

Transport Processes and Large Deformation During Baking of Bread

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A model of multiphase transport in a porous medium coupled with large deformation of the porous matrix is developed and applied to the process of bread baking. Transport-governing equations are based on energy conservation and mass conservation of water, water vapor, and CO₂ produced during baking. Deformation is caused by the pressure gradient from internal evaporation and CO₂ generation. Temperature, moisture, and pressure changes in turn are affected by deformation. Bread is assumed to be viscoelastic, mechanical properties of which are functions of temperature. Geometric nonlinear effects are considered in the mechanics problem. Results are compared with those from baking experiments and literature data. Vapor pressure inside the matrix is likely to be lower than the equilibrium vapor pressure. Convective heat transfer is small compared to heat conduction and evaporation–condensation of water vapor promotes heat transfer to the inside. Rate of CO₂ generation, mechanical properties of dough, and gravity together determine the final shape of the bread. © 2005 American Institute of Chemical Engineers AIChE J, 51: 2569–2580, 2005

Keywords: coupled transport and deformation, evaporation, viscoelasticity, food processing, model

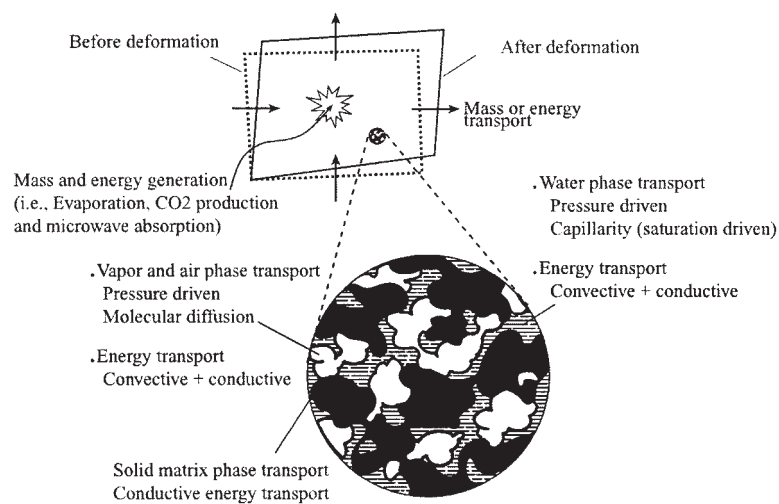
Introduction

Although baking of bread has a history of a few thousand years,¹ our engineering understanding of bread baking is still quite limited. Even today, “cook and look” still seems to be the dominant method to improve bread baking for better taste, color, or aroma. One of the possible reasons is that baking involves many complex physical and chemical processes such as heat and moisture transfer, deformation, starch gelatinization, and other biochemical reactions. Moreover, these processes are coupled and influence each other. Although biochemical reactions are crucial to bread quality such as flavor

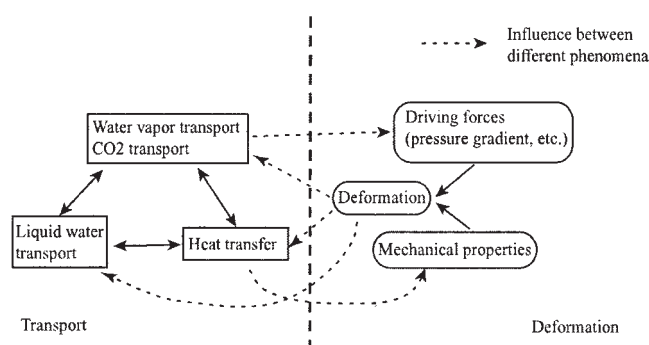
and color, these reactions are directly affected by changes of temperature, moisture content, and volume during baking, which are also of great importance and constitute the subject of this study. Understanding of these fundamentals will help provide a more rational basis for improving bread quality, making it consistent, and automating the process.

Physical processes and material properties related to transport and deformation in the bread baking process are shown in Figure 1. Transport involves four phases: solid, liquid water, water vapor, and CO₂. Water vapor and CO₂ are the major gases in the bread,² so other gases are neglected here. There are many transport modes in bread baking. Heat transfer occurs in all phases and influences moisture transfer. CO₂ generation mainly occurs between 40 and 60°C and is therefore influenced by heat transfer. On the other hand, convection of gas and liquid may contribute to heat transfer.

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(a) System diagram of the coupled transport and deformation in porous media



(b) Coupling mechanisms in the baking process

Figure 1. Physical processes in bread baking.

Deformation is a result of transport, driven by pressure inside the bread. Mechanical properties of bread change with temperature and moisture content. In turn, deformation affects transport through dimension change, porosity, and effective thermal conductivity and so on. Therefore, transport and deformation form a very complex picture in bread baking.

There have been a few modeling studies on baking in the past, which usually focus on only one aspect of the overall picture—transport without volume change³ or volume expansion without considering transport.^{2,4} Because transport and volume expansion are strongly coupled in baking, some questions have not been adequately answered by previous simplified models. For example:

(1) How is moisture removed? Water in bread is in two forms: liquid water and vapor. Previous models usually lump all mechanisms in an effective diffusivity.^{5,6} There are many modes of moisture transport, such as diffusion, capillarity, and pressure-driven flow; using just one parameter—the effective diffusivity—cannot describe all these changes. To better understand the baking process, transport in different phases and through different mechanisms must be considered.

(2) Are convection and evaporation important in baking? Previous modeling studies rarely consider the effect of convection. In addition, starch gelatinization occurs in bread baking,

which tends to limit the movement of water and makes moisture transport and evaporation different from these phenomena in other heating processes. No evaluation of such factors has been reported in the literature.

(3) How to model the deformation and how is it affected by transport processes? Deformation is usually ignored in modeling of transport during bread baking. Some other studies (such as that by Fan et al.²), on the other hand, model the deformation without considering transport. Instead of solving the balance equations governing the deformation of bread dough, the model treats the whole bread as a gas bubble. Different behaviors of the crust and the crumb, a key factor for bread deformation, are not available in a bubble model.

Thus, it is critical to couple deformation and transport to get a better understanding of these processes. Some multiphase transport models for porous media have been developed without considering deformation^{7–10} or small deformation.¹¹ Such models are not valid because large deformation occurs during bread baking. In this study, the specific objectives are to: (1) construct a coupled large deformation and multiphase heat- and mass-transfer model for bread baking; (2) explain the transport of heat and moisture and deformation during the baking process.

Model Development

As outlined in Figure 1, the two major physical phenomena involved in bread baking are multiphase transport and large deformation. Governing equations, boundary conditions, and input parameters for these coupled processes in porous media are developed in this section.

