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1 **Bread baking as a moving boundary problem. Part 2: Model validation**
2 **and numerical simulation**

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8
9
10 **Abstract**

11 A simultaneous heat and mass transfer model proposed to describe the bread baking
12 process is validated. The mathematical model is based on a moving boundary problem
13 formulation with equivalent thermophysical properties and includes the moving
14 evaporation front, the evaporation-condensation mechanism and the development of the
15 crust observed during bread baking. The problem is solved over an irregular three-
16 dimensional geometry using the finite element method. Variation in temperature and
17 water content of bread during baking is predicted with high accuracy by the model.
18 Parameter estimation procedure and sensitivity analysis are performed for some
19 thermophysical properties. The proposed formulation and analysis can be applied for
20 other bakery products as well as for similar food engineering applications.

21 *Keywords:* Baking; Stefan problem; Mathematical modelling; Thermophysical
22 properties

23
24

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25

26 **Nomenclature**

27

28	a_w	Water activity
29	C_p	Specific heat, $\text{J kg}^{-1} \text{K}^{-1}$
30	D	Water (liquid or vapour) diffusion coefficient of product, $\text{m}^2 \text{s}^{-1}$
31	D_{va}	Water vapour diffusion coefficient in air, $\text{m}^2 \text{s}^{-1}$
32	e_{abs}	Mean absolute relative error, %
33	f_{crust}	Crust formation factor
34	Gr	Grashof number
35	h	Heat transfer coefficient, $\text{W m}^{-2} \text{K}^{-1}$
36	k	Thermal conductivity, $\text{W m}^{-1} \text{K}^{-1}$
37	k_g	Corrected mass transfer coefficient, $\text{kg Pa}^{-1} \text{m}^{-2} \text{s}^{-1}$
38	k_g^*	Mass transfer coefficient from Eq. (15), $\text{kg Pa}^{-1} \text{m}^{-2} \text{s}^{-1}$
39	M	Molecular mass, g
40	Nu	Nusselt number
41	P	Pressure, Pa
42	Pr	Prandtl number
43	Re	Reynolds number
44	RH	Relative humidity, %
45	Sc	Schmidt number
46	T	Temperature, K
47	t	Time, s
48	W	Water (liquid or vapour) content, kg kg^{-1}
49	WL	Weight loss, %

50

51 **Greek symbols**52 ΔT Temperature range of phase change, K53 ε Emissivity54 η Delta-type function55 λ Heat of phase change, J m⁻³56 ρ Density, kg m⁻³57 σ Stefan-Boltzmann constant, 5.67 10⁻⁸ W m⁻² K⁻⁴

58

59 **Subscripts**60 ∞ Ambient

61 air Air

62 atm Atmospheric

63 f Phase change

64 s Solid or surface

65 sat Saturated

66 w Water

67

68

69 **1. Introduction**

70

71 Simulation can be defined as the process of developing a model of a real system

72 and carrying out experiments through the model, with the aim of studying, analyzing,

73 designing or re-designing, controlling and predicting a certain real process. Besides the

74 validation of the model, numerical simulation does not imply field experiments; it only

75 includes the development of a mathematical model and computational effort, mostly
76 more inexpensive than *real* tests. In addition, simulation gives the possibility of
77 working under standardized operative conditions, minimizing the uncertainties of
78 complex processes, especially those which are traditional non automated processes. In
79 this way, it will be very useful to have an accurate mathematical model for bread baking
80 simulation.

81 Thus far, the baking process has been mostly modelled as a simultaneous heat
82 and mass transfer (SHMT) problem, though different hypotheses were suggested for
83 describing the internal mechanisms of transport. For instance, the evaporation-
84 condensation theory proposed by Sluimer and Krist-Spit (1987) to explain the rapid
85 heating of porous dough during baking was incorporated in a model of SHMT in dough
86 and crumb, not involving the crust zone (de Vries et al., 1989). Good results were
87 obtained when comparing experimental and simulated core temperature values,
88 suggesting that the evaporation-condensation mechanism should be included in a model
89 for bread baking. In this way, Thorvaldsson and Janestad (1999) took into account
90 evaporation and condensation of water for modelling the drying of bread crumb and
91 developed a model for heat, liquid water and water vapour transfer including an
92 empirical parameter named as evaporation rate (i.e. times per second the vapour content
93 is set at the saturated partial water vapour pressure). Another approach was taken by
94 Lostie et al. (2002) to incorporate evaporation-condensation in a model for the “heating
95 up” period of cake baking; this mechanism was included in the heat balance through an
96 effective thermal conductivity.

97 On the other hand, Zanoni et al. (1994) proposed a mathematical model for
98 baking of mould bread assuming that the variation of moisture content and temperature
99 of the product is determined by the formation of an evaporation front at 100 °C. To

100 solve the model, it was established that when the bread reaches 100 °C, evaporation at a
101 constant temperature takes place until all the unbound water is evaporated, and the heat
102 of evaporation is obtained from the difference between the supplied heat and the heat
103 transferred towards the core by conduction (i.e. $dT/dt = 0$). Respect to biscuit baking,
104 Özilgen and Heil (1994) included the loss of latent heat via loss of water in the energy
105 balance equation to take account of evaporation in the product. Though good correlation
106 was observed between experimental and simulated values of temperature and water
107 content, the authors reported an extensive use of empirical parameters, besides this type
108 of formulation is not recommended for being in conflict with fundamental mass
109 conservation laws (Zhang and Datta, 2004). For the “crust and crumb” period of cake
110 baking, Lostie et al. (2004) introduced in a lumped model an empirical parameter to
111 control the front evaporation velocity.

112 Finally, two opposite viewpoints were applied to model the bread baking
113 process. Zheleva and Kambourova (2005) used the phenomenological theory of Luikov
114 (1975) to develop a SHMT model, but the experimental heating curves were not well
115 reproduced in their work. In contrast, Zhang and Datta (2006) presented a coupled
116 model for multiphase heat and mass transfer using a mechanistic approach; acceptable
117 results were obtained when comparing experimental and simulated data. Further
118 information about the state of the art in mathematical modelling of the baking process
119 can be found elsewhere (Mondal and Datta, 2008; Sablani et al., 1998).

120 From the literature review, it can be concluded that mathematical modelling of
121 bread baking is still a major challenge in food engineering. So far, the experimental
122 heating and drying curves observed during the process could not be well reproduced by
123 numerical simulation; particularly, the characteristic sigmoid trend of the temperature
124 variation at the bread core. In addition, accurate expressions for thermophysical

125 properties of bread are still unavailable or available only for a narrow range of operative
 126 conditions, i.e. temperature below 100 °C.

127 As a part of a comprehensive study of the bread baking process (Purlis, 2007),
 128 the aim of this article was to validate the mathematical model previously developed
 129 using a moving boundary approach, which includes the two main features of bread
 130 baking: the evaporation-condensation phenomena and the moving evaporation front
 131 (Purlis and Salvadori, 2008). Furthermore, a second objective was to propose new
 132 expressions for some thermophysical properties of bread by considering the moving
 133 boundary formulation and carrying out parameter estimation and sensitivity analysis.

134

135 **2. Mathematical model: Thermophysical properties**

136

137 In the first part of this study we developed a mathematical model considering
 138 bread baking as a moving boundary problem (MBP), beyond other assumptions (Purlis
 139 and Salvadori, 2008). The governing equations and the corresponding boundary
 140 conditions are summarized below.

141 Heat balance equation:

$$142 \quad \rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) \quad (1)$$

143 Mass balance equation:

$$144 \quad \frac{\partial W}{\partial t} = \nabla \cdot (D \nabla W) \quad (2)$$

145 Boundary conditions:

$$146 \quad -k \nabla T = h(T_s - T_\infty) + \varepsilon \sigma (T_s^4 - T_\infty^4) \quad (3)$$

$$147 \quad -D \rho_s \nabla W = k_g (P_s(T_s) - P_\infty(T_\infty)) \quad (4)$$

148 where $P_s = a_w P_{sat}(T_s)$ and $P_\infty = RH P_{sat}(T_\infty)$.

