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DEVELOPMENT AND SENSITIVITY ANALYSIS OF CFD-BASED BREAD BAKING MODEL

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Abstract

Bread baking stands as one of the earliest and most important industrial processes, wherein the dough undergoes complex chemical and physical transformations leading to the final product. Regarding process optimization, bakeries historically relied on the "cook and look" method because providing a proper physical description of the process is highly challenging. Our ultimate and long-term goal is to provide a methodology to optimize the energy consumption of the industrial bread-baking process. In this contribution, we delineate the fundamentals of design and implementation of the fully resolved CFD model of internal mass and heat transfer inside the bread. The external transfer limitations are employed using the external transfer coefficients. The model results are validated and cross-verified with existing literature, and the model sensitivity to the variations of the evaporation coefficient and solid heat conductivity is examined. Evaporation coefficient influences especially the total moisture content and the surface temperature, while the solid heat conductivity affects the center bread temperature significantly.

Keywords: CFD, bread baking, OpenFOAM.

1 Introduction

Bread has historically been among the first staple foods produced by humans and it continues to be one of the most commonly manufactured baked goods worldwide. Therefore, the practice of baking bread is widely understood on a global scale [1]. During the baking process, the dough is subjected to "appropriate temperatures" for a "appropriate time" in the ovens [2]. This process induces complex chemical and physical transformations, including starch gelatinization, water evaporation and condensation, carbon dioxide emission, crumb and crust formation, and volume expansion accompanied by the creation of pores [3]. Furthermore, the finished bread must conform to standardized quality benchmarks, which are evaluated primarily based on texture (specifically, crust percentage), moisture content, coloration (browning), structure, and sensory evaluations [4]. This makes proper modeling of the baking process multi-physical and rather challenging, leading to the persistence of the "cook and look" method in the industry to ascertain the "appropriate time and temperatures" [3].

The continuous advancements in numerical mathematics and computational capacity are expanding the applicability of computational fluid dynamics (CFD) across various fields. Our long-term objectives are to (i) create a validated CFD model for simulating bread baking in industrial ovens, (ii) decrease the model's computational expense through conventional model order reduction techniques, and (iii) employ the model to lower energy consumption during the baking process.

In order to accurately simulate the baking process, it is essential to address both (i) the external transport of mass, momentum, and heat within the oven, and (ii) the internal transport of mass and heat within the bread, while ensuring they are appropriately coupled, see Fig. 1a. Our idea is to achieve this coupling using *multi-region* approach as available in OpenFOAM. In particular, the external transport outside the bread will be modeled by an unstable version of the Reynolds-averaged Navier-Stokes equations. The development of a model for internal transport, see Figure 1b, is a primary objective of this study. Additionally, this paper examines the model's sensitivity to variations in parameters that are challenging to determine experimentally.

