keywords: Bread baking, heat and mass transfer, model.

1. Introduction

With energy consumption close to 300 000 tons-equivalent-oil per year, bread baking represents a non negligible part of the energy demand of the French Food sector. An improvement of the energy efficiency of the oven would make it possible to reduce the energy request for this sector and consequently the CO_2 emissions. Before the optimization phase, it is necessary to evaluate the energy needs of the product. This stage needs an increased knowledge and a modeling of the transfer mechanisms in the product, here, a porous medium: bread. Bread is a complex medium in which occur of many physical phenomena during baking: heat and mass transfers (CO_2, liquid water, vapor water), swelling with the formation of a porous structure and various physico-chemical reactions (gelatinization, surface browning: Maillard reaction…).

In this paper, we present physical model designed to describe mass and heat transfer within the porous material during baking. The second part describes the numerical model implemented and the simulated results obtained.

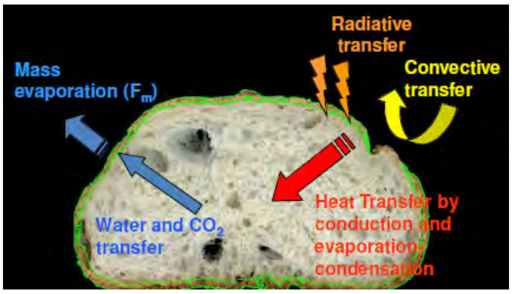

Figure 1. Heat and mass phenomena in bread.

2. Governing equations

A mathematical model based on heat and mass transfer in porous media is used to model the baking of bread. It is derived from mass balance of constituents in different phases: liquid water (l), water vapour (v), CO_2 gas (CO_2). The state variables are the temperature T, the water content W and the total gas pressure P_g. This conservation-based approach was developed for drying theory by Whitaker [1] and Philip and De Vries [2] and used by another authors (Zhang et al. [3]).

2.1. Hypothesis

In this problem, the hypotheses used are:

- medium is homogeneous,
- local thermodynamic equilibrium is achieved,
- liquid phase (l) is not compressible: $\rho_l = cst$,
- the gaseous phase (g) consists of a perfect blend of gas: carbon dioxide (CO_2) and vapour (v), whose equations read as follows:

$$\rho_g^i = \frac{P_j M_j}{RT} \text{ for } j=(v, CO_2) \text{ with } P_g = P_v + P_{CO_2}$$

and $\rho_g^i = \rho_v^i + \rho_{CO_2}^i$ (i: intrinsic)

- radiation and convection are negligible within the material,
- moisture content is the fraction between liquid water mass and dry solid mass: $W = \frac{m_l}{m_s}$.

2.2. Mass conservation

Liquid water phase $$\frac{\partial \rho_l}{\partial t} + \vec{\nabla} \cdot \vec{n}_l = -\vec{K}$$

Vapour phase $$\frac{\partial \rho_v}{\partial t} + \vec{\nabla} \cdot \vec{n}_v = \vec{K}$$

CO_2 phase $$\frac{\partial \rho_{CO_2}}{\partial t} + \vec{\nabla} \cdot \vec{n}_{CO_2} = 0$$

These equations show the matter flows, which are derived from the Fick's law for diffusion and by Darcy's generalised equations giving the mean filtration velocity fields of the liquid and gaseous phases.

Liquid water flux

$$\vec{n}_l = D_l^W \vec{\nabla} W$$

Liquid water diffusion in bread is only due to capillary diffusivity. The measurement of capillary pressure is difficult to obtain, so we have used an expression of the diffusion coefficient obtained by Ni et al. [4], with the parameters of Zhang and Datta [5].

$$D_l^W = C_{k2} \rho_s \exp(-2.8 + 2W)\varepsilon$$

with ε, the porosity and $C_{k2} = 10^{-6}$ a coefficient.

Vapor flux

$$\vec{n}_v = -\rho_v^i \frac{kk_{rg}}{\mu_g}\left(\vec{\nabla} P_g - \rho_g^i \vec{g}\right) - \rho_g^i D_{eff} \vec{\nabla} \omega_v$$

ω_v being the mass fraction of the vapour in the gaseous phase, given by:

$$\omega_v = \frac{m_v}{m_g}$$

CO_2 flux

$$\vec{n}_{CO_2} = -\rho_{CO_2}^i \frac{kk_{rg}}{\mu_g}\left(\vec{\nabla} P_g - \rho_g^i \vec{g}\right) - \rho_g^i D_{eff} \vec{\nabla} \omega_{CO_2}$$

Moisture content equation

This equation is established by liquid water and vapour mass conservation equation sum.

$$\rho_s \frac{\partial W}{\partial t} + \vec{\nabla} \cdot \left[\left(D_l^W + D_v^W\right)\vec{\nabla} W + D_v^T \vec{\nabla} T + D_v^{P_g} \vec{\nabla} P_g\right] = -\left(\beta_1 \frac{\partial T}{\partial t} + \beta_2 \frac{\partial W}{\partial t}\right)$$

Terms with beta coefficient are obtained from vapor phase conservation equation. By including the gradients of the state variables in the expressions of mass flow, the diffusion coefficients appear (see appendix). This model is based on Salagnac et al. [6] developments.

