

Quality prediction of bakery products in the initial phase of process design

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Abstract

The development of food production processes is facilitated by tools which explore the interaction between process design, operation conditions and product characteristics. In this work an approach how to set-up a simulation model is presented for the phenomena and transformations which occur during baking and which fix the product quality. The simulation model has three consecutive parts: mass and heat transport in the product, transformations concerning starch state transition and color, and the formation of quality attributes (color, softness, crispness and staling). The model for mass and heat transfer is based on laws of conservation and expressed in partial differential equations for spatial products. The starch state transition and color formation are a mixture of qualitative and quantitative information, while the product quality model is mainly based on qualitative information. The model is applied to three bakery products: bread, biscuit and a cake-type. The results show that the model estimates the product quality and its transformations as a function of dough composition, baking and storage condition. The results fit well to observed changes of properties and product quality during baking.

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Industrial relevance: Food industries require tools to evaluate processing options in the feasibility phase of process design. Therefore, simulation of process models is important for this purpose. However, knowledge of different aspects is subject to area of expertise (for example heat and mass transfer versus product quality formation) and often these areas are hardly connected. This work presents a systematic modeling approach for the dominant processes during baking and their interconnection. The main functions of the model are to explore the consequences of choices in design, to rank design options and to find in what direction properties will change when operational conditions change. Moreover, the model can be used for sensitivity analysis to explore on what items further information must be gathered.

1. Introduction

Nowadays, the life cycle of products in the food industry decreases and new or modified products are more frequently introduced to the market. As a consequence, the period for product and process development becomes shorter. Modification of old products or introduction of new products starts by making an inventory of desired product quality. Next, a feasibility study defines the main concept of the product and a

global design for the production system. The feasibility phase allows creativity to explore several directions and searching for different alternative solutions. To be efficient in the feasibility phase a systematic working procedure is necessary. In the chemical industry the working procedures are supported by conceptual process design methodologies (CPD). This methodology is used in the chemical industry to find a description for the production plant through the following activities: arrangement of unit operations, routings of product and energy, the estimation of required process conditions, the composition of the streams and the required energy (Douglas, 1988; Siirola, 1996; Wibowo & Ng Ka, 2001). These procedures extensively rely on process models for the analysis, evaluation and prediction of the physical state of the product.

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There are some examples of the use of models in the food equivalent of conceptual process design. Bruin (1999) showed the importance of the phase diagram for food product and process design and Diefes, Okos, and Morgan (2000) performed the design of a milk powder production plant by ranking of process alternatives based on flow sheet calculations in order to achieve high product quality (safety) with low energy costs. In this case, besides mass and energy balances, the kinetics for microbial growth and vitamin degradation were used to predict quality. Wibowo and Ng Ka (2001) used properties of the most important ingredients as a starting point of designing creams and paste products. Here models were used to evaluate the rheological properties of the products. Meeuse, Grievink, Verheijen, and vander Stappen (2001) and Jadhav, van der Stappen, Boom, Bierman, and Grievink (2002) worked on a mixing process for mayonnaise. The final product is composed of three different components, and models are used to estimate the final composition after the mixing process.

The requirements for models used in the initial phase of process design for the food examples above, however, differ from chemical industry. The difference is that the information about formation of food products is based on the knowledge domain of the designer and mostly not defined in quantitative relations. Fryer (1994) emphasizes that lack of information and the qualitative character complicates product and process design for foods. Other reasons for the complexity are the simultaneous occurrence of product transformations and the subjectivity of food product quality due to consumer preferences. Therefore, specifying product quality attributes, translating these into a quantitative model and making a link with the process are the main challenges for food process design.

The bakery industry is considered as an example of a strongly experience based sector where the products have a long history but modification of existing products is still important. Due to the experience-based character of the industry only limited information is captured in models. So, for this sector, it is paramount to have a solution dealing with limited information for quick product and process design. For example during baking gelatinization which is essential for crumb and crust formation, occurs simultaneously with volume changes due to gas expansion. Part of the available knowledge of these transformations is given in well defined models as heat and mass transfer relations; the others appear as qualitative descriptions (for example softness and crispness of product). Bakery products are also judged on their color, which is result of reactions that occur during baking due to heating. The components involved in these reactions are known, but the correlations of these reactions with temperature and water activity are not yet fully described. Furthermore, bakery products are spatial products in which temperature and water gradients arise during baking. As a consequence texture and color properties depend on the position in the product. Because in product valuation consumers make distinction between parts of the product (e.g. crisp on the edge and soft in the center) spatial temperature and water models are needed for prediction of local texture and color.

The objective of this paper is to present a systematic approach, which captures the most dominant physical phenomena and

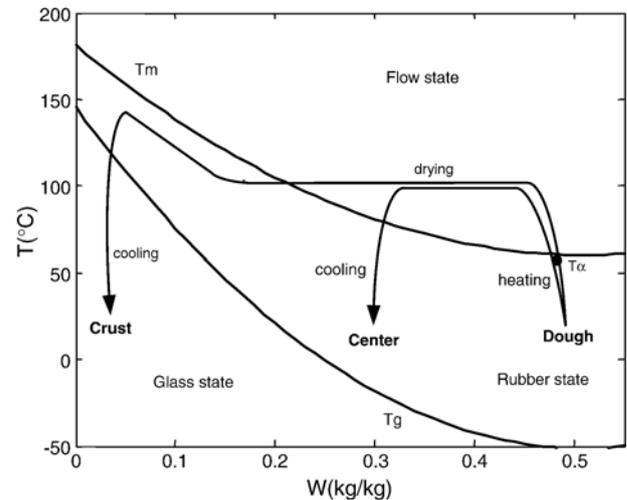


Fig. 1. Schematic state diagram during bread baking. T_m is melting temperature for starch. The glass transition temperatures (T_g) for protein and starch. T_α is the gelatinization temperature for starch. The arrows present the courses of the center and crust of a product during baking.

product transformation during baking. In this approach modeling the interconnection between input, heat and mass transfer, product transformation and product quality attributes represents the total behavior of the product. The final model is used to simulate and to explore product quality in the early phase of process design. The simulation shows how product attributes are modified by changing the initial composition and process variables during baking and allows the ranking of different processing alternatives.

2. System description of baking

Bakery production concerns a series of processing steps such as mixing, baking, cooling and storage during which a number of product transformations take place. Baking is the central process in bakery production and here quality such as size extension, brownness; texture and flavor is formed due to consequence of physical and chemical changes in the product (Sablani, Marcotte, Baik, & Castaigne, 1998). During baking, transformations, which depend on the course of water content and temperature, are decisive for the final product quality (Thorvaldson & Jenested, 1999). These transformations are coupled and influence each other (Zhang & Datta, 2006).

The most dominant phase transitions in bakery product are starch gelatinization, protein denaturation, water evaporation, starch retrogradation, water crystallization and glass transition. The phase transition temperatures are dependent on the composition; especially on the water content but are also influenced by other small molecules which significantly alter the water activity. However, they are relatively insensitive to changes in protein and lipid composition as long as they form minor components. Fig. 1 shows the several transition temperatures for starch as a function of the water content (derived from Farhat, Blanchard, Descamps, and Mitchell (2000) with sugar content as in wheat bread). Such state diagrams, as introduced by Levine and Slade (1990), are increasingly used in structured

product design as a way to comprehend the transformations that occur along the process path for a given location in the product (Cuq, Abecassis, & Guilbert, 2003).

The process paths for the bread center and surface in Fig. 1 reflect the three stages of baking which occur after the dough is placed in the oven.