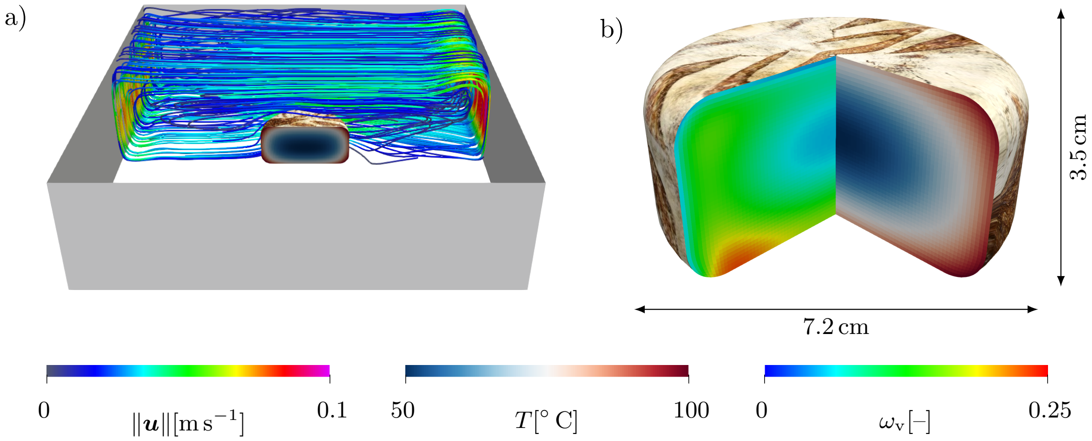

Figure 1: a) Bread inside the oven with the streamlines colored by the velocity, b) contours of the water vapors content (ω_v) and temperature T after 4 minutes of the baking.

2 Mathematical model

In this section, we delineate the model of internal transport in bread as developed in this study by providing the mass balances, the enthalpy balance, the geometry of the model, the boundary conditions and the overall solution algorithm. The bread dough is treated as a pseudo-homogeneous medium comprising three distinct phases: solid wheat (s), liquid water (l), and gas (g), each represented by the volumetric fractions α_s, α_l, and α_g, respectively. Furthermore, the gaseous phase consists of water vapor (v) and CO_2 (c).

2.1 Mass transfer

Liquid water transfer The mass transfer of the liquid water occurs only through the evaporation/condensation mechanism, where liquid water first evaporates on the hotter side of the pores into gas, then it diffuses through pores as water vapor, and finally it condenses on the cooler side of the pores. The liquid water balance can be then written as,

$$\frac{\partial(\alpha_\mathrm{l}\,\rho_\mathrm{l})}{\partial t} = -\dot{m}^\mathrm{ev}\,, \tag{1}$$

where ρ_l is liquid water mass density. The water evaporation rate $\dot{m}^\mathrm{ev}$ is defined based on [1],

$$\dot{m}^\mathrm{ev} = \begin{cases} k^\mathrm{e}\,\alpha_\mathrm{l}\,\rho_\mathrm{l}\dfrac{T-T_\mathrm{s}}{T_\mathrm{s}} & T > T_\mathrm{s} \\ k^\mathrm{c}\,\alpha_\mathrm{g}\,\rho_\mathrm{g}\,\omega_\mathrm{v}\dfrac{T-T_\mathrm{s}}{T_\mathrm{s}} & T < T_\mathrm{s} \end{cases} \tag{2}$$

where T, ρ_g and ω_v are in order temperature, gas mass density, and the mass fraction of the water vapors in the gas. The saturated temperature T_s is calculated from the local water vapor pressure using the Antoine equation. Finally, k^e and k^c stand for the evaporation and condensation constants, which are quite difficult to determine rigorously [1]. To reduce a number of parameters of the model, we assume $k^\mathrm{c} = 1\,000\,k^\mathrm{e}$, which keeps the order of the condensation rate similar to the evaporation rate. Furthermore, the evaporation constant k^e is the subject of the model sensitivity analysis present in this contribution.

Gas transfer In addition to the condensation/evaporation mechanism described in the previous paragraph, the gas inside the bread is transferred due to the pressure gradient according to the

Darcy law of permeability, which we define according to [3] as

$$\dot{\boldsymbol{m}}_\mathrm{g} = -\rho_\mathrm{g}\frac{\kappa_\mathrm{g}}{\mu_\mathrm{g}}\nabla p_\mathrm{g}\,, \tag{3}$$

where κ_g is the Darcy permeability, and μ_g is the gas dynamic viscosity. The gas mass density is expressed using the gas ideal law,

$$\rho_\mathrm{g} = \frac{p_\mathrm{g} M_\mathrm{g}}{RT}\,, \tag{4}$$

where M_g, and p_g are the gas molar mass and the pressure, respectively. The rate of CO_2 generation by fermentation is evaluated based on [3] as,

$$\dot{m}^\mathrm{gen}_{\mathrm{CO_2}} = R_0 \exp\left[-\left(\frac{T-T_m}{\Delta T}\right)^2\right], \tag{5}$$

where R_0, ΔT, and T_m are kinetic constants taken from [3]. The conservation of the gas phase in the bread can be then written as,

$$\frac{\partial(\alpha_\mathrm{g}\,\rho_\mathrm{g})}{\partial t} + \nabla\cdot\dot{\boldsymbol{m}}_\mathrm{g} = \dot{m}^\mathrm{ev} + \dot{m}^\mathrm{gen}_{\mathrm{CO_2}}\,, \tag{6}$$