149 In the MBP formulation *equivalent* thermophysical properties are defined including the
 150 phase change (i.e. water evaporation) occurring during the process (Bonacina et al.,
 151 1973). In this way, available values or expressions in literature for bread properties were
 152 not always adequate when the mathematical model was validated against experimental
 153 data (results not shown). Thus, we proposed new expressions for some thermophysical
 154 properties and performed a parameter estimation procedure by comparing simulated
 155 with experimental data. Following, detailed discussion about bread properties and
 156 transfer coefficients is presented.

157

158 **2.1. Specific heat**

159

160 An equivalent specific heat is defined as a function of temperature and water
 161 (liquid or vapour) content, including the *enthalpy jump* at the temperature of phase
 162 change (Bonacina et al., 1973):

$$163 \quad C_p(T, W) = C_p'(T, W) + \lambda W \eta \quad (5)$$

164 where (Zanoni et al., 1994):

$$165 \quad C_p'(T, W) = C_{p,s}(T) + WC_{p,w}(T) \quad (6)$$

$$166 \quad C_{p,s} = 5T + 25 \quad (7)$$

$$167 \quad C_{p,w} = (5.207 - 73.17 \cdot 10^{-4} T + 1.35 \cdot 10^{-5} T^2) 1000 \quad (8)$$

168 In Eq. (5), η is a Delta-type function, i.e. the sum of two smoothed Heaviside functions,
 169 centred in T_f with range ΔT . This smoothed enthalpy peak replaces the Delta function in
 170 order to achieve large but finite values in the phase transition temperature range as was
 171 suggested by Bonacina et al. (1973).

172

173 **2.2. Thermal conductivity**

174

175 We propose an effective thermal conductivity that includes the evaporation-
 176 condensation mechanism in the model. This expression for thermal conductivity, as well
 177 as for the other bread properties, is valid for dough, crumb and crust, since a smoothed
 178 Heaviside function with parameters T_f and ΔT is used to obtain a continuous function
 179 for the entire range of operative conditions of baking (Purlis, 2007):

$$180 \quad k(T) = \begin{cases} \frac{0.9}{1 + \exp(-0.1(T - 353.16))} + 0.2 & \text{if } T \leq T_f - \Delta T \\ 0.2 & \text{if } T > T_f + \Delta T \end{cases} \quad (9)$$

181 Thermal conductivity increases with bread temperature following a sigmoid trend until
 182 the phase change occurs (Figure 1); it rapidly increases above 60 °C since evaporation-
 183 condensation dominates at high temperatures while conduction at low temperatures (de
 184 Vries et al., 1989), though both mechanisms are present during all the baking process.

185 The behaviour of the proposed thermal conductivity below 100 °C is similar to
 186 the experimental one obtained by Jury et al. (2007) with a line source probe in pseudo
 187 non-isothermal conditions, during the thawing-baking phase of part baked bread
 188 production. Though a parallel model for thermal conductivity was adjusted by Jury et al.
 189 (2007), it is not adequate for temperature values greater than 80-85 °C since high
 190 thermal conductivity is predicted (results not shown). Respect to the crust, a value from
 191 literature is used (Rask, 1989); the low thermal conductivity of this zone is due to the
 192 low water content.

193

194 **2.3. Density**

195

196 Assuming the dough porosity equal to 75%, an apparent density is defined as
 197 follows (Hamdami et al., 2004):

$$198 \quad \rho(T) = \begin{cases} 180.61 & \text{if } T \leq T_f - \Delta T \\ 321.31 & \text{if } T > T_f + \Delta T \end{cases} \quad (10)$$

199 Density for solid that appears in the mass transport boundary condition (Eq. (4)) is equal
 200 to 241.76 kg m⁻³ (Hamdami et al., 2004).

201

202 **2.4. Mass diffusivity**

203

204 An effective diffusion coefficient of liquid water or water vapour is defined as a
 205 function of bread temperature:

$$206 \quad D(T) = \begin{cases} 110^{-10} & \text{if } T \leq T_f - \Delta T \\ f_{crust} D_{va}(T) & \text{if } T > T_f + \Delta T \end{cases} \quad (11)$$

207 Moisture diffusivity in dough and crumb (i.e. temperature below 100 °C) is obtained
 208 from Thorvaldsson and Janestad (1999).

209 With regard to crust, an expression depending on diffusivity of water vapour in
 210 air is proposed by defining a crust formation factor (f_{crust}). This factor is related to the
 211 tortuosity of the crust structure and the experimental observation that the generation of a
 212 crust restricts the diffusion of internal water vapour to the oven ambient (Hasatani et al.,
 213 1991; Wählby and Skjöldebrand, 2002). Further, Zhang and Datta (2006) showed by
 214 scanning electron microscopy (SEM) the microstructure of crust: pores tend to be
 215 smaller than in the crumb region, resulting in a dense porous matrix and thus increasing
 216 the resistance to mass transport. By simulating the model in order to agree numerical
 217 results with experimental data, the crust formation factor was found to be equal to

218 0.0013. So, effective moisture diffusivity in bread varies between $1 \cdot 10^{-10}$ and $6.4 \cdot 10^{-8}$
 219 $\text{m}^2 \text{s}^{-1}$ in the temperature range 25-120 °C, which is in agreement with literature data.

220

221 2.5. Water activity

222

223 Water activity is defined as the ratio of water vapour pressure in the product at a
 224 certain temperature and water content versus the vapour pressure of pure water at the
 225 same temperature. Knowledge about a_w variation is important since it establishes the
 226 driving force for mass transfer between the food surface and the surrounding ambient
 227 (Eq. (4)). In this work, we use the Oswin model (Lind and Rask, 1991) with the
 228 parameters estimated by Zhang and Datta (2006):

$$229 \quad a_w(T, W) = \left[\left(\frac{100 W}{\exp(-0.0056T + 5.5)} \right)^{-1/0.38} + 1 \right]^{-1} \quad (12)$$

230

231 2.6. Heat and mass transfer coefficients

232

233 The convective heat transfer coefficient is obtained from Nusselt number
 234 correlations, according to the experimental baking conditions. For this aim, bread is
 235 assumed to be a cylinder with an equivalent diameter as the characteristic length,
 236 calculated by averaging height and width data of the cross-section of samples. The
 237 following expressions are used for the natural and forced convection modes of the oven
 238 used in baking tests, respectively (Perry and Green, 1997):

$$239 \quad Nu = 0.53 (Gr Pr)^{1/4} \quad (13)$$

$$240 \quad Nu = 0.683 Re^{0.466} Pr^{1/3} \quad (14)$$

241 Respect to heat transfer by radiation, the emissivity of bread surface is considered equal
242 to 0.9 (Hamdami et al., 2004).

243 The mass transfer coefficient was firstly determined using the Chilton-Colburn
244 analogy (Perry and Green, 1997) from the heat transfer coefficient and oven air
245 properties data:

$$246 \quad \frac{h}{k_g^*} = \frac{M_{air}}{M_w} P_{atm} C_{p,air} \left(\frac{Sc}{Pr} \right)^{2/3} \quad (15)$$

247 However, the values obtained from Eq. (15) produced much more water loss in the
248 numerical simulations than that registered in baking tests, suggesting that the actual
249 mass transfer coefficients may be lower. Besides, the heat-mass transfer correlation
250 does not take into account the crust development, which diminishes the mass transport
251 from the bread surface to the oven ambient. Therefore, we propose a corrected mass
252 transfer coefficient by incorporating a correction factor, which can be estimated from
253 experimental data of weight loss (see Table 1).