Governing equations

Four mass species considered in this model are solid, liquid water, water vapor, and CO₂, all of which are assumed to be continuous in the porous medium and have the same temperature at any spatial location. Water vapor and CO₂ are assumed to be ideal gases. Governing equations for multiphase transport in a porous medium are developed based on conservation of energy and the three mass species, as follows:

Energy Conservation

$$\frac{\partial(\sum \rho_i c_{pi})T}{\partial t} + \sum \rho_i c_{pi} \nabla \cdot (v_i T) = \nabla \cdot (k \nabla T) - \lambda I_v \quad (1)$$

Liquid Water Conservation

$$\rho_s \frac{\partial M}{\partial t} + \frac{\rho_s M}{V} \frac{\partial(\nabla \cdot \mathbf{u})}{\partial t} = -\nabla \cdot \mathbf{n}_w - I_v \quad (2)$$

Water Vapor Conservation

$$n(1-S) \frac{\partial(p_v M_v / RT)}{\partial t} + \frac{(1-S)\rho_v}{V} \frac{\partial(\nabla \cdot \mathbf{u})}{\partial t} = -\nabla \cdot \mathbf{n}_v + I_v \quad (3)$$

CO₂ Conservation

$$n(1-S) \frac{\partial(p_c M_c / RT)}{\partial t} + \frac{(1-S)\rho_c}{V} \frac{\partial(\nabla \cdot \mathbf{u})}{\partial t} = -\nabla \cdot \mathbf{n}_c + I_c \quad (4)$$

In Eq. 1, the energy related to CO₂ generation is assumed to be negligible. The vapor and CO₂ fluxes \mathbf{n}_v and \mathbf{n}_c are attributed to the total pressure gradient and binary diffusion^{12,13}

$$\mathbf{n}_v = -\rho_v \frac{k_g}{\mu_g} (\nabla p_v + \nabla p_c) - M_v CD_{eff,g} \nabla x_v \quad (5)$$

$$\mathbf{n}_c = -\rho_c \frac{k_g}{\mu_g} (\nabla p_v + \nabla p_c) - M_c CD_{eff,g} \nabla x_c \quad (6)$$

Liquid water transport is attributed to the water pressure gradient and can be described using Darcy's Law

$$\mathbf{n}_w = -\rho_w \frac{k_w}{\mu_w} \nabla p_w \quad (7)$$

Because the evaporation rate I_v is unknown, Eqs. 2 and 3 are combined to form the total moisture equation

$$\rho_s \frac{\partial M}{\partial t} + \frac{\rho_s M}{V} \frac{\partial(\nabla \cdot \mathbf{u})}{\partial t} + n(1-S) \frac{\partial(p_v M_v / RT)}{\partial t} + \frac{(1-S)\rho_v}{V} \frac{\partial(\nabla \cdot \mathbf{u})}{\partial t} = -\nabla \cdot \mathbf{n}_w - \nabla \cdot \mathbf{n}_v \quad (8)$$

where the evaporation rate I_v is eliminated. The evaporation rate I_v in the energy Eq. 1 is substituted using the vapor Eq. 3. Vapor pressure at a given temperature and moisture content is available for a hygroscopic material, that is,

$$p_v = p_v(T, M) \quad (9)$$

Equations 1, 4, 8, and 9 constitute the four equations with the four unknown parameters T , M , p_v , and p_c .

The governing equation for deformation is based on the *principle of virtual work* (PVW). Using a nonlinear mechanics convention in the updated Lagrange (U.L.) format, one has¹⁴

$$\int_V (\mathbf{S} + \Delta \mathbf{S}) \delta \boldsymbol{\varepsilon} dV = \int_V \mathbf{f} \delta \mathbf{u} dV \quad (10)$$

In Eq. 10, \mathbf{S} is Kirchhoff stress and $\boldsymbol{\varepsilon}$ is the Green strain in the updated geometry at time t . The Kirchhoff stress increment is

$$\Delta \mathbf{S} = \mathbf{D}[\Delta \boldsymbol{\varepsilon} - \Delta \boldsymbol{\varepsilon}^{(n)}] \quad (11)$$

In the above equations, Δ means increment. It is assumed here that the elasticity matrix can be expressed as

$$\mathbf{D} = E \mathbf{D}_0(\nu) \quad (12)$$

where \mathbf{D}_0 is related only to Poisson's ratio.¹⁴ The nonelastic strain in Eq. 11 can be written as

$$\Delta \boldsymbol{\varepsilon}^{(n)} = [\mathbf{D}^{(n)}]^{-1} \mathbf{S} \Delta t \quad (13)$$

It is assumed that the nonelastic behavior of dough can be described by a Maxwell model. The classical one-dimensional (1-D) Maxwell model in tension for small deformation has the form

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^{(e)} + \dot{\boldsymbol{\varepsilon}}^{(n)} = \frac{\dot{\boldsymbol{\sigma}}}{E} + \frac{\boldsymbol{\sigma}}{\eta} \quad (14)$$

where $\boldsymbol{\sigma}$ is the stress, $\boldsymbol{\varepsilon}$ is the strain, and the relaxation time τ is defined as

$$\tau = \frac{\eta}{E} \quad (15)$$

It is well known (see, for example, Christensen¹⁵) that a Maxwell model, although typically classified as a "fluid" model, can in fact be used to model a continuum of material behavior, from "solid"-like to "fluid"-like. This can be accomplished by the appropriate choice of the relaxation time: low τ models,

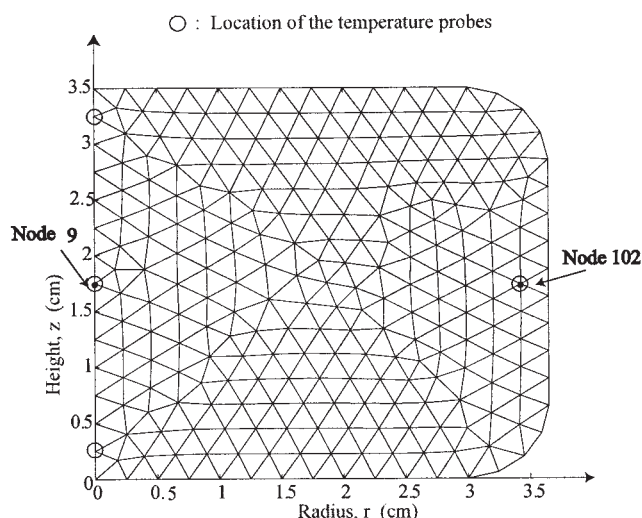


Figure 2. Initial geometry and mesh used in the modeling study.