Water vapor transfer Finally, to complete the description of the mass transfer, the water vapors diffuse in the gas and hence the vapor balance can be written as,

$$\frac{\partial(\alpha_\mathrm{g}\,\rho_\mathrm{g}\,\omega_\mathrm{v})}{\partial t} + \nabla\cdot(\omega_\mathrm{v}\dot{\boldsymbol{m}}_\mathrm{g}) - \nabla\cdot(\rho_\mathrm{g}\,D^\mathrm{eff}\nabla\omega_\mathrm{v}) = \dot{m}^\mathrm{ev}\,, \tag{7}$$

where D^eff is the effective diffusive coefficient of the vapors in CO_2 calculated as suggested in [3],

$$D^\mathrm{eff} = D\,\left[(1-1.11\,S)\alpha_\mathrm{g}\right]^{1.33}\,, \tag{8}$$

where D is the binary diffusion coefficient of the water vapors in CO_2, and S is the water saturation.

2.2 Enthalpy transfer

The enthalpy in the bread is transferred by the standard convection and conduction mechanisms and by the described evaporation/condensation mechanism. Therefore, we use the enthalpy balance in the form,

$$\frac{\partial(\sum_k \rho_k\alpha_k c_{p,k}\,T)}{\partial t} + \nabla\cdot(c_{p,\mathrm{g}}T\,\dot{\boldsymbol{m}}_\mathrm{g}) - \nabla\cdot(\lambda^\mathrm{eff}\nabla T) = \dot{m}^\mathrm{ev}\,{}_\Delta H^\mathrm{ev}\,, \quad k=\{\mathrm{s,\,l,\,g}\} \tag{9}$$

where summation index k stands for all phases, $c_{p,k}$ is the phase heat capacity, and H^ev is the evaporation enthalpy. The effective heat conductivity λ^eff is evaluated as the weighted sum of the heat conductivities of the individual phases,

$$\lambda^\mathrm{eff} = \alpha_\mathrm{l}\lambda_\mathrm{l} + \alpha_\mathrm{g}\lambda_\mathrm{g} + \alpha_\mathrm{s}\lambda_\mathrm{s}\,, \quad \lambda_\mathrm{l}\approx\lambda_\mathrm{s}\approx 10\,\lambda_\mathrm{g}\,. \tag{10}$$

Multiple more advanced methodologies have been proposed for the calculation of effective thermal conductivity, as seen, e.g., in [3, 5]. However, the variation in λ^eff values is high and strongly influenced by the composition of the dough [6]. Due to the uncertainty regarding the specific composition of the experimental dough modeled in this study, we opted to choose λ_s as the second parameter for sensitivity analysis in this contribution. Note that the resulting effective heat conductivity in the dough during baking varies in the range of $\lambda^\mathrm{eff}\approx(0.3;0.5)\,\lambda_\mathrm{s}$.

2.3 Model geometry and boundary conditions

Model geometry The geometry of the model is prepared to match the experimental work of Zhang et al. [3], who baked cylindrically shaped loafs of bread. We utilize the axi-symmetry of the cylinder to create the two-dimensional computational mesh depicted in Figure 2b. Furthermore, Zhang et al. [3] measured the temperature evolution during baking at two probe points in the center and on the bread surface highlighted in Figure 2a in blue and red, respectively.