254

255 **3. Geometry modelling**

256

257 In general, transport phenomena are often simulated over simple regular
258 geometries, e.g. an infinite slab for unidirectional transfer, due to complexity for
259 representing the real geometry of the system (usually irregular) and then generating a
260 mesh or grid over such domain. However, it would be desirable to solve a model using
261 the real geometry of food; in mathematical modelling of bread baking only Zhang and
262 Datta (2006) considered a 2D irregular domain for simulation.

263 In this work, French bread (baguette) is considered as a three-dimensional object
264 having a constant irregular cross-section. To construct the geometry of bread, the

265 irregular boundary of the cross-section is obtained from a digital image of dough sample
266 by the following image processing procedure (Figure 2):

267

- 268 1. Conversion of original RGB image to grey-scale format.
- 269 2. Adjustment of image intensity values to increase the contrast.
- 270 3. Noise reduction by filtering to enhance image quality.
- 271 4. Segmentation through a global threshold value: a binary image is obtained where
272 black colour (pixel value equal to 0) represents the background and white colour the
273 sample (pixel value equal to 1).
- 274 5. Boundary detection and interpolation of a subset of boundary pixels by a closed B-
275 Spline curve (a continuous approximation to the discrete boundary of binary
276 images).

277

278 The B-Spline curve representing the real boundary of bread cross-section is converted
279 into a 2D solid region, which is then extruded in the axial direction to construct the final
280 3D geometry of bread. For further details about geometry modelling the reader should
281 be referred to Goñi et al. (2007). Geometry modelling was performed in MATLAB[®]
282 and COMSOL Multiphysics[™] (version 3.2). Different geometric models were
283 constructed since homogeneity respect to shape and dimensions of samples is difficult
284 to achieve when dealing with bread dough.

285

286 **4. Baking tests**

287

288 Experimental data of the bread baking process was necessary to validate the
289 mathematical model, though in this work it was also used to estimate some parameters

290 of the model (see Section 2). It should be noted that independent experimental
291 information was used to perform the model validation and parameter estimation,
292 respectively. Two baking conditions, i.e. natural convection ($v = 0$ m/s) and forced
293 convection ($v = 0.9$ m/s), and three oven temperatures were used: 180, 200 and 220 °C.
294 Temperature and water content profiles, crust kinetics and weight loss variation were
295 determined experimentally. Further details about baking experiments and variables
296 measurement can be found in the first part of this article (Purlis and Salvadori, 2008).

297

298 **5. Numerical solution**

299

300 The finite element method was used to solve the SHMT problem; the numerical
301 procedure was implemented in COMSOL Multiphysics and MATLAB software. A
302 mesh consisting of ca. 3600 deformed tetrahedrons (for well approximating the irregular
303 shape of bread geometry) was used in all simulations. The solver used is an implicit
304 time-stepping scheme, which implies that it must solve a possibly nonlinear system of
305 equations at each time step. It solves the nonlinear system using a Newton iteration, and
306 it then solves the resulting systems with an arbitrary COMSOL Multiphysics linear
307 system solver. The time step taken by the algorithm is variable, but it was ensured to be
308 small enough in order to do not miss the latent heat peak corresponding to water
309 evaporation.

310 For describing the equivalent thermophysical properties according to the moving
311 boundary formulation, a smoothed Heaviside function was used with parameters: $T_f =$
312 100 °C and $\Delta T = 0.5$ °C. Heat and mass transfer coefficients (Table 1) were calculated
313 using an equivalent diameter equal to 0.0587 m for bread samples (average value of all
314 baking tests). Relative humidity (or vapour pressure) in oven ambient was assumed to

315 be negligible. Baking simulation time was fixed to 30 min; solution time was about 25
316 min using a PC with AMD Sempron™ Processor 2800+ 1.60 GHz and 512 MB RAM.

317

318 **6. Results and discussion**

319

320 **6.1. Model validation**

321

322 Typical three-dimensional distribution of temperature and water content in bread
323 at the end of baking (30 min) is shown in Figure 3; though only one baking condition is
324 shown, all simulations produced similar results in qualitative terms. The proposed
325 mathematical model allows identifying clearly the two characteristic zones of bread, i.e.
326 the crumb (inner region) and the crust (outer region). The crumb does not exceed 100 °C
327 and its moisture content remains constant, while at the crust, the temperature increases
328 tending to oven temperature and dehydration occurs. The same picture was observed
329 during the experimental tests of bread baking.

330 Figure 4 presents the predicted temperature distribution and heat flow variation
331 in the middle cross-section of bread (considering the axial axis) during baking. These
332 numerical results well reproduce the simultaneous heat and mass transfer occurring in
333 bread during baking. Until 15-20 min, temperature increases in the entire domain due to
334 the inward heat flux from oven ambient; however, dehydration takes place only at the
335 surface i.e. the outer zone where temperature is above 100 °C. Then, formation and
336 progressive thickening of the crust happen, which avoid mass transfer from bread core
337 to oven air. Besides, the crumb reaches almost 100 °C at this stage, so the movement of
338 the evaporation front becomes the determining step of the process. In other words, the
339 energy arriving to the bread surface is transferred towards the evaporation front to

340 produce the outward water vapour flux. Respect to the evaporation front, it can be
 341 defined as the zone where the moisture gradient is maximum (Zhang and Datta, 2004):
 342 the proposed mathematical model well agrees with such definition (Figure 4d).

343 Representative temperature profiles obtained from the model along the vertical
 344 axis of the middle cross-section of bread are shown in Figures 5 and 6. Temperature
 345 variation presents the same behaviour as in experimental baking of bakery products,
 346 including bread. It is important to note that temperature at the crumb rises until reaches
 347 100 °C asymptotically, not exceeding this value during the process (30 min). On the
 348 other hand, crust temperature increases continuously up to 100 °C, when water
 349 evaporation occurs, and then rises again following the oven temperature trend. It can
 350 also be seen the advance of the evaporation front inside bread, separating the crumb and
 351 the crust (Figure 6).

352 Beyond the good qualitative representation of the baking process given by the
 353 proposed model, a comparison between the experimental and predicted temperature
 354 values were done involving both the crumb and the crust zones. The goodness of the
 355 model prediction was assessed by the mean absolute relative error defined as:

$$356 \quad e_{abs} (\%) = \frac{100}{n} \sum_{i=1}^n \left(\frac{|T_{experimental} - T_{predicted}|}{T_{experimental}} \right)_i \quad (16)$$

357 where n is the number of temperature values taken into account. In our baking tests, the
 358 sampling time was equal to 5 sec, so $n = 360$ for 30 min baking. The calculated
 359 prediction errors are summarized in Table 2, while Figures 7 and 8 show the
 360 comparison between experimental and simulated temperature profiles in crumb and
 361 crust zones, respectively.

362 As can be seen, the mathematical model predicts very well the variation of
 363 crumb temperature for all baking conditions. Respect to the crust zone, the model

364 reproduces the experimental trend in an acceptable way, but prediction errors were
365 higher than in the crumb case. This is probably related to experimental measurement
366 aspects: placing a thermocouple at dough surface and acquiring temperature values at a
367 depth less than 5 mm (crust mean thickness at the end of baking) is not an easy task. In
368 addition, dough suffers expansion during baking, which can produce a modification in
369 the original thermocouple location. In many cases, the thermocouple end is enclosed by
370 the dough matrix and temperature measurement actually corresponds to the air inside
371 bread. Nevertheless, some successful runs were obtained (Figure 8), which demonstrate
372 the ability of the proposed model to well describe the temperature variation in bread
373 crust as well as in bread crumb.

