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1 **Bread baking as a moving boundary problem. Part 1: Mathematical**
2 **modelling**

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8
9
10 **Abstract**

11 A mathematical model for the bread baking process is developed in this work.
12 Experimental data (temperature, water content, weight loss, crust thickness) obtained
13 during baking is used to well understand the simultaneous heat and mass transfer
14 occurring during the process. The evaporation-condensation mechanism is responsible
15 for the rapid heating of the porous matrix and takes place either in a closed (dough) or
16 open (crumb) structure. The existence of a moving evaporation front inside bread,
17 which is a determining step of baking, is incorporated in a model applying a moving
18 boundary formulation with equivalent thermophysical properties. The approach
19 proposed here can be extended to other similar processes such as baking of other
20 products (e.g. biscuit, cake), high-temperature drying, cooking and roasting.

21 *Keywords:* Simultaneous heat and mass transfer; Phase change; Stefan problem

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25 **Nomenclature**

26

27 a_w Water activity28 \tilde{C} Equivalent heat capacity, $\text{J m}^{-3} \text{K}^{-1}$ 29 C Heat capacity, $\text{J m}^{-3} \text{K}^{-1}$ 30 C_p Specific heat, $\text{J kg}^{-1} \text{K}^{-1}$ 31 D Water (liquid or vapour) diffusion coefficient, $\text{m}^2 \text{s}^{-1}$ 32 H Enthalpy, J m^{-3} 33 h Heat transfer coefficient, $\text{W m}^{-2} \text{K}^{-1}$ 34 k Thermal conductivity, $\text{W m}^{-1} \text{K}^{-1}$ 35 k_g Mass transfer coefficient, $\text{kg Pa}^{-1} \text{m}^{-2} \text{s}^{-1}$ 36 P Water vapour pressure, Pa37 RH Relative humidity, %38 S Interface position, m39 T Temperature, K40 t Time, s41 W Water (liquid or vapour) content, kg kg^{-1}

42

43 **Greek symbols**44 δ Delta function45 ε Emissivity46 λ Heat of phase change, J m^{-3} 47 ρ Density, kg m^{-3} 48 σ Stefan-Boltzmann constant, $5.67 \cdot 10^{-8} \text{W m}^{-2} \text{K}^{-4}$

49

50 **Subscripts**51 ∞ Ambient

52 f Phase change

53 s Solid or surface

54 sat Saturated

55

56

57 **1. Introduction**

58

59 Baking of bread (and bakery products in general) can be defined as the process
60 which transforms a dough basically made of flour, water and leavening agents in a high
61 quality product with unique sensorial features. In particular, French or white bread is the
62 most popular type of bread, and is distinguished for having a crunchy and brown crust, a
63 sponge and light crumb with soft texture and intermediate moisture, and a typical
64 flavour. All these quality aspects are result of a series of physical, chemical and
65 biochemical changes occurring during baking, i.e. formation of a porous and open
66 structure, volume expansion, water evaporation, starch gelatinization, protein
67 denaturation, carbon dioxide production (leavening agents), crust formation, and
68 development of browning (Maillard reaction and caramelization).

69 From a transport phenomena point of view, bread baking has been considered as
70 a simultaneous heat and mass transfer (SHMT) problem in a porous medium. So far,
71 some efforts have been made to well understand and therefore predict and control the
72 bread baking process, including both experimental and theoretical approaches. Sluimer
73 and Krist-Spit (1987) found that the temperature increase in a gas-free dough piece
74 proceeds much slower than in a fermented dough, showing that heat conduction is of

75 minor importance in dough baking. So, they suggested the principle of Watt or
76 evaporation-condensation as the major mechanism of heat transport in baking. The
77 theory of evaporation and condensation was proposed by Henry in 1939 (cited by de
78 Vries et al., 1989); this process can be divided into four steps:

79

- 80 1. Water evaporates at the warmer side of gas cells, absorbing latent heat of
81 vaporization.
- 82 2. Vapour migrates through the gas phase.
- 83 3. Vapour condenses at the colder side of the gas cell, setting free its latent heat.
- 84 4. Heat and water are transported by conduction and diffusion, respectively, through a
85 dough membrane to the warmer side of the next gas cell, where the series of
86 processes can start all over again.