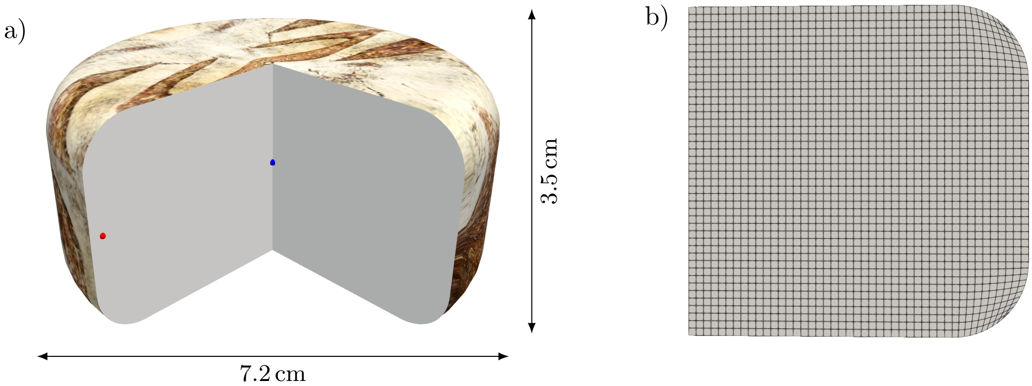

Figure 2: a) Bread with its dimensions and the temperature measurement probe points highlighted in blue and red, and b) used computational mesh.

Table 1: Boundary conditions for all the variables.

	free surface	bottom
α_l	$\boldsymbol{n}\cdot\nabla\alpha_\mathrm{l} = 0$	$-(\boldsymbol{n}\cdot\nabla\alpha_\mathrm{l}) = 0$
p_g	$\boldsymbol{n}\cdot\dot{\boldsymbol{m}}_\mathrm{g} = k_\mathrm{M}\left[\rho_\mathrm{g}-\rho_\infty\right]$	$-(\boldsymbol{n}\cdot\dot{\boldsymbol{m}}_\mathrm{g}) = 0$
ω_v	$-\rho_\mathrm{g}\,D^\mathrm{eff}(\boldsymbol{n}\cdot\nabla\omega_\mathrm{v}) = k_\mathrm{M}\left[\rho_\mathrm{v}-\rho_{\mathrm{v},\infty}\right]-\omega_\mathrm{v}(\boldsymbol{n}\cdot\dot{\boldsymbol{m}}_\mathrm{g})$	$-\rho_\mathrm{g}\,D^\mathrm{eff}(\boldsymbol{n}\cdot\nabla\omega_\mathrm{v}) = 0$
T	$-\lambda^\mathrm{eff}(\boldsymbol{n}\cdot\nabla T) = k_\mathrm{H}\left[T-T_\infty\right]-c_{p,\mathrm{g}}T\rho_\mathrm{g}(\boldsymbol{n}\cdot\dot{\boldsymbol{m}}_\mathrm{g})$	

Boundary conditions The boundary conditions employed are adopted from [3]. We consider external transport limitations characterized by the external mass (k_M) and heat (k_H) transport coefficients at the bread's free surface. During the experiment, the bread is put on a thin metal holder, implying that at the bread bottom, the temperature boundary condition can be same as that of the free surface. However, mass transport through the bread's bottom is constrained. All the boundary conditions are listed in Table 1. Note that subscript '∞' denotes state of the variable in the oven.

2.4 Solution algorithm

The solution of the described set of partial differential equations is performed using a custom-developed OpenFOAM solver. The algorithm of the solution is the segregated one, and the solution is iterative. This means that in each time step, equations (1), (6), (7), and (9) are sequentially solved until the residuals of all variables do not fall below 10^{-10}.