There are 459 axisymmetric triangular elements and 258 nodes. Circles indicate the locations of temperature probes in the experiment.

fluid-like; and high τ models, solid-like behavior. Several examples of publications in which the authors have used the Maxwell model to describe dough behavior can be seen in Maache-Rezzoug et al.¹⁶ and Ramkumar et al.¹⁷ Generalizing the Maxwell model to the large-deformation situation of interest in this work, one then has (see Eq. 12)

$$D^{(n)} = \eta D_0(v) \quad (16)$$

The right-hand side of Eq. 10 is the work done by internal pressure and gravity. The forces in component form can be written as

$$f_i = -\frac{\partial(p_v^{l+1} + p_c^{l+1})}{\partial x_i^{l+1}} + \rho^{l+1} g_i \quad (17)$$

Displacement \mathbf{u} is solved through Eq. 10 and geometry of the computation domain is updated at the end of each time step. This formulation can be used for large deformation, as would be true for bread baking, given that nonlinear strain and stress have been considered here.

Initial and boundary conditions

An axisymmetric geometry, as shown in Figure 2, is used as the initial state (before deformation). The initial conditions are given by

$$T = T_0 \quad M = M_0 \quad p_c = 1.013 \times 10^5 - p_v(T_0, M_0) \quad (18)$$

$$\mathbf{u} = 0 \quad (19)$$

The boundary conditions at the line of symmetry are given by

$$\frac{\partial \phi}{\partial r} = 0 \quad \text{at} \quad r = 0 \quad (20)$$

where ϕ represents T , M , and p_c . Moisture loss at the top and the side surfaces occurs through convection and there is no surface traction for the mechanics problem. Therefore

$$\mathbf{n}_m|_s \cdot \mathbf{n} = h_m(\rho_v - \rho_{vf}) \quad (21)$$

$$\mathbf{S} \cdot \mathbf{n} = 0 \quad (22)$$

Heat transfer occurs through convection and radiation. Modeling of radiation requires the emissivities of bread, gas, oven surface, and computation of geometric relationships between bread and oven. Consideration of radiative heat exchange is simplified by including the radiative effect in an overall heat-transfer coefficient. In this way, the influence of the oven on the bread, in terms of heat transfer, can still be maintained through the heat-transfer coefficient and gas temperature. The boundary conditions at the top and side surfaces therefore can be written as

$$\mathbf{q}|_s \cdot \mathbf{n} = h(T - T_f) \quad (23)$$

The bottom of the bread is supported during experimentation using a metal screen. Because the screen is thin and the area of the metallic part of the screen is much smaller than that of the bread bottom, the same heat and moisture transfer boundary conditions are used at the bottom as those at the top and the side of the bread.

The mechanics boundary condition at the line of symmetry is

$$u_r = 0 \quad \text{at} \quad r = 0 \quad (24)$$

At the bottom surface, special considerations are necessary. Initially, when the bread dough is soft, it tends to relax as a result of gravity. The plate stops the bottom surface from going downward at that time. After heating for some time, the outer region of the bottom surface may tend to go up as a result of the tension from the upper part of the bread. To realize this, displacement of a bottom node is monitored at the end of the first iteration in each time step. If the displacement is negative, it is forced to be zero for this time step. If it is positive, traction at that node is set to zero so that it can go up freely. For the first iteration, this can be written as

$$\mathbf{S} \cdot \mathbf{n} = 0 \quad (25)$$

After the first iteration,

$$\begin{cases} u_z = 0 & \text{if } u_z < 0 \text{ at the end of the first iteration} \\ \mathbf{S} \cdot \mathbf{n} = 0 & \text{if } u_z \geq 0 \text{ at the end of the first iteration} \end{cases} \quad (26)$$

Material properties and input parameters

Some of the input parameters are shown in Table 1 and the rest are discussed in detail in this section. Not all parameters are available for the exact material and process. One of the

Table 1. Some Input Parameters Used in Modeling of Bread Baking

Item	Value	Unit
1. Initial moisture content*	0.54	kg water/kg dry solid
2. Initial temperature*	27	°C
3. Initial dough density*	305.4	kg/m ³
4. Initial gas volume ratio ³¹	0.61	
5. Initial porosity (calculated based on 3 and 4)	0.72	
6. Density of dry flour (calculated based on 3, 4, and 5)	705	kg/m ³
7. Conductivity of solid matrix ³²	0.309	W/mK
8. Oven gas temperature*	190	°C
9. Convective heat transfer coefficient ¹⁸	10	W m ⁻² s ⁻¹
10. Convective mass transfer coefficient ¹⁸	0.01	m/s
11. Vapor pressure of water in surrounding air**	0	Pa

*Parameters measured experimentally in this study.

**Assumed value based on actual heating condition.

goals of this paper is to identify the likely ranges of parameter values through sensitivity analysis of the process and by comparing with experimental observations.

Thermal Conductivity. Thermal conductivity of multiphase porous materials has been shown to be somewhere in between that predicted by series and parallel models and is higher than that of a series model. A model that predicts thermal conductivity in between the series and the parallel models is¹⁸

$$k = k_s^{(1-n)} k_w^n k_g^{n(1-S)} \quad (27)$$

This model is used here to predict the dough's thermal conductivity k as it changes during baking.

Gas Diffusivities and Permeabilities. Diffusivity of water vapor in CO₂ in the pores is given by⁹

$$D_{eff,g} = D_{vc}[(1 - 1.11S)n]^{4/3} \quad (28)$$

where D_{vc} is the binary diffusivity between vapor and CO₂.

Permeability is for pressure-driven flow and is related to structure, such as pore size and connectivity. Pore size ranges from about 1 μ m to several millimeters and obtaining an accurate value for the permeability is difficult. Measurement of permeability of dough at different baking stages has not been reported. In preliminary studies, it is found that large permeability causes almost no pressure buildup inside the dough. Permeability of 2.5×10^{-12} m² is chosen such that appreciable internal pressure appears to generate deformation. During the later stages, small pores still dominate the crust and the intrinsic permeability value of 2.5×10^{-12} m² is used, based on sensitivity analysis, such that internal pressure can be formed to cause deformation. The intrinsic permeability value for the crumb is chosen to be 10^{-11} m² because it is known that the crumb region has much larger pore size and better pore connectivity. Even higher intrinsic permeability does not make a substantial difference in the internal pressure distribution and pressure drop mainly occurs across the crust region. Gas relative permeability is chosen as⁹

$$k_{gr} = \begin{cases} 1 - 1.1 & \text{for } S < 0.9 \\ 0 & \text{for } S \geq 0.9 \end{cases} \quad (29)$$

Overall permeability is the product of intrinsic permeability and relative permeability, that is,

$$k_g = k_m k_{gr} \quad (30)$$

Liquid Water Diffusivity and Permeability. Transport of liquid water in bread during baking is affected by starch gelatinization around 60°C. Before gelatinization, free liquid water may still exist. During gelatinization, starch absorbs a large amount of water,¹⁹ drastically reducing the mobility of water. Here the relationship between water capillary diffusivity and moisture content in the dough is based on Ni et al.,⁹ as follows

$$D_w = C_d \rho_w \exp(-2.8 + 2M)n \quad (31)$$

The coefficient C_d is chosen as 1.0×10^{-9} such that diffusivity at the end of baking (about 1.2×10^{-7} m²/s) matches the diffusivity reported for heating of bread.²⁰

Bread crumb pores are very large because of CO₂ generation, which means a large intrinsic permeability for the fluids that are filling the pores and are flowing in the porous structure. However, liquid water is strongly bound to starch and may not even be continuous. Therefore relative permeability for liquid water is chosen to be zero, which means there is no pressure-driven liquid water flow in baking.