87

88 When dough is transformed into crumb, the gas phase becomes continuous and the last
89 step is not necessary. Evaporation-condensation will continue until the temperature of
90 the whole crumb has achieved 100 °C (Sluimer and Krist-Spit, 1987).

91 Since evaporation-condensation produces a water vapour transport towards the
92 thermal core of the bread, it would be possible that the local moisture content increases
93 during baking. By using a fibre optic instrument, Thorvaldsson and Skjöldebrand (1998)
94 measured an increase in the water content of bread core after temperature had reached
95 70 ± 5 °C, and suggested that the water is not free to move until the pore structure is
96 opened up and becomes continuous. However, the fibre optic method is sensitive to the
97 structure and temperature of the sample, and has to be improved (Wagner et al., 2007).
98 On the other hand, Wagner et al. (2007) found an increase in moisture content at the
99 core during the first minutes of baking when temperature did not exceed 65 °C, tending

100 to confirm the possible occurrence of the evaporation-condensation mechanism even in
101 a closed porous structure (i.e. dough).

102 Zanoni et al. (1993) reported a phenomenological model where the variation in
103 temperature and water content of bread during baking is determined by the formation of
104 an evaporation front at 100 °C. The progressive advancing of this evaporation front
105 towards the inside of the product results in the formation of two separate regions: the
106 crust, where moisture is very low and temperature asymptotically tends to the oven
107 temperature; and the crumb, where moisture is constant and temperature asymptotically
108 tends to 100 °C (Zanoni et al., 1994). In this way, only external zones of bread suffers
109 dehydration during baking; the development of the crust avoids the diffusion of internal
110 water vapour in the bread to the outside (Hasatani et al., 1991; Wählby and
111 Skjöldebrand, 2002). A similar interpretation of cake baking was given by Lostie et al.,
112 who divided the process in two periods, namely the “heating up” period and “crust and
113 crumb” period, delimited by the formation of a dry crust at the batter heated surface
114 (Lostie et al., 2002a, 2002b, 2004).

115 Another suggested hypothesis for bread baking is based on the mathematical
116 model proposed by Luikov (1975) to describe SHMT during drying (Zheleva and
117 Kambourova, 2005). This phenomenological approach applies the concept of
118 irreversible thermodynamics and includes the effect of temperature on the water
119 transport (i.e. *thermodiffusion*). Conversely, Zhang and Datta (2006) proposed a
120 mechanistic basis to describe the bread baking process, involving dough deformation
121 and multiphase heat and mass transfer. Further information about the state of the art is
122 available elsewhere (Mondal and Datta, 2008; Sablani et al., 1998).

123 Thus far, many hypotheses have been proposed to explain the mechanisms of
124 heat and mass transfer occurring in bread during baking. However, numerical results

125 obtained from mathematical models based on the suggested theories are still not in well
126 agreement with reported experimental findings (see further discussion in concomitant
127 paper). As a part of a comprehensive research on bread baking (Purlis, 2007), the
128 objective of this first article was to develop a mathematical model to correctly describe
129 the water content and temperature variation in bread during baking. For this aim,
130 various hypotheses were evaluated and discussed through the use of experimental data.
131 Discussion about thermophysical properties of bread, solution and validation of the
132 model and numerical simulation of the baking process are presented in the second part
133 of this article (Purlis and Salvadori, 2008).

134

135 **2. Materials and methods**

136

137 **2.1. Bread samples**

138

139 Samples were prepared using a standard recipe for French bread: wheat flour
140 (100%), water (54.1%), salt (1.6%), sugar (1.6%), margarine (1.6%), and dry yeast
141 (1.2%). Dough was made by mixing the ingredients for 10 min in a home multi-function
142 food processor at constant speed. Then individual samples of 100-150 g (cylindrical
143 shape, ca. 0.15 m length, 0.04 m diameter) were formed and placed in a perforated tray.
144 After 1.5 h proving at ambient temperature, samples duplicated their volume.