1. Heating phase where dough is gradually warmed up to evaporation temperature (~100 °C). Yeast or baking powder produce CO₂ inside the dough at temperatures between 40–60 °C (Zhang & Datta, 2006). The pressure in the dough increases due to presence of CO₂ gas and water vapor. During the heating phase the proteins will denaturize and form a solidified network at the thermosetting temperature. Around the gelatinization temperature T_{α} , part of the crystalline starch will swell into an amorphous rubbery state. In presence of enough water the gelatinization of starch occurs at temperatures between 60–80 °C (Zanoni, Schiraldi, & Simonetta, 1995) and is required to form the characteristic sponge network. Because the protein thermosetting and starch gelatinization temperature are within the same range, both phenomena are simultaneously observed and frequently lumped to a single transformation in baking heuristics. Within the model we therefore choose to track only the state change of starch.
2. The drying phase is the following step. Now, water evaporates and the surface of the product, which is in direct contact with the heated air, will be dehydrated first. Several studies indicate that during the drying period not only the evaporation but also the condensation in the product is an important mechanism ruling the heat and mass transfer. This phenomenon is known as the evaporation–condensation principle (see for example Thorvaldson & Jenested, 1999; Zhang & Datta, 2006). Here water evaporates and generates vapor near the surface, but because the temperature

decreases towards the center of the product the vapor, which is transported into the product due to diffusion or Darcy flow (Zhang & Datta, 2006), will condense towards the center.

The increasing partial water pressure and the presence of CO₂ inside the dough cause product extension, which results in an increase of product size. The gelatinization and protein thermosetting reactions that occurred in the heating phase have altered the rheological properties such that the extension results in the bread crumb and crust formation. (Cuq et al., 2003; Zanoni et al., 1995).

Sugars together with protein will produce browning compounds, which give color to the product that lead to irreversible changes (Cuq et al., 2003). The required relative high temperature for these reactions to occur will typically only be reached in the outer zones, once they are sufficiently dried to have a low water activity and corresponding high evaporation temperature.

The duration of this phase depends on the initial water content of the dough and is ruled by the heat and mass transfer.

3. Cooling phase. The phase following on drying concerns cooling where the temperature of the product decreases together with a moderate change of water content. The remaining water content determines the state of the product after cooling. The cooled crust will be far below the high glass transition temperature (T_g) due to its low water content. Therefore it will transform during the cooling phase from a rubbery to the glassy state which is essential for the crust crispness (Cuq et al., 2003). The crumb with a high water content will remain soft (rubber state) after cooling to room temperature because it is above the corresponding T_g . However, the gelatinized part of the starch can slowly (re) crystallize in a process called retrogradation because it is below melting temperature of those crystallites (T_m). The effect of retrogradation is loss of firmness due to physical changes of the

Table 1
Analysis of interactions in the system

Quality	Composition	Structure	Mechanical properties	Required transformation	Model required	Model Input
Crumb	- Water	Volume fraction Maintaining structure	Elasticity	Gelatinization	Thermodynamic properties: $T_g, T_m, T\alpha$ Gelatinization and retrogradation kinetics Thermosetting kinetics	Composition (S,W,Z) Process temperature Process temperature
	- Starch			Retrogradation		
	Protein			Thermosetting		
Softness	- Water	-	Elasticity	Gelatinization	Thermodynamic properties: $T_g, T_m, T\alpha$ Gelatinization and retrogradation kinetics	Composition (S,W,Z) Process temperature
	- Starch			Retrogradation		
	Lipids					
Crispness	- Water	-	Elasticity	- Gelatinization	Thermodynamic properties: $T_g, T_m, T\alpha$ Gelatinization and retrogradation kinetics	Composition (S,W,Z) Process temperature
	- Starch			- Retrogradation		
	Lipids					
Staled	- Starch	-	Elasticity	- Gelatinization	Thermodynamic properties: $T_g, T_m, T\alpha$ Gelatinization and retrogradation kinetics	Composition (S,W,Z) Process temperature
	- Water			- Retrogradation		
	Lipids					
Size (volume)	-	-Extension (oven rise)	-	-Gas extension	Kinetic of oven rise	Composition (W) Process temperature
Brownness	- Melanoidin	-	-	- Mailard reaction	Kinetic of browning reaction	Composition (W) Process temperature
	- Caramel			- Caramelization		

Note: Initial composition of dough: (S) Sugar, (W) Water, (Z) starch.

Protein maintains the structure. As the thermosetting reactions of protein fall together with the gelatinization reactions there is no separate model for the protein used. Lipids are hardly affected due to heating. There is no transformation reaction. Lipids may affect kinetic parameters but literature information is minimal.

product (staling). The retrogradation rate diminishes near the glass transition temperature and therefore can long term storage of bread best be done under the corresponding T_g of the crumb (Schiraldi, Piazza, Brenna & Vittadini, 1996).

3. Modeling approach and considerations

Since the intention of this work is to build a generic baking model suitable for an initial exploration of process alternatives with respect to the resulting quality attributes, the model should fulfill the following requirements:

- Being applicable to a broad range of bakery products.
- Cover the interconnections between sub processes
- Concern only the most critical variables involved in the transformations
- Provide a direct mapping from the state variables to quality related attributes

In the modeling approach only the dominant phenomena and transformations are modeled. Although the accuracy of the model predictions will be limited, it learns to understand the phenomena that occur in the product and how the phenomena are connected and will also help to find which additional experiments are required to improve the prediction.

Table 1 presents an inventory of relevant variables. It starts with quality as observed by the consumers in the left column. These qualities are characterized by the composition, mechanical and structural properties of the product. Water content and the state of starch, proteins and lipids characterize texture properties. Thermosetting reactions for protein solidify the crumb network in the product. As these reactions fall almost together with the gelatinization of starch (Cuq et al., 2003) and

because starch is the dominating component for the structural properties, the protein model is omitted in this work. Lipids are hardly transformed during baking, but they may affect the kinetic parameters in the relations for softness, crispness and staling. Information from literature is still too limited to get information on how lipids affect these parameters.

The formation of melanoidins by the Maillard reaction is important for the color. Baking of most products is finished before caramelisation and carbonization reactions at temperatures above 150 °C start. The degree of extension is responsible for the changes in volume.

These state variables are the result of a number of transformations that take place in the product. During baking the transformations change the state of components into the final quality. The transformations are driven by heat and mass transfer which depend on the energy input and initial composition of the dough. The changes of the physical and chemical properties may affect the mass and heat transfer in the system (e.g. heat conductivity depends on the water content, or permeability depends on gelatinization), but literature study showed that these effects are insufficiently known and therefore they are not yet included in this work.

Fig. 2 gives an overview of the connection of these processes, the inputs and the resulting quality as outputs. The total model has three parts: the heat and mass transfer model, the state changes due to the heat treatment (transformation model) and the product quality model. Setting up a model for heat and mass transfer is rather straightforward by using laws of conservation and additional constitutive equations. The transformation model is more difficult to define, as well as the modeling of the product quality as a function of the transformations. Information given in the literature is a mixture of qualitative rules, experimentally observed correlations and

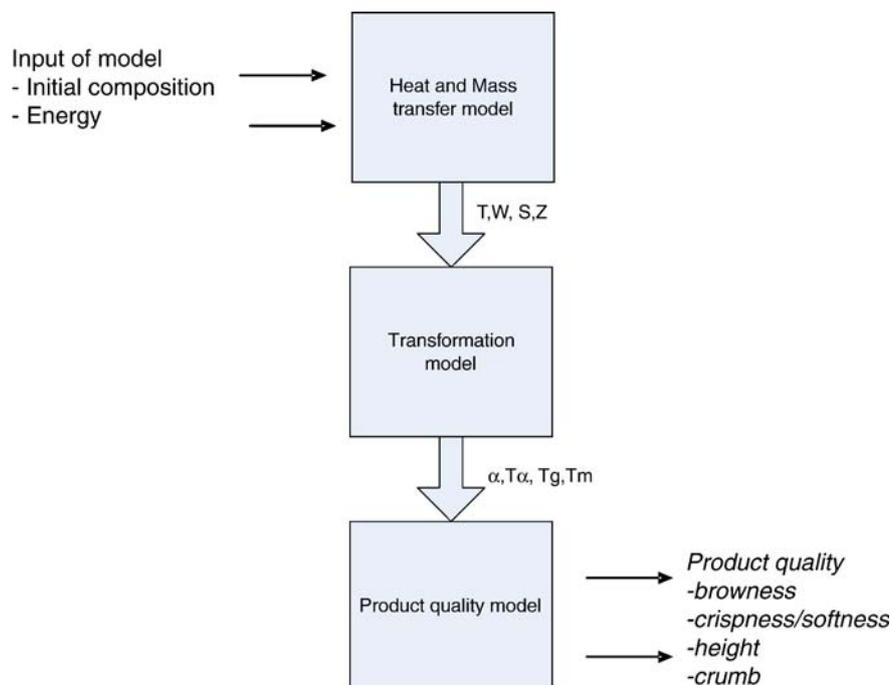


Fig. 2. Sequential model with three steps.