Rate of CO₂ Generation. Generation of CO₂ is considered to arise from yeast only because yeast is more often used in bread baking. The following form of temperature dependency is assumed for the rate of CO₂ generation

$$R = R_0 \exp\left(-\frac{T - T_m}{\Delta T}\right)^2 \quad [\text{kg CO}_2/\text{kg flour} \cdot \text{s}] \quad (32)$$

The CO₂ generation rate I_c in Eq. 4 is

$$I_c = \rho_s R \quad (33)$$

This model of CO₂ generation is consistent with experimental observation.¹⁹ The parameters T_m and ΔT in Eq. 32 are chosen to be 40 and 10°C, respectively, such that CO₂ generation occurs mostly between 20 and 60°C with a peak at 40°C, whereas the parameter R_0 is chosen to be 1×10^{-4} such that the total amount of CO₂ generated is approximately that reported for a typical baking process.¹⁹

Water Activity. In some previous studies on multiphase heat and mass transfer,^{8,9} it has been assumed that water and

water vapor are in equilibrium at a spatial location in the porous media at any temperature and moisture content. This assumption is adopted here as well, which enables vapor pressure to be obtained using Eq. 9.

Vapor pressure is related to available water activity a_w , which is defined as the ratio of equilibrium vapor pressure in porous media at a certain temperature and moisture content vs. the vapor pressure of pure water at the same temperature,²¹ that is,

$$a_w = \frac{p_v}{p_{v, \text{sat}}} \quad (34)$$

Baking is a dynamic process with rapid changes in temperature and moisture content. Water activity data in dough during such a rapid process are unavailable. Water activity data from Lind and Rask²² are used initially because they include values for dough and bread crust at temperatures of 30 and 90°C, respectively, perhaps the closest available data for bread baking. Water activity at other temperatures is interpolated or extrapolated based on these two data points. When the water activity model in Lind and Rask²² is used, much faster moisture loss and slower temperature increase are found in simulation of baking process, which suggests that actual vapor pressure may be lower. As a matter of fact, it is reported²³ that the time to reach equilibrium is about 180 min for a 3- to 5-g sample in an 18-mL container at around 32°C. In such a small container, only a very small amount of water from the sample is needed for the wet sample to reach equilibrium with the surrounding moist air. There is little change in the surface moisture content during the equilibration process. Therefore the moisture diffusion inside the sample is not a major limiting factor for equilibrium. On the other hand, gas diffusion from the wet surface of the sample to the surrounding air has a timescale of 50 s based on vapor–air binary diffusivity of $2.3 \times 10^{-5} \text{ m}^2/\text{s}$.¹² Therefore, the long time needed to reach equilibrium could be limited only by the affinity of water molecules to the solid matrix. During a 20-min baking process, most likely the vapor pressure is lower than equilibrium vapor pressure, especially considering that starch strongly absorbs water during gelatinization once the temperature reaches 65°C.

The nonequilibrium approach has been used in some numerical packages^{24,25} without much justification. Considering that vapor pressure at the material surface may be lower than that at equilibrium, a correction factor has been used for the mass-transfer boundary condition.²⁶ Because of the unavailability of real-time water activity or vapor pressure for bread baking, different water activity models have been tested in this study. It is found that if the literature water activity that corresponds to equilibration over a long time²² is used, computed moisture loss from bread is much faster than that measured from our experiment, which will be shown later in this paper. This seems to confirm the hypothesis that vapor pressure during baking is not under equilibrium with water inside the dough. If lower vapor pressure is assumed, as shown in Figure 3, temperature and moisture history from modeling do match the experimental results. Of course, delicate experimentation is needed to verify how far the vapor pressure is from equilibrium during a dynamic heating process. Such experimentation is only beginning for pure water²⁷ and is outside the scope of the current study.

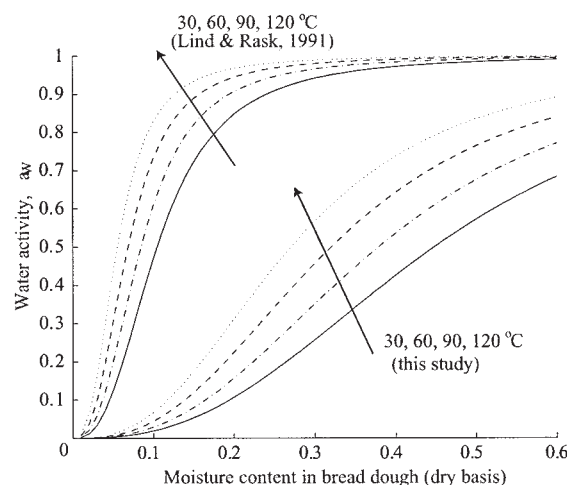


Figure 3. Water activity for dough measured after a long-time equilibrating process and the reduced water activity that matches the temperature and moisture content history in baking experiment.

Based on this discussion, the lowered water activity shown in Figure 3 is used in this study.

Viscoelasticity. In light of the unavailability of rheological data for the dough as the temperature and composition change during baking, the Maxwell model is used that includes a viscous and an elastic unit in series. It can display basic features such as initial relaxation and the surface being set at the later stage. A model for the viscous component follows (Fan et al.).² Relaxation time for wet dough is about 2 s at room temperature based on our experimental observation and results reported by Keentok et al.²⁸ Starch gelatinization around 60°C and protein coagulation at about 71°C tend to solidify the dough¹⁹ and lead to a sharp increase in relaxation time. The relaxation time has been reported to be about 20 s after baking for 10 min at 210°C.²⁹ Expansion is mainly influenced by strength of the crust whose moisture content has an approximately inverse trend with temperature. Relaxation time as a function of moisture content only is given in Itaya et al.³⁰ Alternatively, it can be expressed in terms of temperature. Based on experimental observations and understanding of the process, we formulate the relaxation time as a function of temperature

$$\tau = 9 \left[\frac{2}{\pi} \arctan \left(\frac{T - 65}{2} \right) + 1 \right] + 2 \quad (35)$$

The elastic modulus can be deduced after determination of viscosity and relaxation time.