145

146 **2.2. Baking tests**

147

148 Dough samples were baked in an electrical static oven (Ariston FM87-FC, Italy)
149 under two different baking conditions, depending on air velocity: natural convection (v

150 = 0 m/s) and forced convection ($v = 0.9$ m/s). Experiments were carried out by using
151 three oven temperatures: 180, 200 and 220 °C. The perforated tray with the samples was
152 placed in the central zone of the oven in order to achieve a homogeneous distribution of
153 heat and mass fluxes. Baking tests were divided into three groups according to the
154 variable(s) being registered: temperature, water content and crust thickness, and weight
155 loss of bread; this was necessary since experimental protocol was different for each
156 measurement.

157

158 **2.3. Temperature measurement**

159

160 Temperature inside bread samples and in oven ambient was measured using T-
161 type thermocouples (Omega, USA) connected to a data logger (Keithley DASTC, USA)
162 which was incorporated to a PC; sampling time was set to 5 sec in all cases. It is worth
163 to note that thermocouples had to be inserted in the product before the proving stage
164 because dough easily collapses if any pressure is done over the surface just before
165 baking, since is a porous liquid matrix at that moment. Moreover, the proving step was
166 carried out inside the oven (turn off) to allow any movement of thermocouples while
167 introducing the tray inside the chamber. Thermocouples were placed in different
168 positions of dough between the centre and the surface along the axial axis; final
169 locations of thermocouples were determined after baking. Each baking condition was
170 done by duplicated using four bread samples each time.

171

172 **2.4. Water content, crust thickness and weight loss measurement**

173

174 Water content was measured in five different regions along the vertical axis of
175 the central cross-section (1 cm thickness) of bread samples: lower, central and upper
176 crumb, and lower and upper crust (Figure 1). Sampling was performed every 10 min for
177 180 and 200 °C, and every 7 min for 220 °C baking temperature. Also, moisture content
178 of unbaked dough was determined. Water content values were calculated by drying the
179 samples in a vacuum oven (Gallenkamp, United Kingdom) at 80 °C, until constant
180 weight was achieved. Crust thickness was determined using a calliper in the same
181 experiments as water content. Several measures of each sample were recorded and then
182 an average value was obtained for each baking time.

183 Weight loss during baking was assessed by weighing the tray with samples
184 (outside the oven) every 5 min. It is worth to note that this procedure took about 5 sec
185 each time, thus it was assumed that no significant perturbation was introduced in
186 measurement. All tests were done by duplicate with the oven under steady regime
187 condition.

188

189 **3. Experimental results**

190

191 **3.1. Temperature**

192

193 Temperature variation at different regions of bread during baking is shown in
194 Figure 2; only one baking condition is illustrated for simplicity though all experimental
195 runs presented a similar behaviour. Firstly, it can be seen the set-up profile followed by
196 the oven air temperature during the initial phase of baking, certainly due to the
197 experimental protocol established in subsection 2.3. Once the set value for air
198 temperature is achieved the oven controls this parameter with ± 3.3 °C accuracy showing

199 an oscillating tendency. Temperature at bread surface (0 cm position) described a
200 similar variation as air temperature, increasing almost constantly until 120 °C was
201 reached and then following the oven temperature behaviour.

202 On the other hand, in the core zone of bread (at 2 cm from surface) the
203 temperature slightly increased during the first 10 minutes since thermal gradient had not
204 been established yet, but then a rapid temperature raise was observed achieving a
205 maximum heating rate of 11.6 °C/min at 16 minutes baking. Since 20 minutes, the core
206 temperature stopped increasing and described a plateau at 98 °C until the end of baking.
207 Notice from Figure 2 the sigmoid shape of temperature variation at the centre of bread,
208 which is very similar to the ones obtained during heating of multi-dimensional
209 moistened objects (Sommier et al., 2005). In the intermediate zone (0.5 and 0.6 cm
210 positions), i.e. underneath the surface but not at the core of bread, the temperature
211 variation showed hybrid behaviour between previous descriptions. Initially, temperature
212 increased in a similar way as surface but when values about 98-100 °C were attained, it
213 remained constant in a plateau towards the end of baking. It is worth to note that
214 temperature at the closer position to surface (0.5 cm) left the plateau from 25 minutes
215 and started to increase again above 100 °C.