Energy conservation equation

Heat transfer occurs in three forms: conduction, convection and latent heat moved outward by the vapor diffusion. The convective term is negligible compared to the latent heat:

$$\rho C_p \frac{\partial T}{\partial t} + \rho_g C_{p,g} \vec{v}_g \vec{\nabla} T = \vec{\nabla} \cdot \left(\lambda \vec{\nabla} T\right) - \vec{K} L_v$$

with $\rho C_p = \rho_s C_{p,s} + \rho_l C_{p,l} + \rho_g C_{p,g}$ and λ, the effective thermal conductivity. The necessary energy for the water vaporisation is obtained by the product of the phase change rate K and the latent heat of vaporisation L_v. The evaporation rate, K, is given by Zhang and Datta [3] and, obtains with the liquid water conservation equation:

$$K = -\rho_s \frac{\partial W}{\partial t} + \vec{\nabla} \cdot \left(D_l^W \vec{\nabla} W\right)$$

Gas pressure equation

The equation for the total pressure of the gaseous phase P_g is obtained from the readings of the mass balance on CO_2.

$$\frac{\partial P_g}{\partial t} = \frac{1}{\gamma_3}\left[\begin{array}{l} -\vec{\nabla} \cdot \left(D_{CO_2}^W \vec{\nabla} W + D_{CO_2}^T \vec{\nabla} T + D_{CO_2}^{P_g} \vec{\nabla} P_g\right) \\ -\gamma_1 \dfrac{\partial T}{\partial t} - \gamma_2 \dfrac{\partial W}{\partial t} \end{array}\right]$$

2.3. Boundaries conditions

The boundaries conditions on air/bread interface are for:

Heat equation

$$-\vec{n} \cdot \left(\lambda \vec{\nabla} T\right) = h(T_{air} - T)$$

with h, the heat coefficient (convection and radiation phenomena).

Water content equation

Evaporated mass flux is equal to the sum of liquid water and vapor water flux.

$$-\vec{n} \cdot \left(D_l^W + D_v^W\right)\vec{\nabla} W = F_m$$

Evaporated mass flux on surface is given by:

$$F_m = k_m \left(\frac{P_t M_v}{RT_{film}}\right) \ln\left(1 + \left(\frac{P_{v,surf} - P_{v,\inf}}{P_t - P_{v,surf}}\right)\right)$$

Gas pressure equation

Atmospheric pressure is considered on bread surface.

$$P_g = P_{atm}$$

3. Physical properties and parameters

Physical properties are chosen for typical French bread.

Vapor pressure and water activity

Vapor pressure is obtained by an equilibrium approach.

$$P_v = a_w P_{vs}$$

The water activity (a_w) have been determined by Lind and Rask [7], Vanin [8], Jury [10], Zhang and Datta [5] with different models.

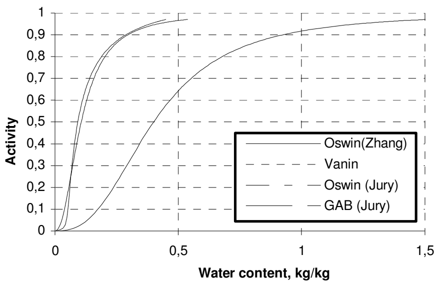

Figure 2. Activity models for bread.

The Oswin model fitted by Zhang and Datta [5] is used.

$$a_w = \left(\left(\frac{100W}{\exp(-0.0056T + 5.5)} \right)^{-1/0.38} + 1 \right)^{-1}$$

Thermal conductivity

Heat transfer in the porous media is described by two phenomena, conduction and evaporation-condensation. Two solutions are developed in bibliography, some authors use multiphase model of conductivity and others an experimental effective conductivity. In this paper, an effective conductivity, taking into account evaporation-condensation and conduction phenomena has been used. The values of thermal conductivity come from experimental data of Jury et al. [10] and have been fitted by Purlis and Salvadori [11].

$$\lambda = \begin{cases} \dfrac{0.9}{1 + \exp(-0.1(T - 353.16))} + 0.2 & if\ T \le T_f - \Delta T \\ 0.2 & if\ T > T_f + \Delta T \end{cases}$$

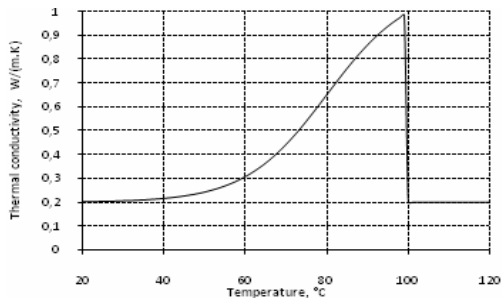

Figure 3. Effective thermal conductivity.