374 The mathematical model was also assessed considering experimental data of
375 total water content (Figure 9). The mean absolute relative error defined in Eq. (16) was
376 calculated using $n = 6$ since experimental sampling was performed every 5 min (Table
377 2). As can be seen, the model predicts very well the decrease in total moisture content,
378 i.e. the weight loss of bread during baking. Respect to the water content distribution
379 inside bread, the model does not include the evaporation-condensation phenomena in
380 the mass balance, so the experimentally observed increase of moisture in bread core can
381 not be predicted. Nevertheless, such increase was between 0.4 and 2.3% in our baking
382 tests (Purlis and Salvadori, 2008), so for engineering purposes the proposed model gives
383 very acceptable results. Finally, the predicted water content of the crust is close to 0.1
384 (dry basis), which is in agreement with experimental data; the simulated kinetics of
385 crust development presents a similar trend to the experimental one, achieving a
386 dehydrated layer of 0.5-0.6 cm thickness at the end of baking.

387

388 **6.2. Parameter estimation**

389

390 As previously mentioned, available values or expressions in literature for some
391 thermophysical properties of bread did not produce good results when the mathematical
392 model was validated against experimental data. Therefore, we performed a parameter
393 estimation procedure; this approach is a common practice in food engineering and it has
394 been also carried out by other authors in the mathematical modelling of the baking
395 process (Lostie et al., 2004; Thorvaldsson and Janestad, 1999; Zhang and Datta, 2006).
396 Note that all baking conditions were used for this aim, but independent experimental
397 information was considered for model validation and parameter estimation steps.

398 Respect to thermal conductivity, we firstly used a linear expression dependent
399 on bread porosity reported by Zanoni et al. (1995). Considering porosity equal to 75%,
400 thermal conductivity values for crumb and crust are 0.393 and 0.165 W m⁻¹ °C,
401 respectively, which is in agreement with other values found in literature (Rask, 1989;
402 Baik et al., 2001). Figure 10 shows the difference in temperature variation at bread core
403 by using these constant values and the expression proposed in the present paper (Eq.
404 (9); Purlis, 2007). Underestimation of temperature above 60 °C by using the literature
405 values/expressions is probably due to not considering the evaporation-condensation
406 contribution to heat transfer. This result reveals the importance of including such
407 mechanism in heat transport, also demonstrated by de Vries et al. (1989) and Jury et al.
408 (2007); the presence of evaporation-condensation is responsible for the typical sigmoid
409 heating curve observed during bread baking.

410 A sensitivity analysis for the effective mass diffusivity defined in Eq. (11) was
411 carried out by simulating the baking process with different values of the crust formation
412 factor. Figure 11a shows that the total water content is highly dependent on this
413 parameter: a low value of f_{crust} represents a high resistance to water vapour transport

414 from the evaporation front to oven ambient, resulting in higher total moisture values
415 than the actual ones (and vice versa). This demonstrates the influence of crust formation
416 and its structural properties on the bread baking process. Finally, Figure 11b presents
417 the sensitivity analysis performed for the mass transfer coefficient, which values
418 obtained from the Chilton-Colburn analogy (Eq. (15), Table 1) were corrected in this
419 work (correction factor < 1). Mass transfer is highly affected by the presence of the
420 crust and thus the model is also sensitive to variations in k_g .

421

422 **7. Conclusions**

423

424 The bread baking process is confirmed as a moving boundary problem, where
425 simultaneous heat and mass transfer occurs in a porous medium. Bread baking is very
426 well described by the mathematical model developed in this work, which is based on a
427 moving boundary formulation including the most important features of the process: the
428 moving evaporation front, the evaporation-condensation mechanism and the
429 development of the crust. The major advantage of this approach is that the use of
430 empirical parameters to control the position of the evaporation front is not required.

431 New expressions for some thermophysical properties of bread are proposed.
432 Baking simulation through the use of the validated mathematical model is very helpful
433 for well-understanding the process and estimating unknown values of some parameters
434 of the model. Sensitivity analysis shows the importance of including the main aspects of
435 the bread baking process in the model formulation. Finally, we expect the above
436 comments should be useful for other food engineering processes with similar
437 characteristics as bread baking.

438

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440

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514 **Figure captions**

515

516 **Figure 1.** Variation of effective thermal conductivity of bread (Eq. (9)) as a function of
517 temperature. Parameters of smoothed Heaviside function: $T_f = 100\text{ }^\circ\text{C}$, $\Delta T = 0.5\text{ }^\circ\text{C}$.

518

519 **Figure 2.** Image processing steps for geometry modelling of bread samples. (a) Original
520 RGB image of a dough cross-section. (b) Binary image obtained by segmentation after
521 grey-scale transformation, intensity adjustment and filtering stages. (c) Original image
522 and its approximated boundary using a B-Spline curve (in red). (d) 2D solid region
523 obtained from the approximated irregular boundary. (e) 3D geometry of bread
524 constructed by extruding the 2D solid region in the length direction.

525

526 **Figure 3.** Simulated (a) temperature ($^\circ\text{C}$) and (b) moisture content (kg water/kg dry
527 matter) distribution for 30 min baking at $200\text{ }^\circ\text{C}$ under forced convection.

528

529 **Figure 4.** (a-c) Distribution of temperature ($^\circ\text{C}$) in the middle cross-section (in length
530 direction) of bread during baking at $200\text{ }^\circ\text{C}$ under forced convection. Arrows represents
531 heat flow. Curve inside bread (10 and 20 min) indicates the isotherm at $100\text{ }^\circ\text{C}$
532 (evaporation front). (d) Contour curve at $100\text{ }^\circ\text{C}$ for 20 min baking at $200\text{ }^\circ\text{C}$ under
533 forced convection. Dots indicate the maximum and minimum moisture gradient.

534

535 **Figure 5.** Simulated temperature profiles inside bread (middle cross-section) for baking
536 at $200\text{ }^\circ\text{C}$ under forced convection. Locations (cm) from upper surface: 0 (surface); 0.1;
537 0.4; 0.6; 0.8; 1.1; 1.6; 2.6 (core).

538

539 **Figure 6.** Temporal evolution (0 to 30 min, every 4.28 min) of temperature along height
540 direction over the middle cross-section, during baking at 200 °C under forced
541 convection.

542

543 **Figure 7.** Simulated (solid line) and experimental (●) crumb temperature during baking
544 at (a) 220 °C under natural convection and (b) 200 °C under forced convection. Only
545 experimental values every 1 min are shown for simplicity.

546

547 **Figure 8.** Simulated (lines) and experimental (symbols) crust temperature during baking
548 at 220 °C under natural convection (solid;●) and 200 °C under forced convection
549 (dashed;△). Only experimental values every 1 min are shown for simplicity.

550

551 **Figure 9.** Simulated (lines) and experimental (symbols) total water content of bread
552 during baking under forced convection. 180 °C (dashdot;□); 200 °C (solid;●); 220 °C
553 (dashed;△).

554

555 **Figure 10.** Temperature variation at bread crumb during baking at 200 °C under forced
556 convection. Dots represent experimental data. Dashed line corresponds to simulation by
557 using Eq. (9). Solid line accounts for simulation with 0.393 and 0.165 W m⁻¹ °C for
558 crumb and crust thermal conductivity, respectively. Only experimental values every 1
559 min are shown for simplicity.

560

561 **Figure 11.** Experimental (dots) and simulated (solid lines) total water content during
562 baking at 200 °C under forced convection. (a) Effect of crust formation factor ($f_{crust} =$
563 0.0013). (b) Effect of mass transfer coefficient ($k_g = 8.46 \cdot 10^{-9} \text{ kg Pa}^{-1} \text{ m}^{-2} \text{ s}^{-1}$).