(sometimes) well established relations; so a mixture of expert information, black-box and white-box models. For this work all qualitative descriptions are translated into quantitative information. The translation is expressed into a range between 0–1, which has the meaning of minimum to maximum values.

4. Heat and mass transfer of product during baking

4.1. The mass balances

The mass balances for liquid water, water vapor and CO₂ gas are given in Eqs. (1)–(3). The changes of liquid water in the product are result of the diffusion and the evaporation rate (I_v). Water vapor is considered as an ideal gas which is in equilibrium with liquid water content. The vapor concentration is a function of diffusion and evaporation rate. The rate of extension (e) describes the change of size (height) correspond to initial height of product.

$$\rho_s \frac{\partial W}{\partial t} + \frac{\rho_s \cdot W}{1+e} \frac{\partial e}{\partial t} = \nabla \phi_w - I_v \quad (1)$$

$$\rho_s \frac{\partial V_v}{\partial t} + \frac{\rho_s \cdot V_v}{1+e} \frac{\partial e}{\partial t} = \nabla \phi_v + I_v \quad (2)$$

$$\rho_s \frac{\partial V_c}{\partial t} + \frac{\rho_s \cdot V_c}{1+e} \frac{\partial e}{\partial t} = \nabla \phi_c - I_c \quad (3)$$

4.2. Energy balance

The energy balance concern conduction, evaporation–condensation, and the water vapor and CO₂ fluxes (Eq. (4)).

$$\rho_s c_p \frac{\partial T}{\partial t} + \frac{\rho_s \lambda}{1+e} \frac{\partial e}{\partial t} = \nabla \cdot (k \nabla T) - \lambda I_v - \nabla \cdot (m_v H_v) - \nabla \cdot (m_c H_c) \quad (4)$$

4.3. The flux equations

Flux equations for Eqs. (1)–(3) are described as follows:

$$\phi_w = \rho_s D_w \nabla W \quad (5)$$

$$\phi_v = \rho_s D_{eff} \nabla V_v - m_v \quad (6)$$

$$\phi_c = \rho_s D_{eff} \nabla V_c - m_c \quad (7)$$

4.4. Constitutive relations and assumptions

The liquid water and water vapor are correlated by the water activity and partial vapor pressure relationship in the sorption isotherm. The evaporation rate (I_v) is solved by combining Eqs. (1), (2) and (4) with Eqs. (8) and (9).

$$V_v = \frac{\varepsilon M_w}{\rho_s R T} a_w \cdot p_v \quad (8)$$

$$a_w = \frac{1.05 W}{0.09 + W} \quad (9)$$

Water vapor and CO₂ are considered as ideal gases and balances are derived from Fick's law and by CO₂ production.

Zhang and Datta (2006) used a general term for production of CO₂ both for yeast or baking soda as:

$$I_c = R_{CO} \rho_s \exp\left(-\frac{(T-T_{ref})}{dT}\right)^2 \quad (10)$$

with R_{CO} as the CO₂ production at T_{ref} .

Mass fluxes of CO₂ and water vapor depend on local pressure differences, kinematic viscosity and permeability of product.

$$m_v = -\frac{\kappa}{v} \frac{V_v}{V_v + V_c} \nabla P \quad (11)$$

$$m_g = -\frac{\kappa}{v} \frac{V_c}{V_v + V_c} \nabla P \quad (12)$$

The changes of size (extension) are caused by the increasing pressure inside the gas cells in dough due to the release of water vapor and CO₂ from baking powder or from yeast (Fan, Mitchell, & Blanshard, 1999; Zhang & Datta, 2006). Zhang and Datta (2006) considered bread as a visco-elastic material for which the deformation can be expressed by the Maxwell equation and it is driven by pressure difference between total pressure inside product (P) and ambient pressure (P_{atm}). The total pressure (P) is the sum of partial water vapor pressure and CO₂ pressure which can be derived from gas ideal law. This work considers the change of size as not only due to visco-elastic but also to elasticity properties that are described by the Kelvin–Voight model.

$$\eta \frac{de}{dt} + Ee = P - P_{atm} \quad (13)$$

4.5. Initial and boundary conditions

The initial values for heat and mass transfer are given by:

$$T = T_0, W = W_0; e(0) = 0; \quad \text{and} \quad p_c(0) = 1.10^5 - p_v(0)$$

The boundary conditions of model are given by Eqs. (14)–(17):

- Fluxes at the surface

$$-k \nabla T = h_c (T_{ext} - T_s) - \lambda \cdot \rho_s \cdot D_w \nabla (W_s) \quad (14)$$

$$-D_v \nabla V_v = h_v (V_{ext} - V_{v,s}) \quad (15)$$

- Symmetry at the center of the product

$$-k \nabla T = 0 \quad (16)$$

$$-D_v \nabla V_v = 0 \quad (17)$$

5. Product transformation model

5.1. Starch gelatinization and retrogradation

Starch gelatinization and retrogradation are starch state transition processes which largely determine the final product texture. If enough water is available the crystalline starch granules will transform into an amorphous rubbery state by adsorption of water; this transformation is named gelatinization (Eliasson, 1993). Retrogradation is the process where the gelatinized starch turns to a non-native crystalline state. This occurs mainly during storage (Farhat, Blanshard, & Mitchell, 1999). With respect to the amorphous–crystalline ratio, the gelatinization and retrogradation will be simply considered as reverse processes (see Fig. 3).

The change of the degree of gelatinization is given by Eq. (18). First order kinetics is adopted to describe the changes of gelatinization and retrogradation (Chinachoti & Vodovotz, 2001; Farhat et al., 1999; Karapantsios, Sakondiou, & Raphaelides, 2002; Zanoni et al., 1995).

$$\frac{d\alpha}{dt} = k_{gel}(T)f_g(\alpha) - k_{retro}(T)f_r(\alpha) \tag{18}$$

where α the degree of gelatinization which ranges from 0 to 1, $k_{gel}(T)f_g(\alpha)$ and $k_{retro}(T)f_r(\alpha)$ the conversion rates for gelatinization and retrogradation are respectively:

$$\begin{aligned} f_g(\alpha) &= (\alpha_{max} - \alpha) \\ f_r(\alpha) &= \alpha \end{aligned} \tag{19}$$

α_{max} is the maximum attainable degree of gelatinization. Fessas and Schiraldi (2000) showed that the maximum degree of gelatinization α_{max} is a function of the water content in the product (see Section 5.1.1).

The gelatinization rate constant $k_{gel}(T)$ and retrogradation rate constant $k_{retro}(T)$ are given in Eqs. (20)–(21) and depend on temperature. Zanoni et al. (1995) found that $k_{gel}(T)$ follows an Arrhenius equation with the activation energy (E_a) of 139 kJ/mol.

$$k_{gel}(T) = 2.8 \cdot 10^{19} \exp\left(\frac{-E_a}{RT}\right) \tag{20}$$

Retrogradation is significantly slower than gelatinization, and takes place mainly during storage. Farhat et al. (1999) reported that the Lauritzen–Hoffman model can be used to express the rate of starch retrogradation.

$$k_{retro}(T) = G_0 \cdot \exp\left[\frac{-U^*}{R(T-T_\infty)}\right] \exp\left[\frac{-K_g}{T \cdot \Delta T \cdot f}\right] \quad \text{if } T < 298^\circ\text{K} \tag{21}$$

with additional information on this expression in Table 2.