3 Results

3.1 Mesh and time step independence study

To examine how the choice of spatial and temporal discretization steps affects the independence of the results, we define the error of the simulation in the variable ϕ with the spatial discretization h and temporal discretization k as,

$$E_h^k(\phi) = \left\| \frac{\boldsymbol{\phi}_h^k - \boldsymbol{\phi}_\mathrm{ref}^\mathrm{ref}}{\boldsymbol{\phi}_\mathrm{ref}^\mathrm{ref}} \right\|, \tag{11}$$

where $\boldsymbol{\phi}_h^k$ is the temporal evolution of the variable ϕ and the notation "ref" denotes the reference simulation with the most fine mesh ($h^\mathrm{ref} = 0.4\,\mathrm{mm}$) for the spatial studies, and smallest time step ($k^\mathrm{ref} = 0.025\,s$) for the temporal studies. Finally, the center temperature of the bread and the total moisture content have been selected as the studied variables.

At first, the time step is fixed at $k = 0.2\,\mathrm{s}$ and we study the influence of the decreasing spatial step. Figure 3a depicts the error development of the center temperature of the bread and the total

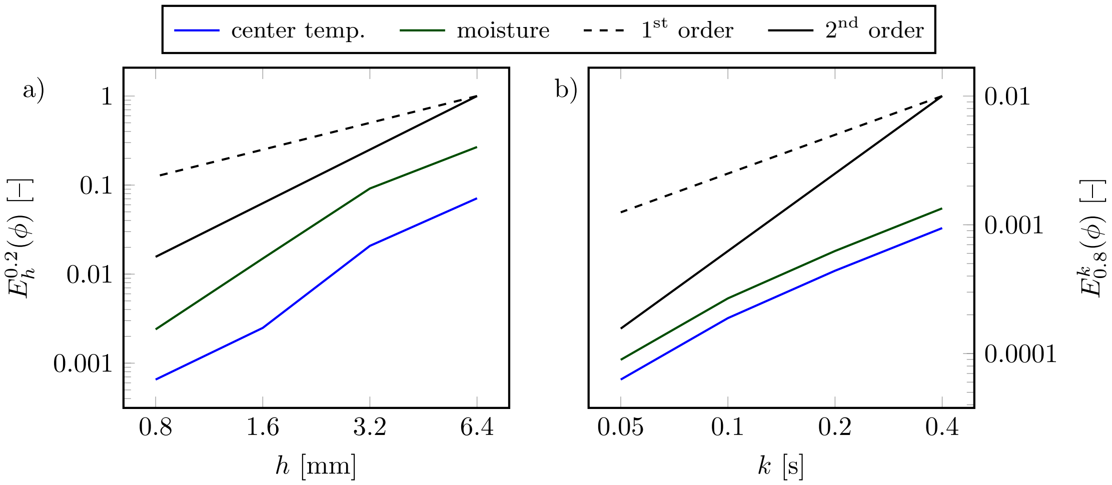

Figure 3: Simulation error development with the increasing a) spatial, and b) temporal time step.

moisture content in bread. The spatial model accuracy for both variables is close to the second order, which is expected for the used finite volume discretization. Moreover, in all future studies we use mesh with the spatial discretization of $h^{\text{used}} = 0.8\,\text{mm}$, where the relative error for both studied variables is far below 1 %.

Similarly, the spatial step is fixed at $h = 0.8\,\text{mm}$ and the temporal discretization is studied in Figure 3b. For the temporal discretization, *Crank-Nicolson 0.9* scheme as implemented in OpenFOAM is used and as such, the second order accuracy would be expected. In the reality, the model seems to be closer to the first order, but the error for the selected time step $k^{\text{used}} = 0.2\,\text{s}$ is below 0.1 %.