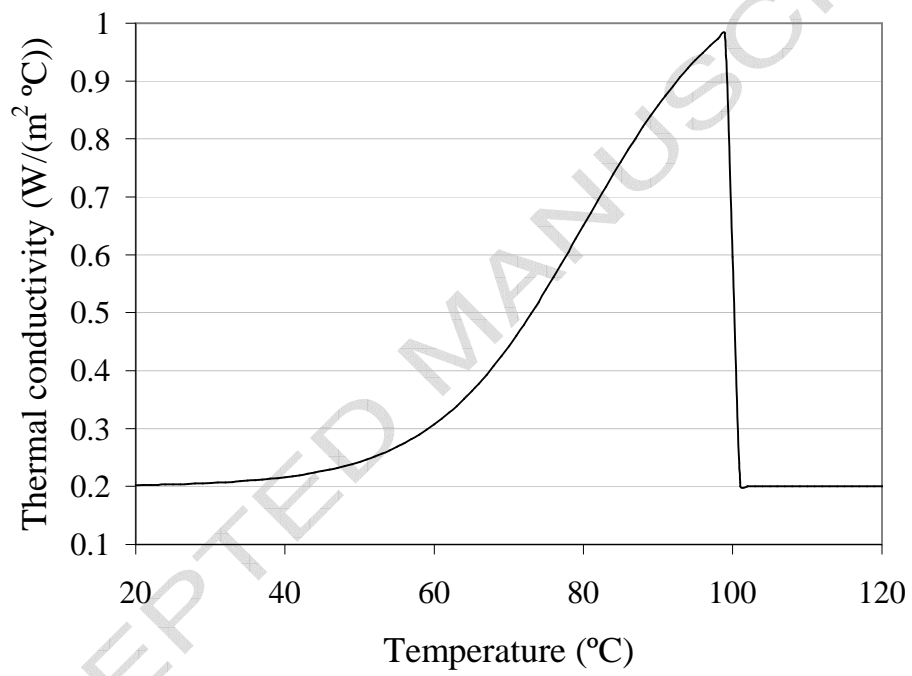


Figure 2

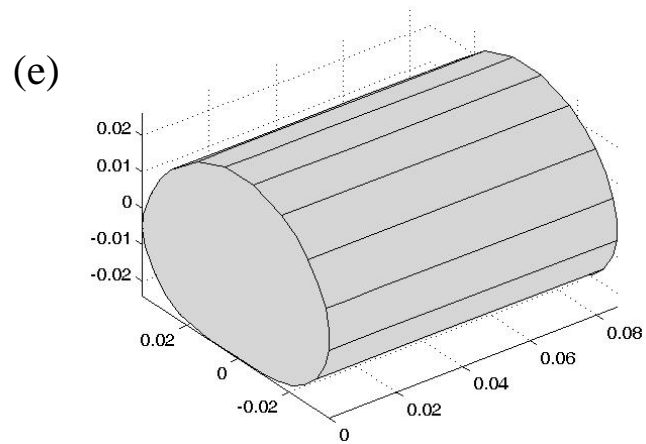
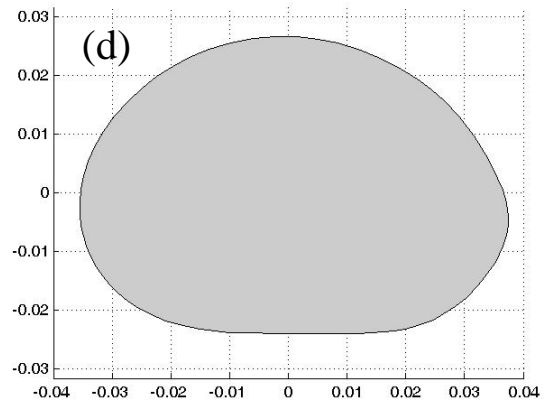
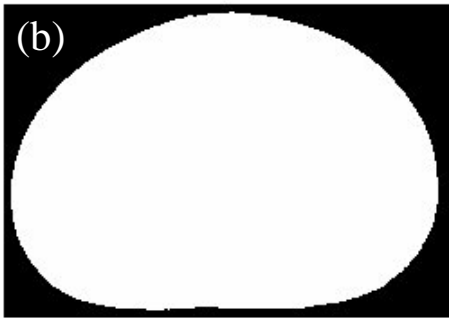


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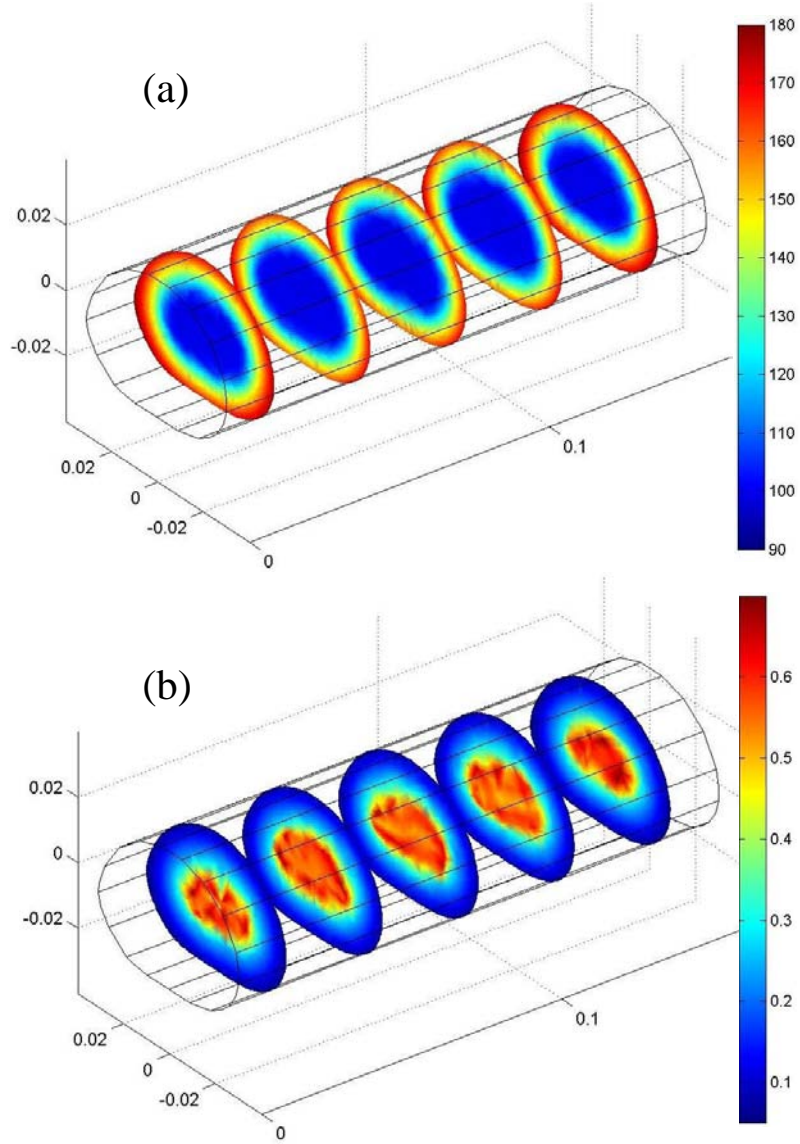