Numerical implementation

The finite-element method is used to solve the governing equations in this study in which linear triangular mesh is used, as shown in Figure 2. Because transport and deformation are fully coupled, the entire set of equations is solved simultaneously. The mesh at time zero is generated using Gambit (Fluent Inc., Lebanon, NH). A constant time step is used for

simplicity and a typical time step is 1 s in this study to reach convergence. Convergence is reached by controlling the relative changes of the independent variables within a time step to be less than a prescribed small value.

Because of the strong nonlinearity of transport and mechanical properties associated with temperature and moisture changes, special consideration has been made to improve numerical performance. For example, permeability is evaluated in the element instead of at the nodes to ensure mass and energy conservation and implicit pressure is used in the PVW equation rather than pressure at the last iteration, to remove numerical oscillation. The computation is carried out on a PC with Pentium III running at 1 GHz. A typical 25-min baking process takes about 250 min of CPU time.

Experiment

For the baking experiment the material used is the Pillsbury dinner roll (The Pillsbury Co., Minneapolis, MN). Before baking, each roll is in the shape of a short cylinder with a diameter of 3.65 cm and a height of 3.5 cm.

Baking is performed in a domestic gas-heated oven that is maintained at $190 \pm 5^\circ\text{C}$. The cylindrical roll (dough) is put into the oven and supported using a thin and flat metal plate. Four fiber-optic temperature probes are placed in the roll, and temperature readings are obtained using a FISO real-time measurement system (FISO Technologies, Quebec, Canada). A consumer digital camcorder is set up to record the history of volume change. The baking process lasts 20 min.

The same baking experiment is carried out to determine the differential weight loss. At certain times, the bread roll is taken out to measure its weight. Each measurement process takes about 2–3 s and does not significantly change the bread weight compared with the weight change when there is no removal from the oven.

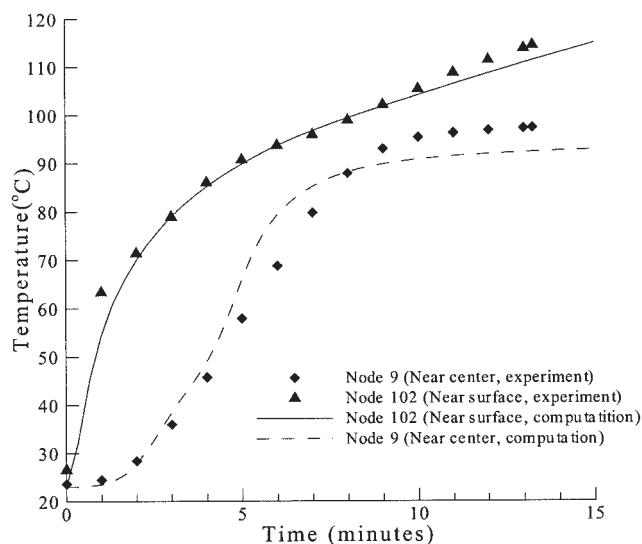


Figure 4. Experimental and computed transient temperature at two locations inside the bread.

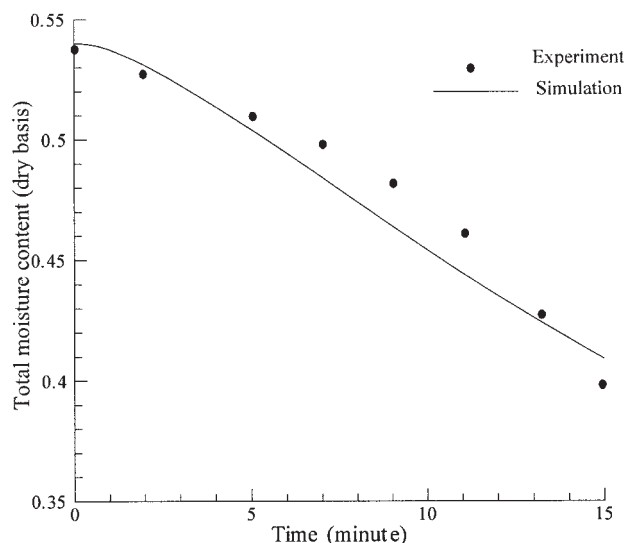


Figure 5. Experimental and numerical results of total moisture change with time during baking.

Results and Discussion

Comparison between experiment and modeling

Temperature Profiles. Temperature probes are placed at four locations of the bread in the experiment, as shown in Figure 2. One is at the center and another is inserted into the bread so that the probe tip touches the bread skin. During the baking process, probes move with the bread deformation. The tip of the second probe above is about 2–4 mm away from the side surface. Nodes 9 and 102 on Figure 2 are closest to these two locations, respectively. Temperatures computed at nodes 9 and 102 are plotted together with the experimental results in Figure 4. Near the surface, the temperature increases rapidly during the first few minutes. When the temperature approaches 100°C , evaporation becomes stronger. Because a greater portion of energy at the bread surface is used for evaporation, the rate of temperature rise decreases. At lower water content, water is held tightly by the starch. Thus the evaporation rate is likely to be small and the temperature can go beyond 100°C . Near the center, however, the moisture content remains high and the temperature does not exceed 100°C . Thus, experimental results agree well with the simulation in terms of temperature history both near the surface and at the center. Because it is difficult to position the probe precisely in the bread dough, this comparison should still be considered somewhat qualitative.

Change of Total Moisture Content. Total moisture content in the bread decreases with baking time, as shown in Figure 5. This trend can be seen in both experiment and simulation, which shows good qualitative agreement.

Volume Change. Experimentally observed shape change during baking is shown in Figure 6. Only half of the bread is shown because of symmetry and to compare with simulation. Computed shape change is shown in Figure 7 and volume change is shown in Figure 8, respectively. Figure 8 confirms that the volume increases substantially in the first few minutes. After about 4 min, volume change is no longer significant. The contours in Figure 7 show how the temperature changes. Ini-

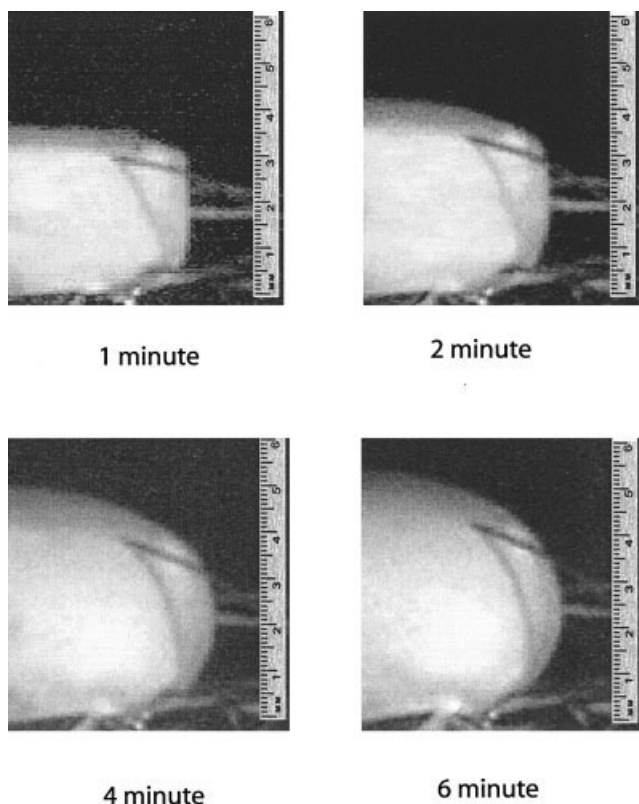


Figure 6. Shape change of the right half of the bread during baking experiment, recorded using a video camera.