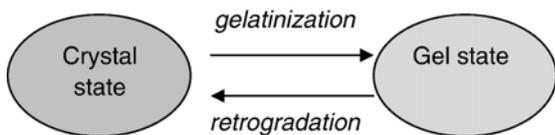


Fig. 3. Changing starch state due to gelatinization and retrogradation.

Table 2
Variables in retrogradation kinetics (Farhat et al., 1999)

Variable	Expression	Unit
G_0	$10^{-10.44W + 5.75}$	1/s
U^*	$-8140W + 8464$	J/mol
K_g	$-3.422 \cdot 10^5 W + 3.2322 \cdot 10^5$	K ²
f	$\frac{2T}{T_m + T}$	[-]
T_∞	$T_g - 30$	K
ΔT	$T_m - T$	K

Because of the limited validity range the retrogradation calculations are started in the cooling phase after baking when the product temperature falls below 25 °C during the baking process and storage.

5.1.1. Calculation of α_{max}

The role of water for gelatinization of starch has been studied (Fessas & Schiraldi, 2000; Karapantsios et al., 2002; Roos, 1995). Roos (1992) states that for a starch–water system, the amount of water bound to starch is equal to 50% of total of starch, while the rest is available for gelatinization. In addition, for the same system, Roos (1995) reported that at least 60% of water (40% starch) is required to achieve complete gelatinization. In conclusion, 20% of water bound to starch and the rest (40% of water) will be available for gelatinization. This gives as a rule that free water and starch require a ratio 1:1 for gelatinization.

For bakery dough which is not only composed of water (W) and starch (Z), other components such as sugar (S) and other water-binding components (C) should be taken into consideration for calculation of maximum gelatinization. Fat as hydrophobic material can be excluded as water binding component. We remark that gelatinization occurs only if the amount of water in dough exceeds 50% of the summed weight of starch and other water binding components. Otherwise there is no gelatinization (Roos, 1995). These findings are based on the composition of dough and in the following expressions the composition of dough is used to calculate α_{max} :

$$\alpha_{max} = \begin{cases} 0 & \text{if } W < 0.5(Z + C) \\ \frac{W - 0.5Z - 0.5C}{Z} & \text{if } 0.5(Z + C) < W < 0.5(3Z + C) \\ 1 & \text{if } 0.5(3Z + C) < W \end{cases} \tag{22}$$

5.1.2. Glass transition and melting temperature (T_g and T_m)

To calculate the retrogradation rate, glass transition (T_g) and melting temperature (T_m) have to be determined. Roos (1995) states that the effect of the product composition on the glass transition and melting temperatures is an important aspect in the design of food products which are subject to well-defined processing and storage conditions. The main components in bakery dough – sugar, starch and water – have effect on glass transition and melting temperature. The work of Farhat et al. (2000) concerning the effect of sugar–starch solution on the glass transition and melting temperature of starch is used in this

Table 3
Regression coefficients for glass transition and melting temperature as a function of composition

Parameters	p_1	p_2	p_3	p_4	p_5	p_6	p_7
T_g	457.10	-396.32	-853.21	716.76	430.27	778.44	-1424.71
T_m	472.69	-180.90	-519.97	419.63	124.46	471.87	-749.88

study. Farhat et al. (2000) performed experiments for the glass transition and melting temperature as a function of sugar/starch ratio ($S/Z=0:100, 10:90$ and $30:70$) and for the water content range of $0-0.5$ kg water/kg total. The expressions for T_g and T_m for bakery products as a function of water content (W) and sugar/starch ratio (S/Z) is extrapolated from the work of Farhat et al. (2000) by non-linear regression (Eq. (23)).

$$T_{g/m} = p_1 + p_2(S/Z) + p_3 \cdot W + p_4(S/Z)W + p_5(S/Z)^2 + p_6(W)^2 + p_7(S/Z)^2 W^2 \quad (23)$$

with p as the estimated parameters which are listed in Table 3.

5.2. Maillard reaction

The Maillard reaction is a non-enzymatic reaction which causes the formation of melanoidins. The melanoidins give an impression of brownness which increases with increasing concentration of melanoidins. The formation of melanoidins by the Maillard reaction follows a zero order kinetic (Eq. (24)) (Bates, Ames, Mac Dougall, & Taylor, 1998; Martins & van Boekel, 2003; Morales & van Boekel, 1998).

$$\frac{dm_e}{dt} = k_{m_e} \quad (24)$$

$$k_{m_e} = k_0 \cdot \exp\left[\frac{-E_a}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right)\right] \quad (25)$$

van Boekel (2001) reported that the activation energy for bakery products is about 100 kJ/mol. K_0 is determined from a correlation between browning reaction rate and water activity, which shows a maximum rate for water activities between 0.7–0.8. This information is not yet sufficient, and to complete the model a reference value is introduced as a standard. This standard is that the level of melanoidins (m_e) equals 1 when a product is exposed for 30 min to a temperature of 90 °C and water activity of 0.93. This statement leads to the next expression for k_0 as function of water activity (Eq. (26)).

$$k_0 = 4.9 \cdot 10^{-3} \frac{\exp(9a_w)}{2 \cdot 10^3 + \exp(11.3a_w)} \quad \text{for } T = 363^\circ\text{K} \quad (26)$$

The water activity (a_w) is taken from Eq. (9).

6. Quality attributes

6.1. Crumb formation

During baking the elastic dough transfers into a fixed structure due to starch gelatinization (Schiraldi et al., 1996). At this moment

Table 4
The composition of Dutch bakery products

Products	Water	Sugar	Starch	Fat	Protein	Other
Krakeling	0.15	0.30	0.26	0.02	0.04	0.22
Wholemal rusk	0.45	0.02	0.33	0.04	0.09	0.07
Bastogne cookie	0.17	0.31	0.29	0.18	0.04	0.00
Knackebrod	0.43	0.04	0.31	0.04	0.08	0.10
Cream cracker	0.20	0.04	0.54	0.14	0.07	0.01
Rusk	0.45	0.05	0.36	0.03	0.09	0.02
Biscuit	0.19	0.15	0.49	0.08	0.07	0.02
Toast	0.45	0.09	0.31	0.02	0.08	0.04
Cookie	0.20	0.24	0.31	0.17	0.06	0.02
Speculas	0.21	0.24	0.31	0.17	0.05	0.02
Cake	0.30	0.23	0.16	0.21	0.06	0.04
Ginger bread	0.40	0.23	0.23	0.01	0.02	0.11
Luxury white bun	0.45	0.04	0.37	0.04	0.07	0.03
White milk bread	0.46	0.05	0.37	0.02	0.08	0.02
Wheat bread	0.45	0.02	0.37	0.02	0.09	0.06
White water bread	0.46	0.03	0.41	0.02	0.07	0.01
Wholemeal bread	0.45	0.04	0.31	0.03	0.08	0.09
Egg cake	0.40	0.28	0.22	0.03	0.06	0.01
Rye bread	0.46	0.05	0.31	0.01	0.06	0.11

crumb, which is a major texture quality, is formed. The degree of gelatinization depends on the actual temperature and water content and is used as a measure for the final level of crumb formation. Examination of Dutch bakery products, with product compositions given in Table 4, by a small panel learned that the degree of crumb increases with the degree of gelatinization (α); see Fig. 4) and reaches a maximum value for $\alpha > 0.5$. Between these levels a linear relation between crumb and gelatinization is used (Eq. (27)).

$$\text{crumb} = \begin{cases} 0 & \text{if } \alpha = 0 \text{ (no crumb)} \\ 2\alpha & \text{if } 0 < \alpha < 0.5 \text{ (moderate crumb)} \\ 1 & \text{if } 0.5 < \alpha < 1 \text{ (crumb)} \end{cases} \quad (27)$$

6.2. Consistency: softness and crispness

The consistency attributes softness and crispness of bakery products are related to the elasticity of the product during consumption. The degree of crispness is related with the difference between product temperature and glass transition temperature (T_g). The glass transition temperature is a function

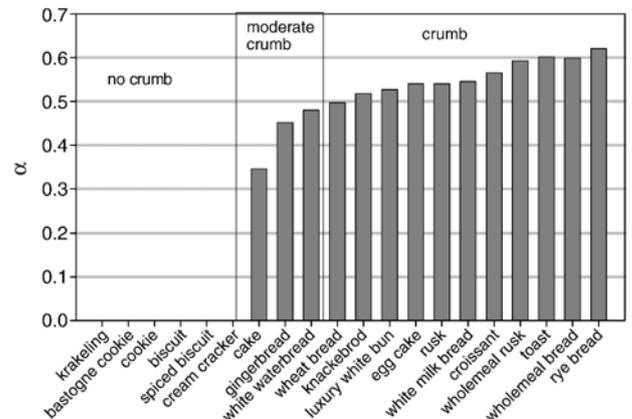


Fig. 4. Total degree of gelatinization for bakery products and crumb classification.