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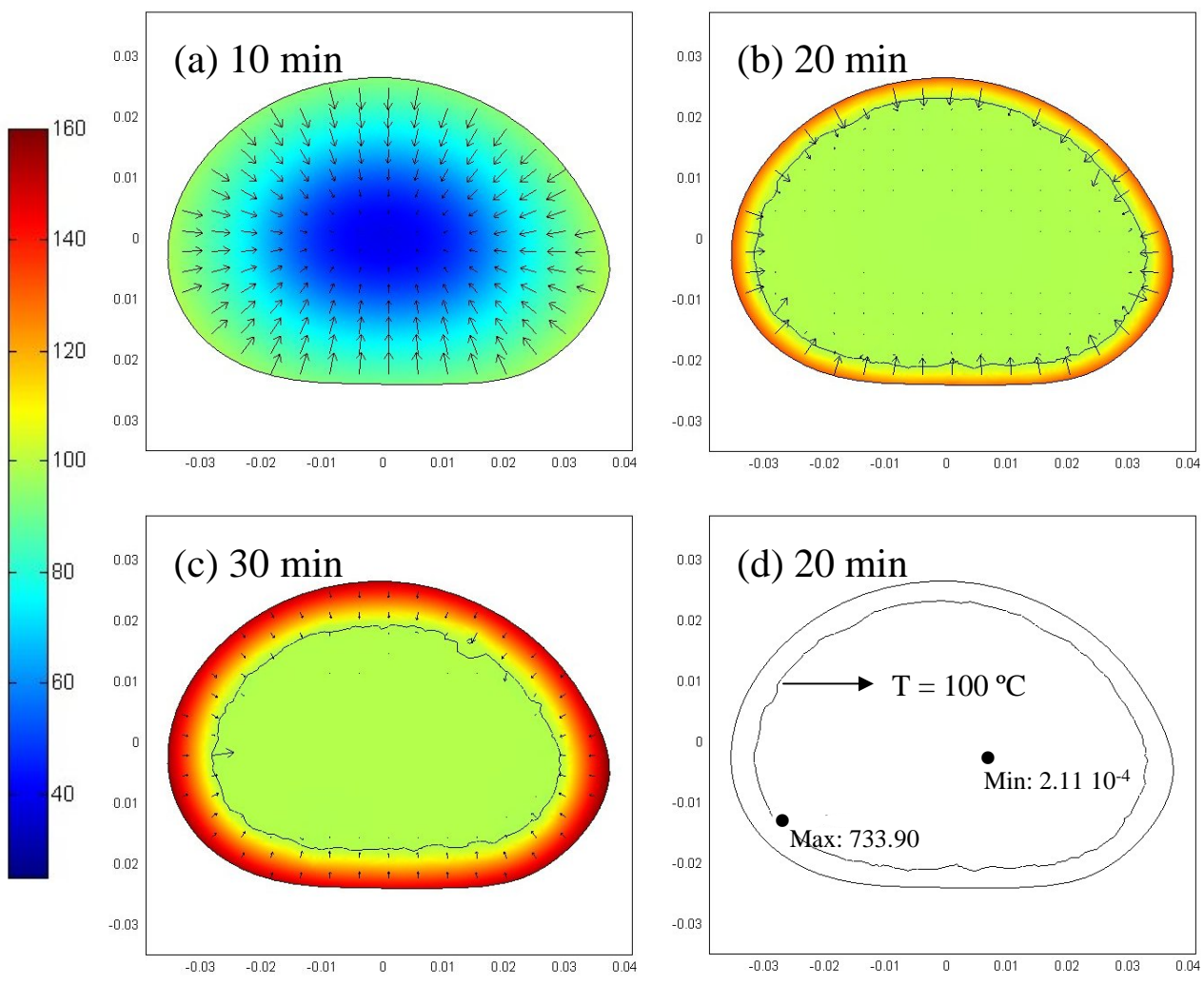


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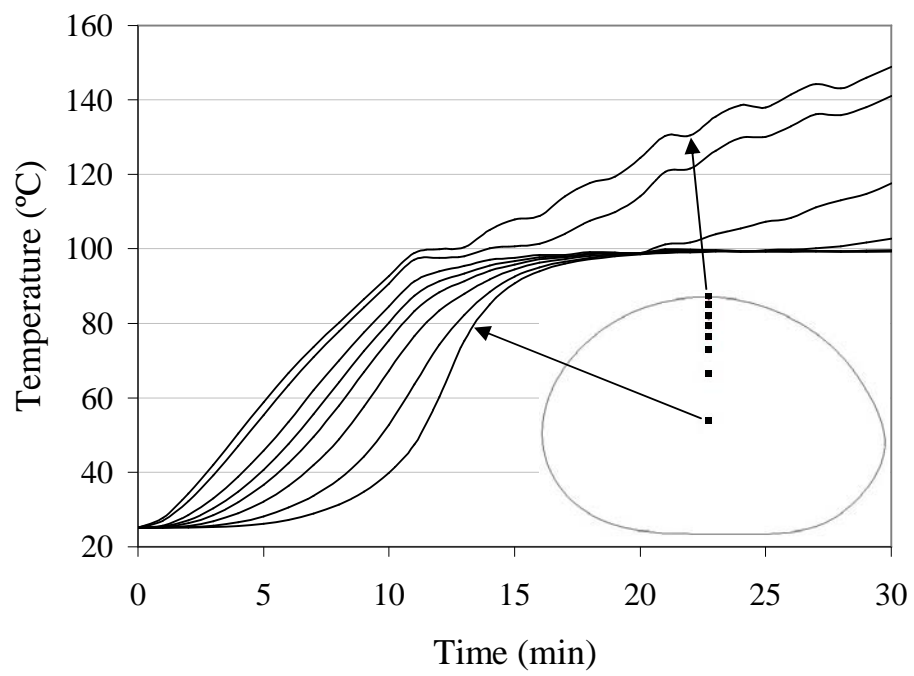


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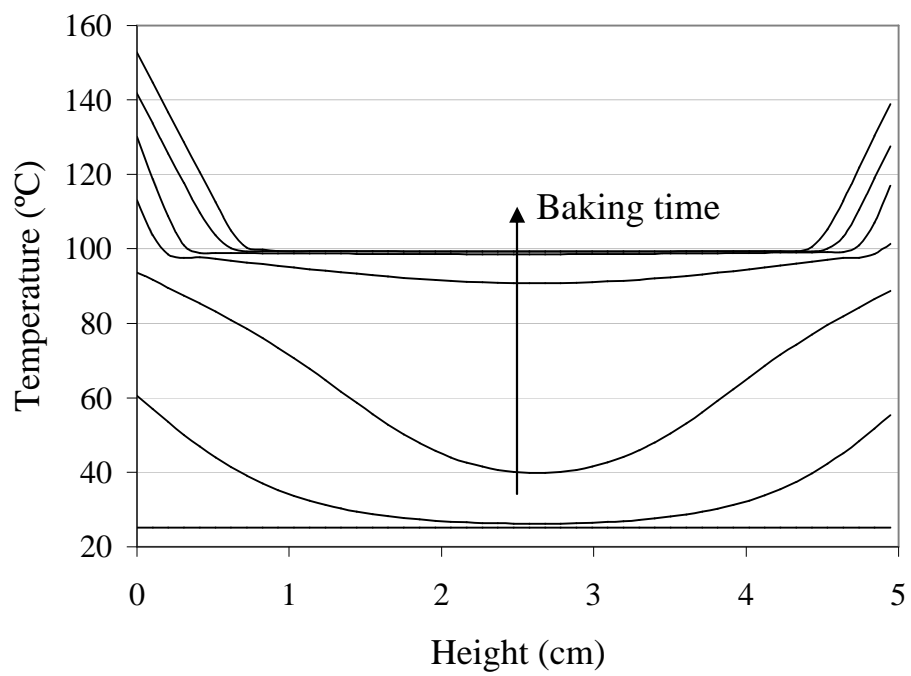