tially, temperature increases quickly in the outer region. As the temperature approaches 100°C , the rate of temperature increase in the surface region becomes slower as a result of evaporation. Only the very outer surface goes beyond 100°C , which becomes dry soon after heating starts.

Comparison with Conjectured Profiles. Conjectured profiles of moisture content, temperature, vapor pressure, and total pressure during bread baking exist in the literature.³³ These profiles are reproduced in Figure 9 at two different time instances. Computations using a 1-D axisymmetric model are performed here to compare with their work. Our simulations, using a fundamental engineering description, predict the profiles in Figure 9 after 1 and 4 min of heating. The simulated trends compare quite well with the postulated trends. This can be seen for all four variables of moisture, temperature, vapor pressure, and total pressure and during initial period as well as toward the end of heating.

Transport of liquid water

Liquid water transport is assumed to be small because of starch gelatinization (see subsection on "Liquid water diffusivity and permeability"). Because precise information about water diffusivity for such complex systems is not available, sensitivity analysis is carried out to verify the validity of the chosen values.

Using water diffusivity two orders higher than that mentioned earlier, the predicted shape after 6 min is shown in Figure 10. By comparing with Figure 7, it can be seen that the

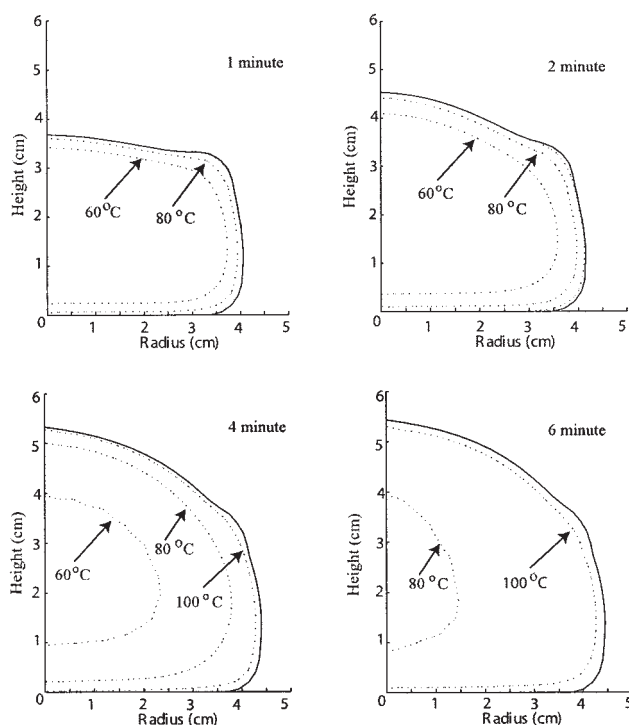


Figure 7. Shape change in bread during baking with temperature contours superimposed, computed using the model.

temperature is generally lower in Figure 10 because larger water diffusivity could bring water to the surface faster and prevent the surface temperature from going higher. As a result, the bread dough would stay longer at a low temperature. Because yeast is always active below about 60°C , as an assumption, the prolonged yeast activity generates more CO_2 and larger expansion, which is not realistic.

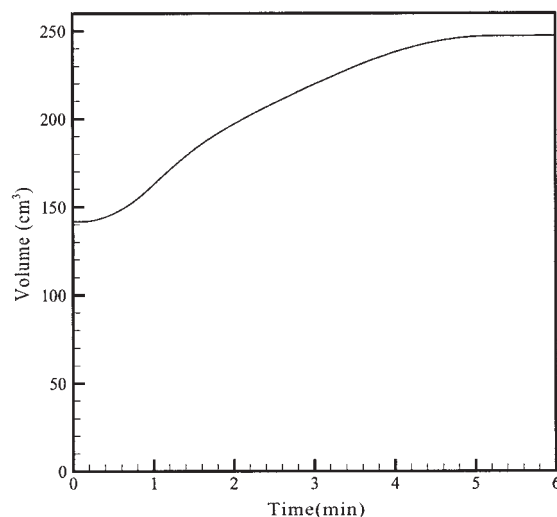


Figure 8. Bread volume change with time, computed using the model.

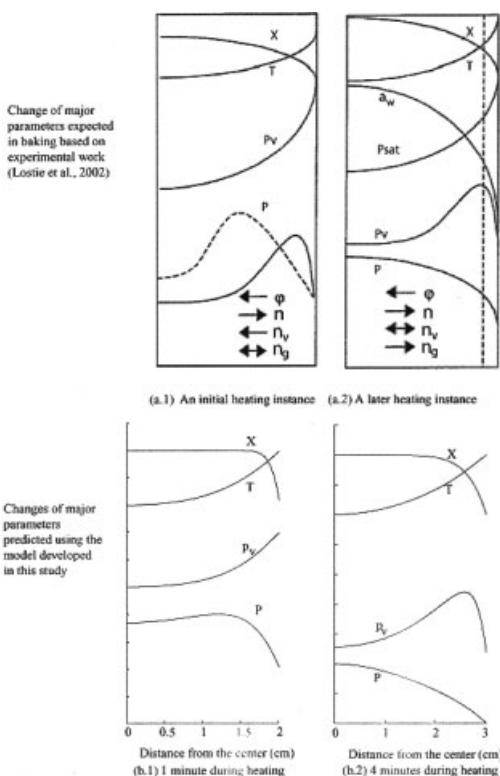


Figure 9. Comparison of profiles of moisture content X , temperature T , partial vapor pressure p_v , and total pressure P at two different times during baking between this study and experimentally based postulation of Lostie et al.³³

Heat-transfer mechanisms in bread baking

During the baking process, there could be three major heat-transfer mechanisms: thermal conduction, convection, and phase change (evaporation–condensation) of water. Heat conduction using an effective conductivity has been the dominant approach for modeling of baking.^{5,6} Performance of this model largely depends on the empirical parameter of effective conductivity. Water evaporation also exists in baking and influences heat transfer. Some studies³⁴ suggest that condensation is also present. During baking, vapor is generated near the surface, picking up a certain amount of heat, and then travels to the inside (in the form of diffusion and/or Darcy flow) and condenses, resulting in transfer of heat from the outer region to the inside. This process is known as evaporation–condensation. Another heat-transfer mechanism is convection. Although phase change or evaporation–condensation involves vapor flow, it should be noted that convection specifically denotes the second term in Eq. 1, which is the heat transferred by all fluids when there is temperature gradient along the path of fluid flow. The effects of convection and phase change are now discussed.