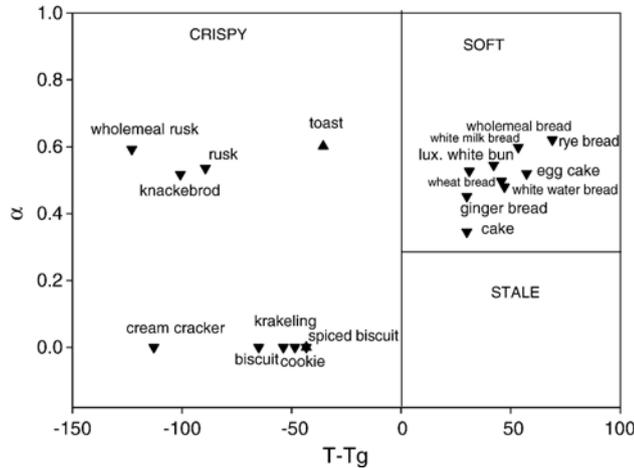


Fig. 5. Crispness and softness of products in terms of the difference between room temperature, glass transition temperature and degree of gelatinization. T_g varies for the products and is calculated from the composition and by using Eq. (23).

of water, sugar and starch content and is given in Eq. (23). Products are evaluated at room temperature; therefore the difference between room temperature and glass transition temperature is used to express crispness and softness.

$$\delta T = T_r - T_g \tag{28}$$

Products with a negative value for (δT) are crispy products and crispness reaches a maximum value (crispness=1) when all water is evaporated which occurs for $(\delta T = -150^\circ\text{C})$. For the degree of crispness between $\delta T = 0$ to $\delta T = -150^\circ\text{C}$ a linear expression is used:

$$\text{crispness} = \begin{cases} 0, & \text{if } \delta T > 0 \\ -\delta T/150, & \text{if } -150 < \delta T < 0 \\ 1, & \text{if } \delta T < -150 \end{cases} \tag{29}$$

Softness is a combined function of the glass transition temperature and degree of gelatinization. A soft product is obtained for $(\delta T > 0)$, but the gelatinization fraction has to be minimal 0.3 otherwise the product is experienced as staled. Maximal softness is obtained when all starch is gelatinized. Comparison of calculated values for Dutch bakery products yield that softness corresponds with the range $(\delta T = 0-100^\circ\text{C})$. From this information the following expressing is defined:

$$\text{softness}(\delta T) = \begin{cases} 0, & \text{if } \delta T < 0 \\ 0.01 \times \delta T, & \text{if } 0 < \delta T < 100, \\ 1, & \text{if } 100 < \delta T \end{cases} \tag{30}$$

and for the degree of gelatinization

$$\text{softness}(\alpha) = \begin{cases} 0, & \text{if } \alpha(t) < 0.3 \\ -\frac{3}{7} + \frac{10}{7} \alpha(t) & \text{if } 0.3 < \alpha(t) < 1 \end{cases} \tag{31}$$

Total softness is calculated as

$$\text{Softness} = \text{softness}(\delta T) \times \text{softness}(\alpha) \tag{32}$$

Fig. 5 shows the valuation of Dutch bakery products for their crispness and softness by using Eqs. (18)–(23), Eqs. (27)–(32) and initial composition for each product (Table 4). From the model follows that crackers, biscuits, *knäckebröd* and toasts fall in the category of crispy products, while bread types and cakes fall in the group of soft products. These results correspond to the consumers experiences. Due to retrogradation the degree of gelatinization of soft products decrease and for $\alpha < 0.3$ the soft products become staled. Crisp products do not retrograde because they are in the glass state.

6.3. Brownness model

Brownness is important for appearance and is influenced by the Maillard reaction which is non enzymatic reaction producing melanoidins (m_e) as a color compound. Moreover, product color is also a function of the initial color of the dough, and the follow-up reactions caramelization and carbonization, which occur when the product temperature is above 150°C . Although oven temperatures above 150°C are being used the temperature of the surface seldom exceeds 150°C . Therefore caramelisation and carbonisation are not considered in this work.

Even though the correlation between melanoidins and color development was reported as linear relation (Martins & van Boekel, 2003), in this work it is assumed that with increasing number of melanoidins, the color will reach saturation and goes to a maximum value (dark brown). This is achieved with the following expression:

$$\text{brownness} = 1 - (1 - \text{brown}(0)) \exp(-0.23m_e) \tag{33}$$

where $\text{brown}(0)$ is the initial brownness of the dough.

Fig. 6 shows the relation between melanoidins and brownness formation. It shows that the color formation goes to a maximum level of brownness in the range of white (brownness=0) to dark brown (brownness=1). Fig. 6 and Eq. (33) also show that the brownness development can start

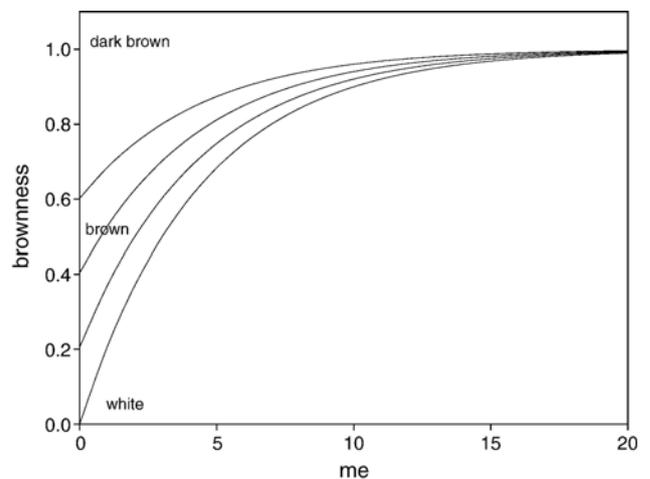


Fig. 6. Correlation between amount of melanoidins and brownness.

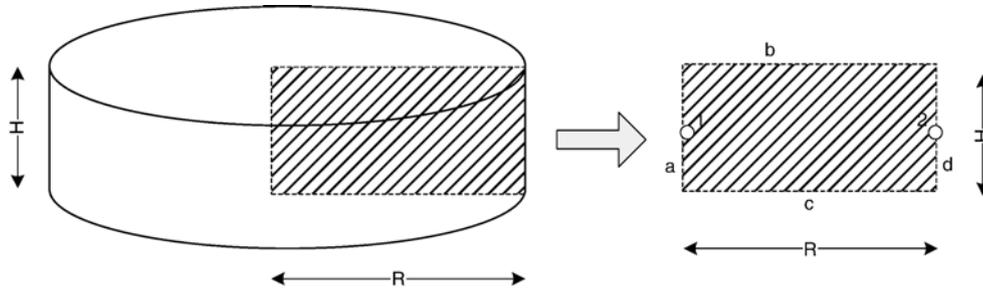


Fig. 7. The simulation domain. a,b,c and d represent the lines for boundary conditions. Points 1 and 2 represent the center and surface characteristic of products.

from different initial color due to other color compounds and melanoidins in the dough.