Figure 7

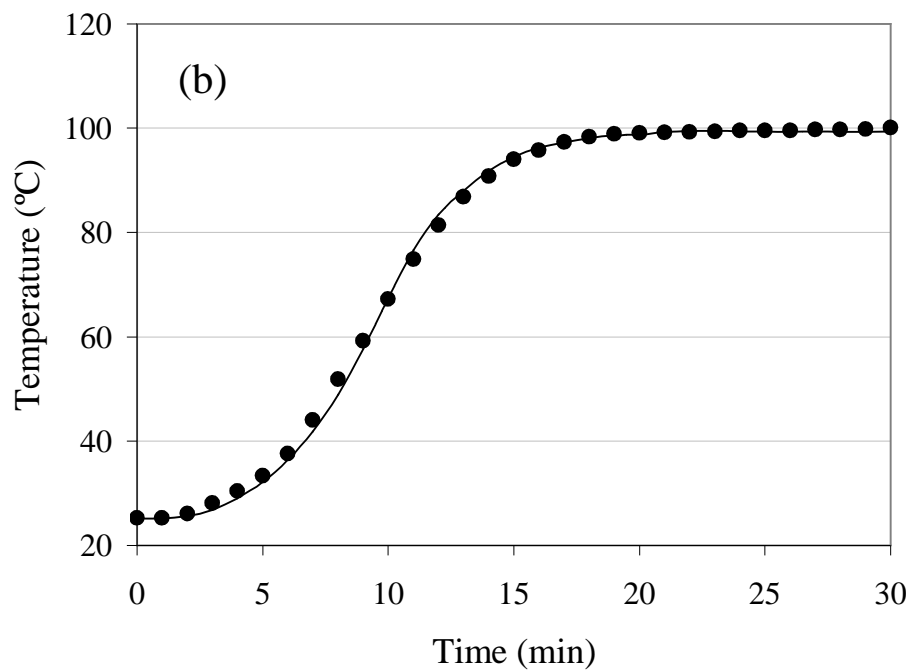
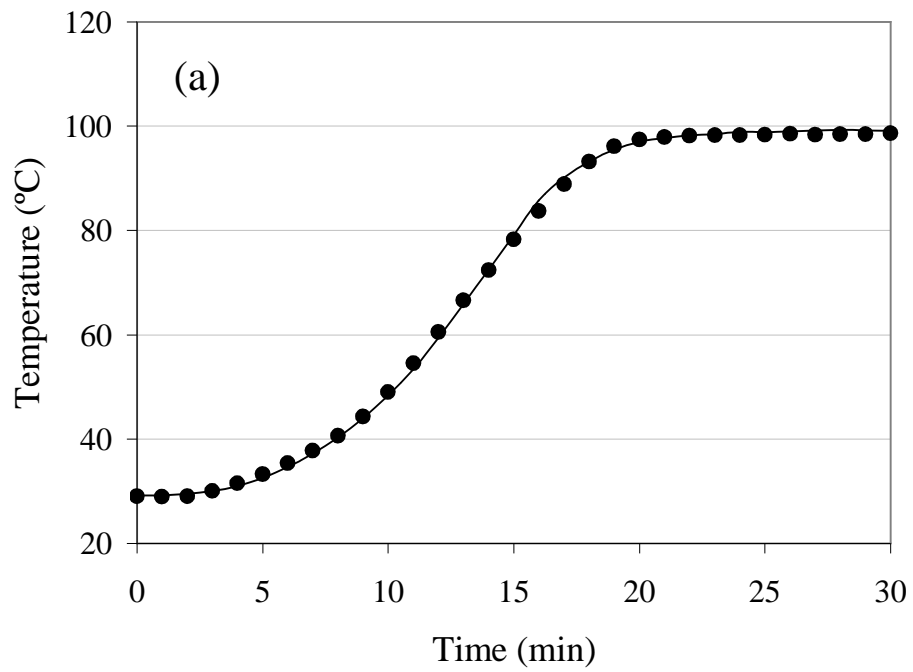