Convective Heat Transfer. The magnitude of convective heat transfer varies with location inside the bread and time. To determine the influence of convection, the effect of convection is calculated at two representative locations and at two representative instances. After 1 min of heating, water velocity near the surface (node 102 on Figure 2), where the moisture gradient is large, is about 10^{-8} m/s based on Fick's law. The velocity of

gases is in the order of 10^{-4} m/s based on Fick's law and Darcy's law, whereas near the center (node 9 on Figure 2), gas velocity is about 10^{-6} m/s. Although water density is nearly three orders of magnitude higher than that of vapor, gas velocity is about four orders higher: so gas convection is dominant. The Peclet number (Pe) for gas, which denotes the relative magnitude of convective heat transfer vs. thermal conduction, has a value near the surface as

$$Pe = \frac{\rho c_p u L}{k} \approx \frac{0.5 \times 1000 \times 2 \times 10^{-4} \times 0.025}{0.1} \approx 0.025 \quad (36)$$

When $Pe \ll 1$, convective heat transfer is considered negligible.³⁵ Therefore, convective heat transfer in baking is not significant near the surface, initially. The pressure gradient is close to zero near the dough's center because of symmetry, and thus convection should be even weaker going toward the center.

Evaporation–Condensation. It is stated in Sluimer and Krist-Spit³⁴ that in baking, heat conduction contributes very little to the delivery of heat from the surface to the inside and the major transport mechanism should be condensation–evaporation. If this is the case, there should exist a vapor flow from the surface toward the inside.

The computed vapor velocity field at 4 min is shown in Figure 11, in which some vapor flow is going toward the inside. Because the magnitude of vapor velocity near the center is much smaller than that near the surface and is hard to see in Figure 11a, Figure 11b reproduces only the direction of vapor flow. To compare the heat transfer by thermal conduction and evaporation–condensation, an enclosure is chosen, as shown in Figure 11c. Heat transfer to the inside of the enclosure through conduction is shown in Figure 11d. It increases first as a result of both the large temperature gradient across the enclosure

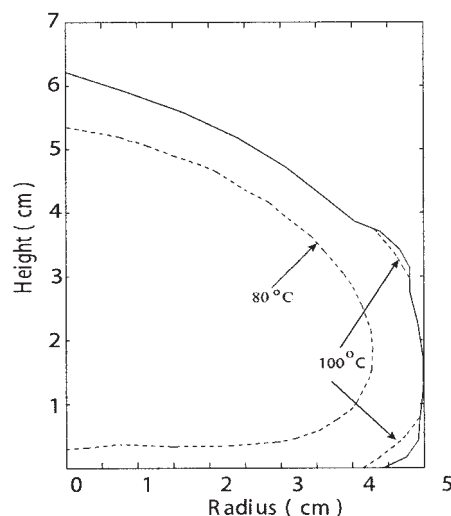


Figure 10. Shape change and temperature contours after 6 min of baking if water diffusivity of 1.0×10^{-7} is used that is two orders larger than the original water diffusivity.

Compare with the 6-min configuration in Figure 7.

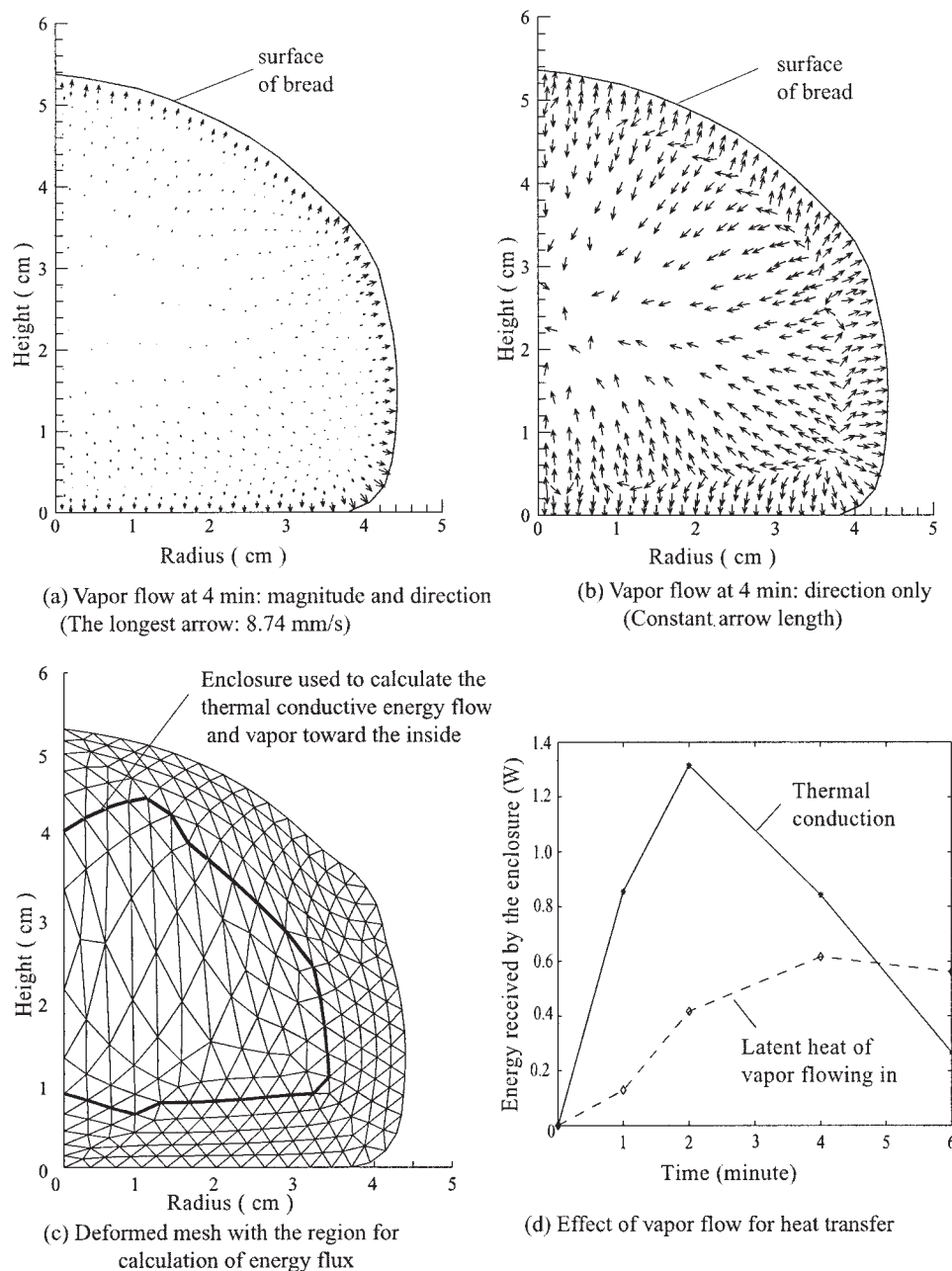


Figure 11. Vapor flow, associated heat transport, and comparison with conduction heat transport.