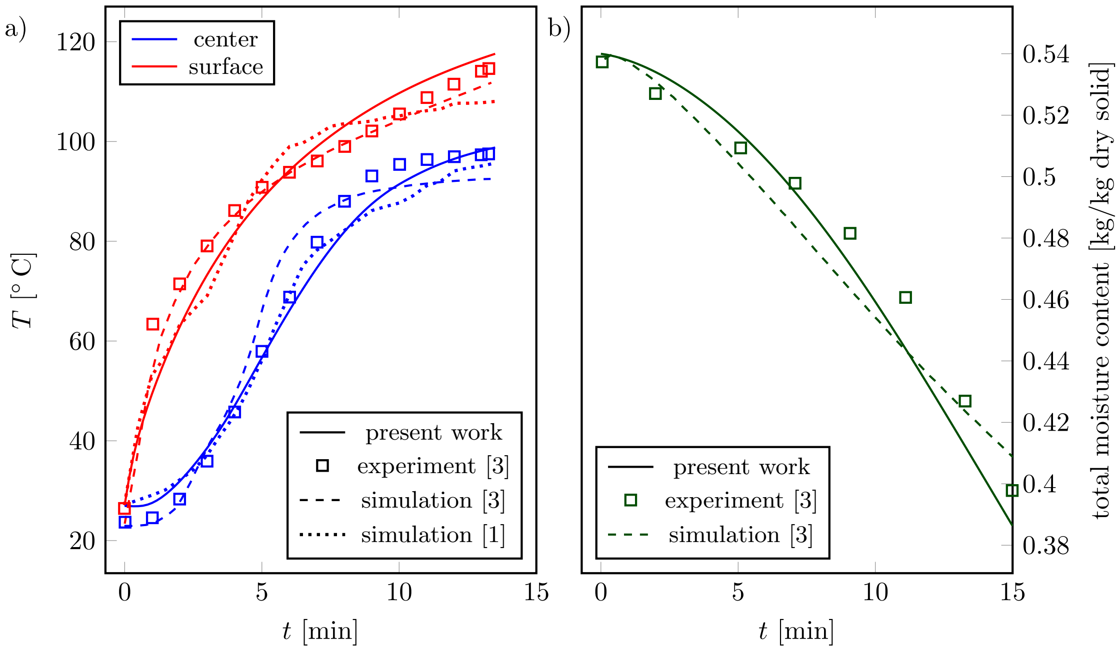

Figure 4: Temporal evolution of the a) surface and center temperature of the bread, b) moisture content inside the bread.

3.2 Model verification and validation

Before the sensitivity analysis of the selected parameters of the model, we first present the verification of the model against simulations of Zhang et al. [3] and Al-Nasser et al. [1], and the validation against experimental work of Zhang et al. [3]. Note that in this subsection, the values of the studied parameters are set to fit the experimental data as best as possible.

As stated in the paragraph Model geometry in the previous section, Zhang et al. [3] measured two temperatures during baking and the total moisture content during baking. The temporal evolution of these is shown in Figure 4. Starting with the comparison of the center (blue) and the surface (red) temperature development depicted in Figure 4a, the present model (solid) predicts the experimental data (squares) quite well. Especially for the center temperature that is crucial for the baking process, the prediction of the model seems to outperform the previous numerical studies [1, 3]. Focusing on the surface temperature, the model slightly underestimates the temperature increase at the start of baking, but the error is within the scatter of the previously published models.

Examining the evolution of the total moisture content during baking in Figure 4b, note that the model of Zhang et al. [3] predicted a practically linear decrease of the total moisture content. The present model seems to better capture the trend of water evaporation, but still the experimental data suggest a higher evaporation at the start of the process and, on the other hand, a lower evaporation at the end of the process.