Figure 8

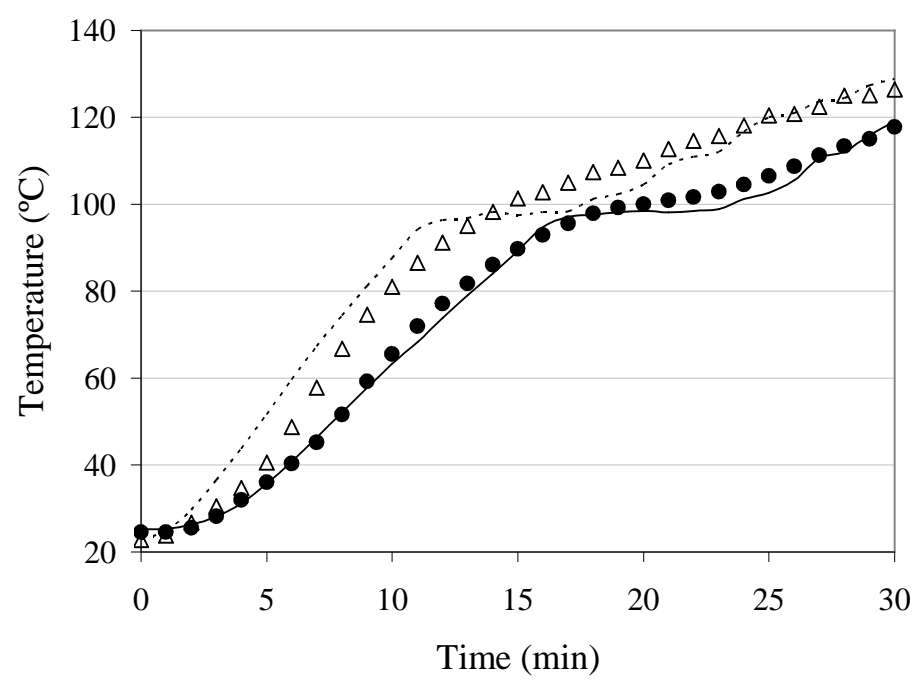


Figure 9

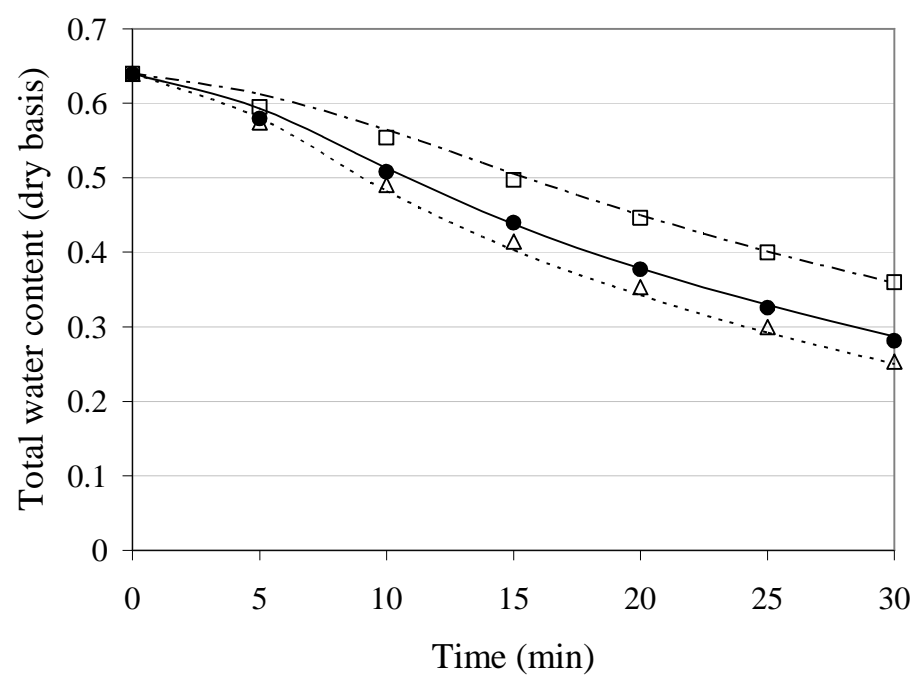


Figure 10

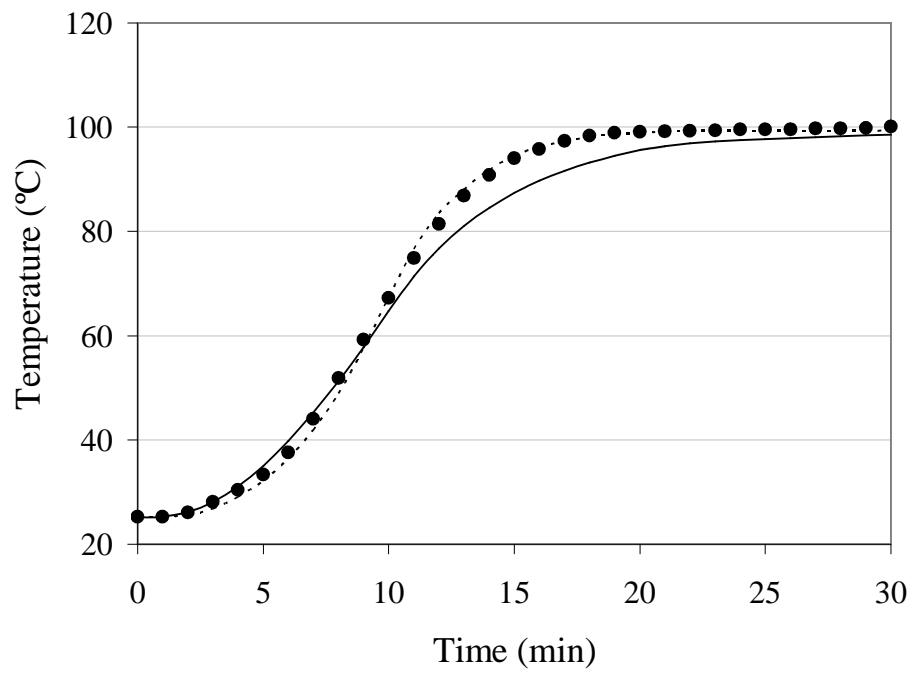


Figure 11

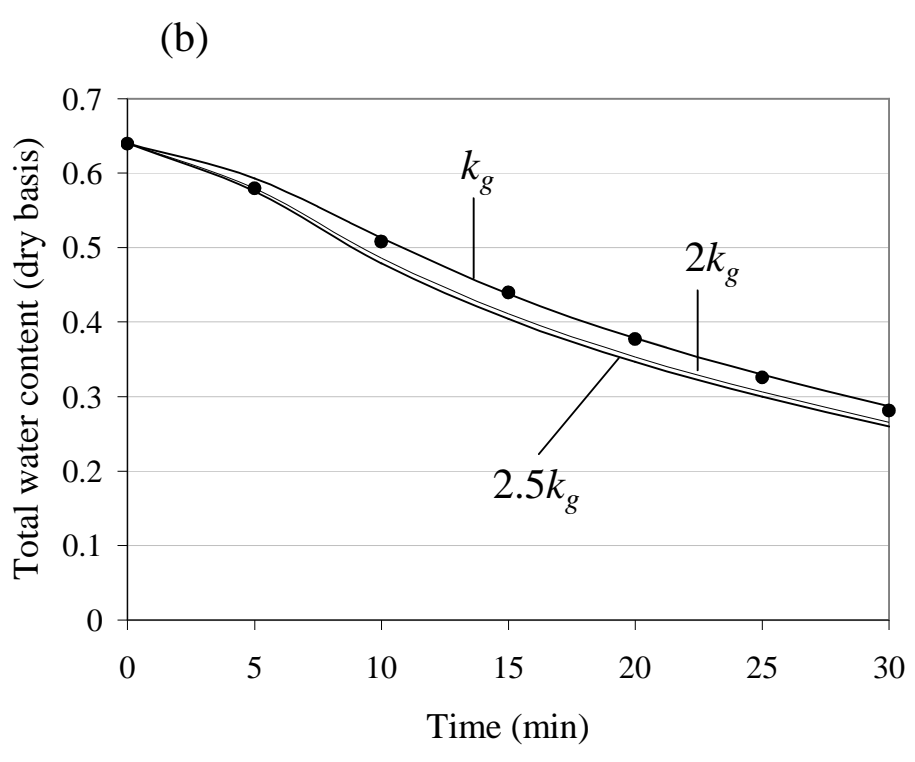
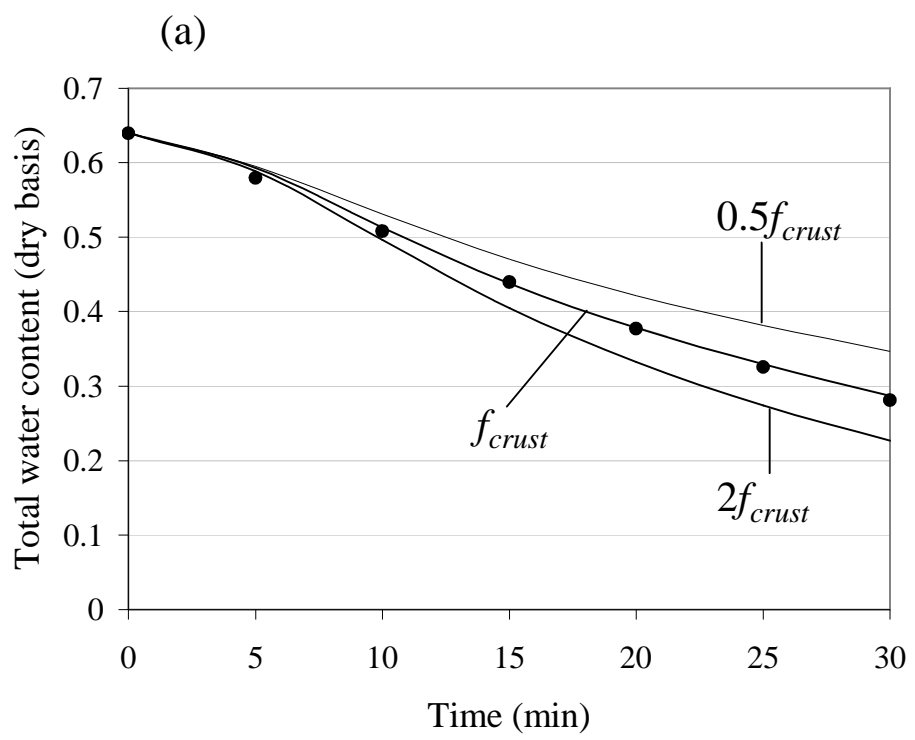


Table 1. Values for heat (h , in $\text{W m}^{-2} \text{K}^{-1}$) and mass (k_g , in $\text{kg Pa}^{-1} \text{m}^{-2} \text{s}^{-1}$) transfer coefficients according to description in Section 2.6. Data for mass transfer coefficient is already corrected by the estimated correction factor, i.e. $k_g = 7.83 \cdot 10^{-2} k_g^*$.

Baking temperature (°C)	Natural convection		Forced convection	
	h	k_g	h	k_g
180	7.34	$4.35 \cdot 10^{-9}$	11.94	$5.08 \cdot 10^{-9}$
200	7.68	$3.38 \cdot 10^{-9}$	11.96	$8.46 \cdot 10^{-9}$
220	7.95	$6.04 \cdot 10^{-9}$	11.97	$8.46 \cdot 10^{-9}$

Table 2. Mean absolute relative error (e_{abs} , Eq. (16)) for crumb temperature ($n = 360$) and total water content ($n = 6$) predictions for 30 min baking. NC: natural convection; FC: forced convection.

	Crumb temperature	Total water content
Baking condition	e_{abs} (%)	e_{abs} (%)
180 °C, NC	1.24	1.12
200 °C, NC	1.53	1.74
220 °C, NC	0.98	0.79
180 °C, FC	1.71	1.17
200 °C, FC	1.48	1.02
220 °C, FC	1.78	1.83
<i>Average</i>	<i>1.45</i>	<i>1.28</i>