7. Simulation method

Bakery products are 3 dimensional products and the quality depends on the position in the product. Heat and mass transfer calculations are done with finite element calculations by multi-physic package of COMSOL 3.2. For the simulation, the bakery products were considered as a cylinder with height (*H*) and radius (*R*) as shown in Fig. 7. The shaded region is the sub domain where the simulation was performed and the two points were used to represent the center (point 1), and the surface (point 2). The symmetrical boundary condition (Eqs. (16) and (17)) is applied at the boundary line a, and the flux boundary condition (Eqs. (14) and (15)) to boundary lines b, c and d. The heat and mass transfer model and the boundary conditions are given in Eqs. (1)–(17).

The model allows the simulation of a variety of bakery products. In the next section three different bakery products (bread, biscuit and cake) illustrate the results for product transformation and product quality. The products and properties are specified in Table 5.

Table 5
Parameter specification for simulated bakery products

Properties	Products		
	Bread	Biscuit	Cake
Size (<i>H</i> , <i>R</i>)	(0.03,0.05)	(0.0025,0.025)	(0.03,0.05)
Baking time (s)	2100	800	2100
<i>T</i> _{oven} (°C)	200 °C	200 °C	200 °C
Initial conditions			
<i>W</i> ₀ (kg/kg)	0.45	0.19	0.30
<i>Z</i> ₀ (kg/kg)	0.37	0.49	0.16
<i>S</i> ₀ (kg/kg)	0.02	0.15	0.23
<i>C</i> ₀ (kg/kg)	0.15	0.09	0.10
<i>m</i> _{e,0}	0	0	0
Brown ₀	0	0	0
Product properties			
ρ_s (kg/m ³)	705	540	880
<i>C</i> _p (J/kgK)	1712.5	1712.5	1951
<i>k</i> (W/mK)	0.4	0.2	0.4
<i>D</i> _{vc} (m ² /s)	2.10 ⁻⁵	2.10 ⁻⁵	2.10 ⁻⁵
<i>D</i> _w (m ² /s)	1.10 ⁻¹⁰	1.10 ⁻¹⁰	1.10 ⁻¹⁰
<i>h</i> _c (W/m ² K)	15	15	15
<i>h</i> _v (m/s)	0.2	0.2	0.2

8. Results and discussion

8.1. Product temperature and water distribution

The predicted temperature and water content for bread, cake and biscuit during baking at an oven temperature of 200 °C are given in Fig. 8. The lines represent the change of temperature and water content in the center and just below the surface. The temperature near the surface of the products increases more rapidly than

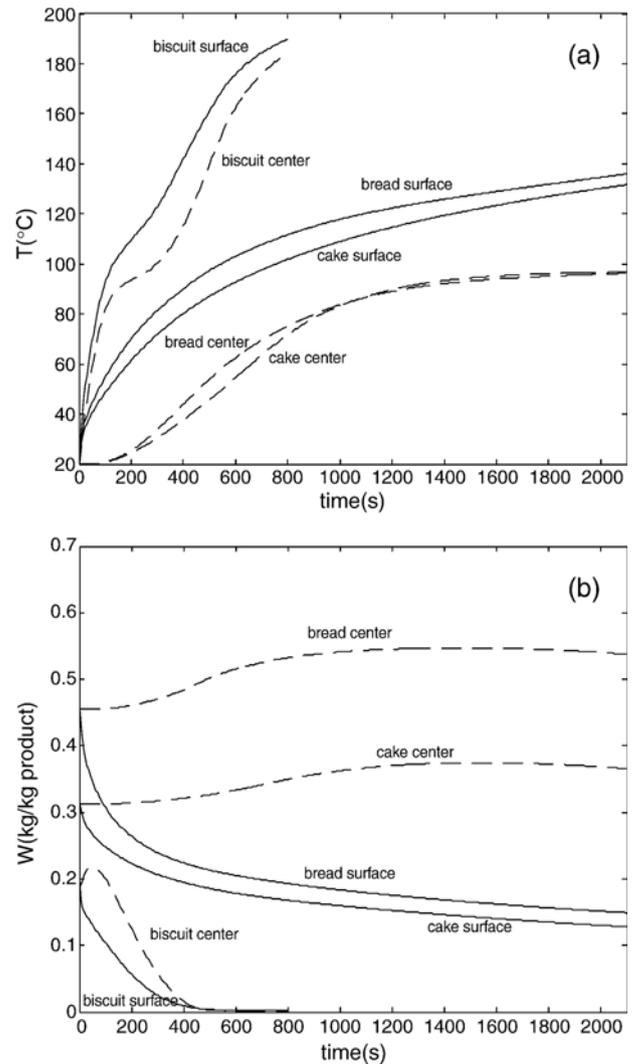


Fig. 8. Temperature (a) and water (b) profiles for three products during baking.

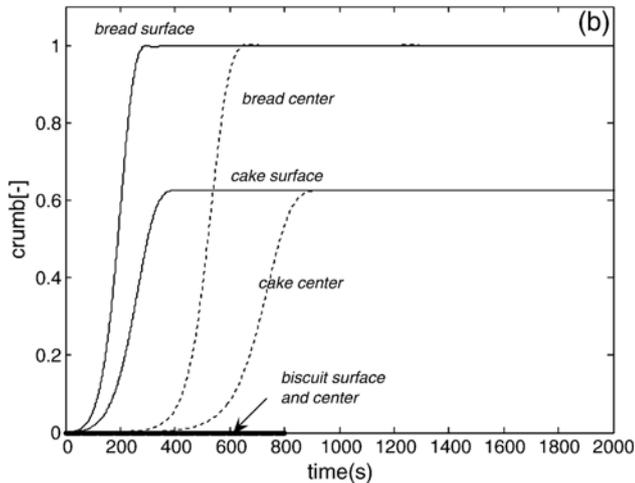


Fig. 9. Crumb formation during baking.

in the center and come closer to the oven temperature. For all products, the temperature in the center remains during some time around the evaporation temperature (100 °C). Due to the relatively high water content the period around 100 °C is longer for bread and cake than for the other products. The center temperature for biscuits, with low water content, remains only a short time at 100 °C and rises when the majority of water has been evaporated.

For all products, the high evaporation rate in the surface region results in rapid decrease of the water content. In the first phase of baking, the water in the center of the products is almost unchanged as the heat does not yet penetrate into the center. Then the water content increases due to the condensation effect. For biscuits the center of the product starts to dry in a third phase and finally the water contents becomes zero. Bread and cake show the same phenomena but with different patterns. The water content in the center increases but due to the larger product dimensions and the limited heat penetration, it takes a long time before the water content in the center starts to decrease. This result corresponds to the work of Thorvaldson and Jensted (1999).

8.2. Crumb formation

Crumb formation is important since it develops the pore structure in the products (Schiraldi et al., 1996). Crumb formation is a result of starch gelatinization which depends on the actual water content, the composition and product temperature. Fig. 9 shows the degree of crumb formation that corresponds to degree of gelatinization formation of the three products. The result shows that degree of gelatinization at the surface is significantly faster than in the center which corresponds with the temperature profile. The simulations (combining Figs. 8 and 9) show that gelatinization is completed at 78 °C for bread and 81 °C for cake; the degree of gelatinization is 0.50 and 0.31 respectively. Biscuit, which has low water content, does not gelatinize. The consequences of gelatinization on the crumb formation are also shown in Fig. 9. In bread full crumb is formed while in cake the degree of crumb is partial because of the degree of gelatinization is below 0.5. The structure in cake is not fully developed and pores formation is partial. For biscuit the crumb is absent.

8.3. Softness and crispness

Softness and crispness are also derived from the degree of gelatinization. During product heating, starch gelatinizes and water evaporates into the oven. Gelatinization affects the mechanical strength of the products which also increases with decreasing amount of water in the product. As a result the products lose first their softness and then become crispy.