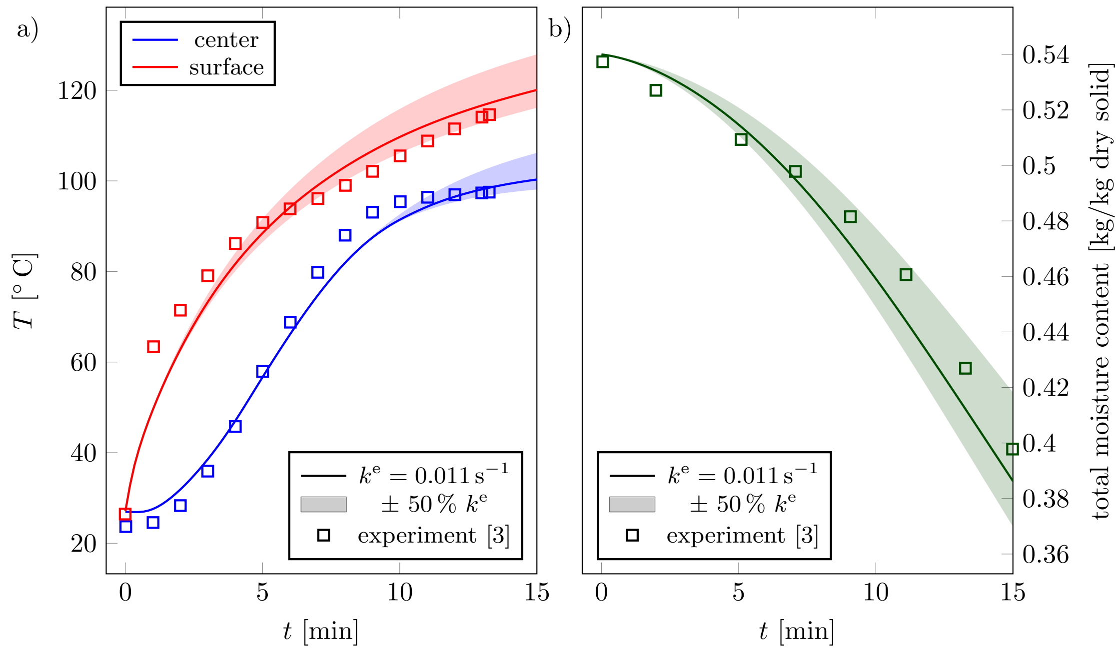

Figure 5: Influence of the evaporation coefficient k^e on the temporal evolution of the a) center and surface temperatures, and b) moisture content inside the bread.

3.3 Model parameters sensitivity analysis

Influence of the evaporation coefficient The first parameter selected for the sensitivity analysis is the evaporation coefficient k^e needed to evaluate the evaporation rate (2). In Figure 5, we present the change in the evolution of the temperature and moisture content with $\pm$ 50 % changes of this parameter. Considering the temperatures in Figure 5a first, note that the value of the evaporation coefficient influences the typical shape of the temperatures development. With low k^e values, both the surface and the center temperatures exhibit a similar trend; see the upper border of the red and blue areas in Figure 5a. On the other hand, with increasing values of k^e, the heat in the center of the bread is used for evaporation and the temperature in the center cannot cross over 100 ° C. Next, the time development of the total moisture content is strongly influenced by the evaporation coefficient value, see Figure 5b. This is expected as the evaporation rate directly influences the amount of evaporated (lost) water.