Diffusivity of vapor water in CO_2 is given by:

$$D_{eff} = D_{vc} \left[(1 - 1.11S)\varepsilon \right]^{4/3}$$

Table 1: Input parameters.

Parameters	Values	Units
Initial moisture content, W_0	0.54	kg of water/kg of dry solid
Initial temperature, T_0	27	°C
Initial pressure, P_{g0}	$1.013\ 10^5$	Pa
Initial dough density, ρ_0	305.4	kg/m^3
Intrinsic density of solid matrix, ρ_s^i	705	kg/m^3
Initial porosity	0.72	-
Oven gas temperature, T_{air}	190	°C
heat transfer coefficient, h	10	W/(m^2.K)
Convective mass transfer coefficient, k_m	0.01	m/s
Vapor pressure in surrounding air, $P_{v,\ inf}$	0	Pa
Gas intrinsic permeability, k	$2.5\ 10^{-12}$	m^2
Gas relative permeability, k_{rg}	$1 - 1.1S$ for $S \le 0.9$ 0 for $S > 0.9$	-
Standard binary diffusivity, D_{vc}	$2\ 10^{-5}$	m^2/s

Bread swelling

To simulate the volume expansion of the bread, different mechanical models exist (Zhang [13], Vanin [8]). In first approximation, we introduced into the model a deformation of the bread coming from numerical results (Zhang [13]). In this case, the volume expansion is a function of time and is given by a radius expression:

$$R(t)=\left(\frac{V_0\,\alpha(t)}{\pi}\right)^{0.5} \quad \text{with:}$$

$$\alpha(t)=\begin{cases} \left.\begin{array}{l} -2\,10^{-4}\left(\frac{t}{60}\right)^5+5\,10^{-3}\left(\frac{t}{60}\right)^4 \\ -4.49\,10^{-2}\left(\frac{t}{60}\right)^3 \\ +1.517\,10^{-1}\left(\frac{t}{60}\right)^2 \\ +4.8\,10^{-3}\left(\frac{t}{60}\right)+0.9968 \end{array}\right\} \text{for } t\le 360\ s \\ 1.7132 \quad \text{for } t>360\ s \end{cases}$$

4. Numerical model

The numerical model was programmed with Comsol Multiphysics®. The geometry is 2D cylindrical. The initial radius of bread is 36.5 mm. A mobile triangular meshing (ALE) with 548 elements is used.

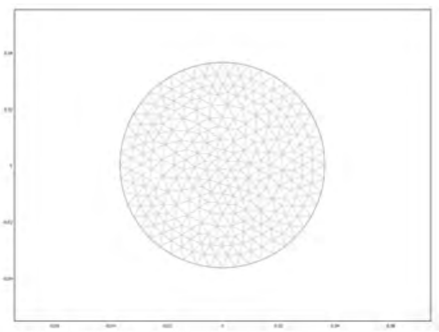

Figure 4. Geometry and mesh.

The equations are simultaneously resolved with a free step time by the solver UMFPACK. A baking of 15 min is calculated in 47 s. All equations are implemented with PDE formulations in general form time dependant:

$$d_a\frac{\partial u}{\partial t}+\nabla\cdot\Gamma=F \quad \textit{inside domain}$$

$$\left.\begin{array}{l} -n\cdot\Gamma=G \\ 0=R \end{array}\right\} \quad \textit{on domain boundary}$$

with u the variable corresponding to T, W and P_g. Equations have to be identified in different PDE terms. It is difficult to implement an equilibrium approach in commercial software due to divergence of heat source term corresponding to phase change. The choice of general form makes it possible to introduce this approach.

Heat source term has been modified to correspond to the PDE general form:

$$\rho C_p\frac{\partial T}{\partial t}+\vec{\nabla}\cdot\left(-\lambda\vec{\nabla}T+D_l^W L_v\vec{\nabla}W\right)=-\rho_g C_{p,g}\vec{v}_g\cdot\vec{\nabla}T$$
$$-D_l^W\vec{\nabla}W\cdot\vec{\nabla}L_v+\rho_s^a\frac{\partial W}{\partial t}L_v$$

5. Results

Simulation has been realised for a 15 min baking in an oven at 190°C. Simulated results are compared with Zhang and Datta [13] experimental data.