Fig. 10 shows softness and crispness of the simulated bakery products. Softness follows the pattern of decreasing water content and becomes zero when the product temperature comes below the glass transition temperature (T_g). When T_g is achieved, the product changes from rubber to glassy state. The glass transition temperature for bread, which has a high water content, is $T_g = -25$ °C and for cake $T_g = -10$ °C, while biscuit has a high glass transition temperature $T_g = 80$ °C. These values explain the differences in the soft and crispness of the products at consumption temperature. Fig. 10 also shows that softness in the center of cake and bread hardly changes, while significant changes in crispness occur in the biscuit

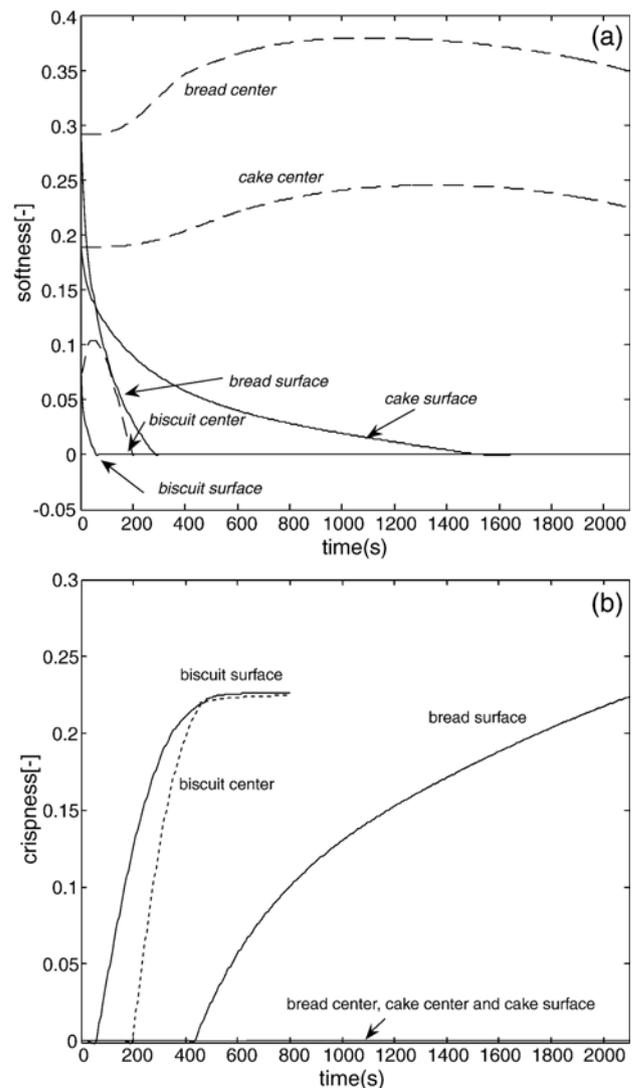


Fig. 10. Softness (a) and crispness (b) development.

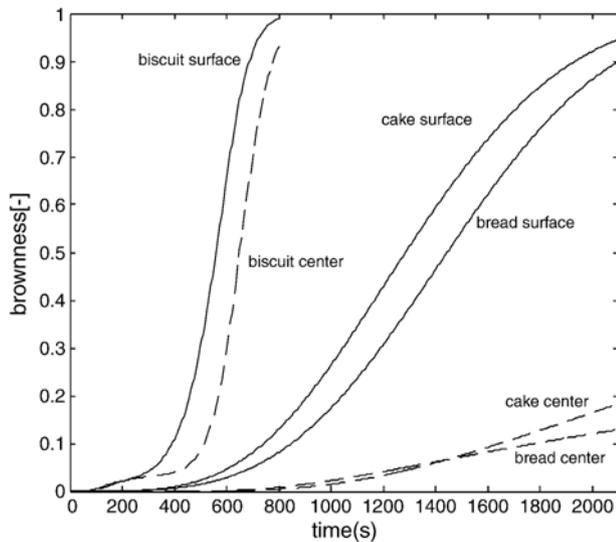


Fig. 11. Development of brownness during baking.

center. This is directly related to current water content in the product which evaporates faster than for the two other products.

8.4. Color

The color, expressed in the level of brownness, is influenced by the composition of the dough, the water content and process conditions during baking process. The Maillard reaction is the main responsible for color development at temperatures below 150 °C.

Fig. 11 shows the development of brownness during baking for the three products due to the formation of melanoidins. The development of brownness on the surface is faster than in the center due to quick increase of surface temperature. The fast increase of temperature together with the fast decrease of the water content in the surface accelerates the Maillard reaction between sugar and amino acids which gives more melanoidins during baking.

Bread shows significant color change at the surface and only a moderate change in the center. This is the result of the high water content and low temperature in the center which gives a low amount of melanoidins.

The formation of melanoidins in biscuit is faster than in the bread. The low water content and small dimension have the effect that water is quickly evaporated and the product is dried out faster. The low water activity would result in a low reaction rate, but the increased temperature effect on color formation surpasses the water activity contribution. Cake shows also a different pattern than bread; the final brownness is higher. This is due to the larger amount of sugar in cake which gives a higher amount of melanoidins.

8.5. Size (height)

The height is a result of the pressure difference between the total pressure in the product and pressure in the oven. The pressure difference causes product deformation resulting in extension of height.

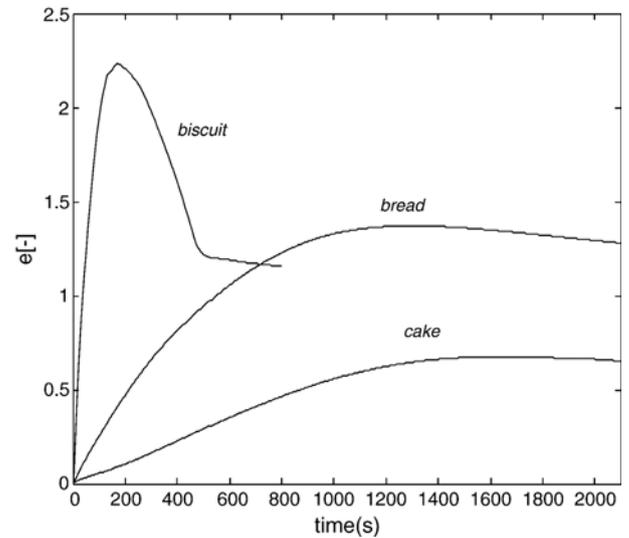


Fig. 12. The extension of product height during baking.

Fig. 12 shows the extension for the three products. The height of the biscuit increases during the first 200 s and starts to decrease when the product structure is open. The pressure difference between product and oven becomes less and at about 400 s the pressure difference is constant. The simulation shows that for biscuits the initial height is doubled (i.e. 100% extension). Bread height increases to a slightly higher value (120% extension), but there is not a prominent maximum in the curve. Cake shows the lowest degree of extension (60%). This also related to degree of gelatinization which is not fully achieved during baking.

8.6. Retrogradation during storage

As biscuits are in the glass state retrogradation does not occur for this product and therefore only retrogradation for bread and cake is presented in Fig. 13. To demonstrate the

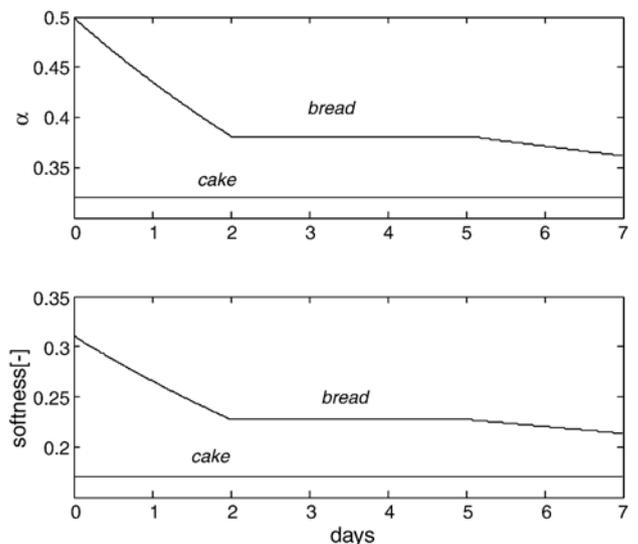


Fig. 13. Changes in degree of gelatinization and softness during storage caused by retrogradation. Temperature is 20 °C for 2 days, then -20 °C for 3 days and finally 5 °C for 2 days.

effects of storage temperature, different settings of temperature are applied: 20 °C (room temperature) for 2 days followed by –20 °C (freezer temperature) for 4 days and 2 days at 5 °C (refrigerator temperature).