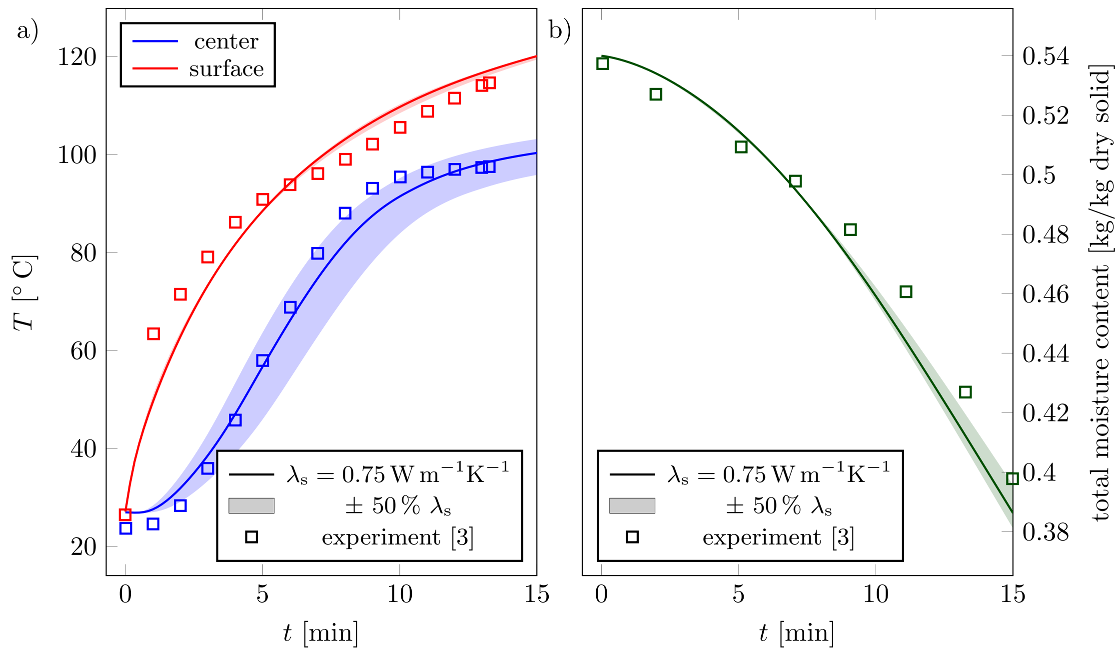

Figure 6: Influence of the solid heat conductivity λ_s on the temporal evolution of the a) center and surface temperatures, and b) moisture content inside the bread.

Influence of the solid heat conductivity Second, the model sensitivity to changes in solid and consequently effective heat conductivity is examined in Figure 6. Note that the heat conductivity value mostly affects the bread center temperature, while as expected, the higher heat conductivity leads to the higher center temperature. The surface temperature and the total moisture content stay almost unaffected.

4 Conclusions

In the present contribution, the comprehensive model for the internal transport inside the loaf of the bread was described and developed. The results of the model were confronted with the available literature and the model was validated and cross-verified. Next, the influence of the evaporation coefficient and the solid heat conductivity has been examined in the model sensitivity analysis. As expected, the evaporation coefficient mostly affects the evolution of the total moisture content in the bread as it directly influences the loss of the water from the loaf. The heat conductivity value mostly influences the bread center temperature, while the surface temperature and the total moisture content are practically uninfluenced. In the future, we plan to couple the developed model with the external model for the mass, momentum and heat transport in the oven.

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References

[1] Al-Nasser, M., Fayssal, I. & Moukalled, F.: Numerical simulation of bread baking in a convection oven. *Applied Thermal Engineering*. vol. 184: (2021). page 116252. doi: https://doi.org/10.1016/j.applthermaleng.2020.116252.

[2] Baldino, N., Lupi, F. R. & Gabriele, D. 4 - fundamentals of food baking processes. In Jafari, S. M., editor, *High-Temperature Processing of Food Products*: Unit Operations and Processing Equipment in the Food Industry: pp. 79–102. Woodhead Publishing: (2023). doi: https://doi.org/10.1016/B978-0-12-818618-3.00008-2.

[3] Zhang, J., Datta, A. K. & Mukherjee, S.: Transport processes and large deformation during baking of bread. *AIChE Journal*. vol. 51 no. 9: (2005). pp. 2569–2580. doi: https://doi.org/10.1002/aic.10518.

[4] Therdthai, N. & Zhou, W.: Recent advances in the studies of bread baking process and their impacts on the bread baking technology. *Food Science and Technology Research*. vol. 9 no. 3: (2003). pp. 219–226. doi: 10.3136/fstr.9.219.

[5] Zúñiga, R. & Le-Bail, A.: Assessment of thermal conductivity as a function of porosity in bread dough during proving. *Food and Bioproducts Processing*. vol. 87 no. 1: (2009). pp. 17–22. doi: https://doi.org/10.1016/j.fbp.2008.04.002.

[6] Rask, C.: Thermal properties of dough and bakery products: A review of published data. *Journal of Food Engineering*. vol. 9 no. 3: (1989). pp. 167–193. doi: https://doi.org/10.1016/0260-8774(89)90039-3.