Figure 5 presents the evolution of temperature obtained in the center and at 1.5 mm of the surface.

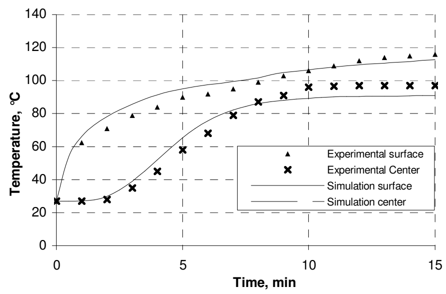

Figure 5. Temperatures in bread.

Temperature evolutions of numerical model are in good agreement with experimental data. The surface temperature increases until the end of baking. At 8 min, the slope break of the curve shows the phenomenon of evaporation. In the center of bread, the temperature increases but stay under 100°C.

Figure 6 presents the evolution of mean moisture content.

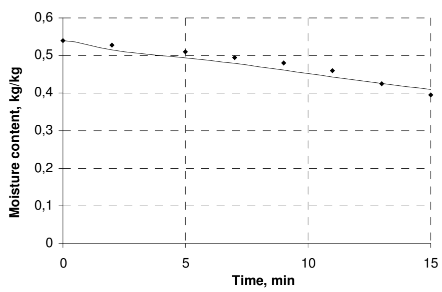

Figure 6. Mean moisture content in bread.

Moisture content evolution corresponds very well to experimental data. The quantity of liquid water decreases almost linearly with time during baking.

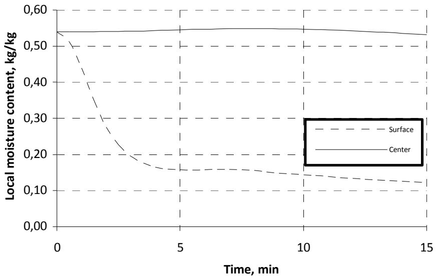

Figure 7. Local moisture content in bread.

As for the local moisture contents, one notices a light increase in moisture content in the center of the bread (dough) during baking. This phenomenon is caused by the evaporation-condensation phenomenon in crumb. In surface (crust), moisture content decreases in few minutes. This evolution corresponds well to typical baking evolution (Wagner [14]).

6. Conclusion

A mathematical model has been developed for bread baking. The numerical model has been computed with Comsol Multiphysics® in deformed mesh. Deformed mesh provide to model bread deformation during baking. Some modifications have been used to compute phase change in heat transfer equation. Temperature and moisture content evolution are in good agreement with experimental data.

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8. Acknowledgements

The authors want to thank the National Research Agency of France (ANR) for its financial contribution (ANR ALIA-BRAISE).

9. Appendix

Vapor diffusion coefficients:

$$D_v^W = -D^{eff}\left(\frac{M_v M_{CO_2}}{M_g RT}\right)\frac{\partial P_v}{\partial W}$$

$$D_v^T = -D^{eff}\left(\frac{M_v M_{CO_2}}{M_g RT}\right)\frac{\partial P_v}{\partial T}$$

$$D_v^{P_g} = -\left[\rho_v^i \frac{k_g}{\mu_g} - D^{eff}\left(\frac{M_v M_{CO_2}}{M_g RT}\right)\frac{P_v}{P_g}\right]$$

CO_2 diffusion coefficients:

$$D_{CO_2}^{W} = -D_v^{W}$$

$$D_{CO_2}^{T} = -D_v^{T}$$

$$D_{CO_2}^{P_g} = -\rho_{CO_2}^{i} \frac{k_g}{\mu_g} - D^{eff}\left(\frac{M_v M_{CO_2}}{M_g RT}\right)\frac{P_v}{P_g}$$

Other coefficients:

$$\gamma_1 = \gamma_3\left[\frac{P_v - P_g}{T} - \frac{\partial P_v}{\partial T}\right]$$

$$\gamma_2 = -\gamma_3\left[\frac{\partial P_v}{\partial W} - \frac{\rho_s\left(P_g - P_v\right)}{\rho_l^i \varepsilon (1-S)}\right]$$

$$\gamma_3 = \frac{\varepsilon M_{CO_2}(1-S)}{RT}$$

$$\beta_1 = \frac{\varepsilon M_v (1-S)}{RT}\left[\frac{\partial P_v}{\partial T} - \frac{P_v}{T}\right]$$

$$\beta_2 = \frac{\varepsilon M_v (1-S)}{RT}\left[\frac{\partial P_v}{\partial W}\right]$$