surface and the expanding enclosure area. Then thermal conduction decreases as the bread approaches equilibrium with the outside. The latent heat of vapor flowing into the enclosure is also calculated in Figure 11d, which is comparable to heat transfer by conduction. The reason is that, although the vapor flow rate n_v is small, the water latent heat per unit mass λ is large. This multiphase model confirms that the evaporation–condensation process exists in baking of bread and it helps heat transfer toward the inside during bread baking.

Changes of shape and size

Volume change of bread is determined by three major factors: generation of gases inside, mechanical properties of

dough, and gravity. From the experimental results in Figure 6 and simulation in Figures 7 and 8, it can be seen that the volume increase in baking mainly takes place in the first 4 or 5 min. During that period, yeast activity is substantial and generates considerable CO_2 . Surface temperature is not too high, so the surface has not been set and the bread expands more easily. Later, yeast activity ceases because of higher temperature. Temperature at the crust region exceeds 100°C (see Figure 4) and becomes very dry. Browning reactions occur between sugars and amino acids above 100°C , leading to the surface color development and greatly increasing the mechanical strength of the crust. Although vapor pressure becomes much higher inside the bread at this stage, not much volume

change is seen because of a crust with high mechanical strength.

Understanding the deformation characteristics actually aids the modeling process. As mentioned earlier, it is difficult to obtain the mechanical properties of bread dough in a large range from room temperature to 150°C in dry crust and wet crumb. It is known that CO₂ production occurs mainly between room temperature and 60°C. The period in which CO₂ is generated in baking coincides with the period when the surface remains unset. This helps us to choose a reasonable model for mechanical properties. For example, use of lower viscosity and elasticity of bread near the crust region would lead to continued expansion beyond what is currently predicted, which is not correct.

To predict the baking more realistically, gravity could not be ignored. Otherwise, the predicted shape of bread would be more like a sphere rather than the one shown in Figure 7, which is flat at the bottom.

The model developed here helps to explain why a closed bubble model as in Fan et al.² is not adequate to simulate the volume expansion in bread baking. A bubble model needs to assume uniform temperature throughout the volume that increases at a certain rate. As discussed above, surface temperature increases differently from inside temperature, which is the key to the volume change in bread baking. Choosing one temperature for the whole bread, as in a bubble model, means that this important information is lost. For example, if the average temperature of the bread is used as the bubble temperature, the surface would be at a lower temperature, which would lead to a collapsed top, as using a larger water diffusivity shown before.

Conclusions

In this work, a mathematical model is developed for fully coupled transport and large deformation processes and is applied to the baking of bread. The model can describe the transient deformation (oven rise) and temperature and moisture distributions in bread baking as a coupled process. Coupling between the transport and deformation is shown to be important in understanding the bread baking process.

During baking, vapor pressure is likely to be lower than equilibrium vapor pressure. Moisture loss occurs mainly in the dough that is close to the heating surface. Convective heat transfer inside the bread is insignificant and can be ignored in modeling of baking. Heat transfer from the surface to the inside is facilitated by vapor generation at regions close to the surface and vapor condensation when going toward the inside. Volume expansion and shape are influenced mainly by rate of CO₂ generation, mechanical properties of dough, and gravity. Particularly in bread baking, these quantities below 70°C are more important in deciding the final shape of bread.

Volume expansion and browning of bread have been studied as influenced by power level in microwave and infrared baking.³⁶ The modeling and analysis presented here help to explain or understand some of their results and therefore are valuable for baking research. In addition, the modeling techniques and analysis can shed light on the general understanding of transport phenomenon, deformation, and their interaction in coupled processes similar to baking, such as rehydration of vegetables, drying of wood, puffing processes, and microwave heating

processes that can include significant internal evaporation and volume change.

Notation

a_w	= water activity
c_p	= specific heat, J kg ⁻¹ K ⁻¹
D	= elasticity matrix
D_{eff}	= effective diffusivity, m ² /s
E	= Young's modulus, Pa
g	= gravity, m/s ²
h	= convective heat transfer coefficient, W m ⁻² K ⁻¹
h_m	= convective moisture transfer coefficient, m/s
I_v	= evaporation rate, kg m ⁻³ s ⁻¹
I_c	= CO ₂ production rate, kg m ⁻³ s ⁻¹
k	= permeability, m/s; thermal conductivity, W m ⁻¹ K ⁻¹
M	= total moisture content, kg water/kg dry material
M_c/M_v	= CO ₂ /water vapor molecular weight, kg/mol
n	= porosity or a component of normal direction
\mathbf{n}	= normal direction when without subscripts
\mathbf{n}	= mass flux when with subscripts, kg/s
p	= partial pressure of a phase, Pa
Pe	= Peclet number, defined in Eq. 36
q	= heat flux, W/m ²
r	= radial coordinate in axisymmetric coordinates, m
R	= universal constant, 8.314 J mol ⁻¹ K ⁻¹
R_c	= CO ₂ generation rate, kg kg ⁻¹ s ⁻¹
S	= water saturation when without index
\mathbf{S}	= Kirchhoff stress when with index, Pa
t	= time, s
T	= temperature, °C
\mathbf{u}/u	= displacement increment vector/component, m
v	= velocity, m/s
V	= volume, m ³
x	= coordinate, m
z	= axial coordinate in axisymmetric coordinates, m

Greek letters

δ	= Kronecker symbol
λ	= latent heat, J/kg
ρ	= density, kg/m ³
τ	= relaxation time, s
ν	= Poisson's ratio
ε	= Green strain
ε	= strain, scalar

Superscripts

l	= time step l
$l+1$	= time step $l+1$
(n)	= nonelastic
(e)	= elastic

Subscripts

0	= initial state
c	= CO ₂
d	= diffusivity
e	= equilibrium
f	= ambient fluid or flux
g	= gas, including air and other gaseous components
gr	= gas relative
i, j, k, l	= dummy indices
in	= intrinsic
m	= total moisture content
s	= solid
S	= surface
sat	= saturated
v	= water vapor
V	= volumetric
w	= liquid water

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