During storage at room temperature the degree of gelatinization lowers due to retrogradation and the product becomes more stale. Retrogradation is enhanced by water uptake from the air around the product (see also contribution of water content in Eq. (21) and Table 3). For cake there is hardly retrogradation because of the higher glass temperature (–18 °C) and the lower water content. Therefore, the product can be stored under room temperature for 1 week with minimal staling. In frozen state the retrogradation of bread is minimized and therefore long term storage under this temperature is recommended to keep quality. However, when bread is stored under refrigerator conditions (5 °C), retrogradation will start again.

8.7. Directions for quality control

The overall influence of control parameters on the selected quality attributes were derived from simulations. The changes in final product quality for bread (composition given in Table 5) were calculated for 20% changes of oven temperature, initial water content, sugar, and starch components. The sensitivity indicators are given in Table 6. The sensitivity changes are categorized into 5 categories: o = changes below ±1%, +/- = moderate changes in the range 1–10% (increase/decrease), ++/-- = significant changes in the range 10–20% (increase/decrease), and +++/---- = major changes above 20% (increase/decrease).

The product surface is directly exposed to the oven temperature. Therefore it is the main variable that affects the product quality attributes (water content, crispness, height and color) of the product at the surface. An increase of the initial water content results in a strong increase of softness in the product center and at the same time crispness of the surface decreases. Crumb formation is highly affected by a decrease of initial water content. Sugar and starch concentrations are mainly important for the crispness of the surface and softness in the

center and no significant changes are found for other quality attributes.

Combination of two opposite sensitivities does not always compensate each other. For example, the effects of changes in crispness at the surface due to increase of oven temperature are surmounted by the effect of increased initial water content.

9. Conclusion

Initial phases in food process design are enhanced by using mathematical models to explore the feasibility of alternatives, to compare alternatives and to reduce the time span for process development. The main objective of such feasibility phase is to rank different production methods with respect to the obtained product quality.

Baking is a process where several transformations occur for which a lot of information is available on specific aspects. To deal with the complexity of the product–process interaction, a systems approach is used, by splitting the process in three sequential parts:

- mass and heat transfer in porous media
- transformations of starch and the formation of color forming components
- quality properties (crumb, crust, color, softness and crispness)

Models of these parts were based on the dominant phenomena in the system. Although the accuracy of the model predictions might be limited, the proposed approach covers the interconnection between the separate parts, it learns to understand the phenomena that occur in the product and will also help to find which additional experiments are required to improve the prediction.

Because of the transport phenomena in bakery products, the qualities depend on the position in the products and also on the size and form of the product. Therefore it is necessary to use spatial models. The model predicts how the quality changes by the choice of the dough composition and energy as input variables.

The transformation of starch is derived from the behavior of polymers as a function of temperature and composition. The

Table 6
The variation of bread quality attributes after baking for changed values of input variables with 20%

Parameter ^a	W		Crumb		Crispness		Softness		Color		Height
	s	c	s	c	s	c	s	c	s	c	
T _{ext} : ↑	--	-	o	o	+++	o	o	--	++	+	+
T _{ext} : ↓	+++	+	o	o	----	-	o	+	----	o	--
W ₀ : ↑	++	+++	o	o	----	o	+	+++	-	o	o
Z↑;	o	o	o	o	-	o	-	+++	o	o	-
S↑;	o	o	o	o	-	o	o	--	o	o	-
T _{ext} : ↑ W ₀ : ↑	-	++	o	o	-	o	+	+++	+	+	++
T _{ext} : ↑ W ₀ : ↓	----	----	----	----	+++	o	o	----	++	+	-
T _{ext} : ↓ W ₀ : ↓	-	--	----	----	-	o	o	----	----	o	----
T _{ext} : ↓ W ₀ : ↑	+++	+++	o	o	----	o	o	+++	----	o	--

The changes of quality attributes are relative to a standard product (as given in previous sections).
 Note: s = surface, c = center, W₀ = initial water content, T_{ext} = oven temperature, Z = starch, S = sugar.
 ↑ = increase of parameter value = 20%, ↓ = decrease of parameter value = 20%.
 o = less than 1% change, + = increase 1–10%, - = decrease 1–10%, ++ = increase 10–20%.
 -- = decrease 10–20%, +++ = increase >20%, ---- = decrease >20%.

^a Other parameters which are not mentioned use standard values.

glass transition, melting and gelatinization temperature are important indicators. The degree of starch gelatinization is used as the main indicator for softness and crispness of the products. In storage the degree of gelatinization decreases by starch retrogradation, which results in staled products. The Maillard reaction is the main reaction for color formation.

Heuristic knowledge on quality attributes was captured by using rules with a minimum and maximum value (0–1 rules). This approach showed realistic predictions for Dutch bakery products and offer therefore good opportunities for use in the feasibility phase of process design.

As the model is not yet calibrated, the model will not give full accuracy. However, the model shows the tendency of the effects of input variables (composition and outside temperature) on the product quality, and is therefore suitable to explore production alternatives and to compare them by ranking in the initial phase of food process design. Moreover, the model supports to understand the interconnection between the phenomena.

Nomenclatures

Notations	Description (unit)
a_w	Water activity
C	Other water binding components (kg kg ⁻¹)
C_p	Heat capacity (J kg ⁻¹ K ⁻¹)
D_v	Gas diffusivity (m ² s ⁻¹)
D_w	Liquid diffusivity (m ² s ⁻¹)
e	Extension of height
f	Fusion factor
E	Elasticity modulus (Pa)
E_a	Activation energy (kJ mol ⁻¹)
G_0	Reference retrogradation rate (s ⁻¹)
I_v	Evaporation rate (Kg m ⁻³ s ⁻¹)
I_c	Production rate of CO ₂ (Kg m ⁻³ s ⁻¹)
h_c	Convective heat transfer coefficient (Wm ⁻² K ⁻¹)
h_v	Mass transfer coefficient (m s ⁻¹)
K	Thermal conductivity of product (W m ⁻¹ K ⁻¹)
K_g	Constant
k_{gel}	Gelatinization rate constant (s ⁻¹)
k_{me}	Reaction rate of Maillard reaction (s ⁻¹)
m_v	Mass flux of water vapor (kg m ⁻² s ⁻¹)
m_e	Melanoidins
m_c	Mass flux of CO ₂ gas (kg m ⁻² s ⁻¹)
M_w	Molecular weight of water (kg mol ⁻¹)
P	Total pressure (Pa)
$P_{v,sat}$	Saturated pressure of water vapor (Pa)
R	Gas constant (J mol ⁻¹ K ⁻¹)
R_{CO}	CO ₂ generation rate (kg kg ⁻¹ s ⁻¹)
S	Sugar content (kg kg ⁻¹)
T_∞	Hypothetical temperature (K)
U^*	Activation energy for product during recrystallization (J mol ⁻¹)
V_c	CO ₂ gas concentration (kg kg ⁻¹)
V_v	Water vapor (kg kg ⁻¹)
W	Water content (kg kg ⁻¹)
Z	Starch content (kg kg ⁻¹)
T_g	Glass transition temperature (K)

T_m	Melting temperature (K)
T_α	Gelatinization temperature (K)
S/Z	Ratio sugar to starch

Greek letters

α	Total degree of starch gelatinization
α_{max}	Maximum gelatinization degree
λ	Evaporation heat (J kg ⁻¹)
ϵ	Porosity
ν	Kinematic viscosity (m ² s ⁻¹)
ρ_s	Density of solid matrix (kg m ⁻³)
κ	Permeability (m ²)
η	Dynamic viscosity (Pa. s)
ϕ	Flux (kg m ⁻² s ⁻¹)

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