216

217 **3.2. Water content, crust thickness and weight loss**

218

219 Figure 3 presents typical variation of water content in bread during baking,
220 where two different situations can be well distinguished. From one side, outer zones of
221 bread suffered dehydration during all the process, which actually leads to the formation
222 of a crust. At the end of baking, values for water content of crust were in the range 5-
223 10% (wet basis), depending on process condition, i.e. high oven temperature and forced

224 convection produced more dehydration. On the other hand, the crumb zone beneath the
225 crust maintained the moisture content of the unbaked dough throughout the baking
226 process. Furthermore, at the core region (central crumb) we detected an increase
227 between 0.4 and 2.3% in the water content respect to initial condition, in all baking
228 experiments, i.e. the bread core increased its moisture during all the process. Bearing in
229 mind that we used the same method for water content measurement as Wagner et al.
230 (2007), our findings complement their results obtained at the very beginning of baking,
231 confirming the occurrence of the evaporation-condensation mechanism during all the
232 process. This implies that evaporation-condensation is not determined by the state of the
233 porous structure (i.e. open or closed), but is a characteristic mechanism given in high
234 moisture porous media.

235 Weight or average moisture content of bread continuously decreased during
236 baking, which is in agreement with the variation in water content at the crust (Figure 4).
237 However, the drying rate was not constant as can be seen from Figure 5. Hasatani et al.
238 (1991) did not observe a constant drying rate period either, and they found that the
239 bread crust was generated from the time when the drying rate achieved the maximum
240 peak and the temperature stopped increasing at 100 °C. So, the drying rate increases up
241 to a crust is formed, but then it begins to decrease due to the enlarging of crust thickness
242 (Figure 6). In this way, the crust avoids further dehydration of bread, acting as barrier to
243 mass transfer towards the oven ambient (Wählby and Skjöldebrand, 2002).

244

245 **4. Mathematical model**

246

247 Beyond the several complex changes occurring in bread during baking, the most
248 characteristic aspects are the rapid heating of bread core and development of a crust.

249 Sluimer and Krist-Spit (1987) proposed the evaporation-condensation mechanism to
250 explain the former, suggesting that heat conduction is of minor importance in dough
251 baking. Certainly, the experimental findings reported in this work together with the ones
252 published by Wagner et al. (2007) confirm the occurrence of evaporation-condensation
253 in the dough/crumb of bread during baking. Secondly, the formation and advancing of
254 an evaporation front towards the core are responsible for the development of a crust
255 which restricts the water vapour diffusion to the outside of bread. Note that bread
256 baking must be considered as a SHMT problem in a porous medium.

257 Thus, bread can be modelled as a system containing three different regions:

258

- 259 1. Crumb: wet inner zone, where temperature does not exceed 100 °C and dehydration
260 does not occur.
- 261 2. Crust: dry outer zone, where temperature increases above 100 °C and dehydration
262 takes place.
- 263 3. Evaporation front: between the crumb and crust, where temperature is ca. 100 °C
264 and water evaporates.

265

266 The evaporation front is actually a moving interface where a phase change happens. The
267 same situation is observed in processes which involve melting and freezing (i.e. solid-
268 liquid phase change), such as metal casting, manufacturing of ice, thermal storage and
269 thawing and freezing of food; and processes with liquid-vapour (evaporation) or solid-
270 vapour phase change (sublimation) such as frying, high temperature drying, spray- and
271 freeze-drying of food and non-food materials (Farid, 2002). All these processes are
272 catalogued as moving boundary problems (MBP), though the second group is more

273 complicated by the vapour diffusion throughout the dried zone of the material (Farid,
274 2002). Therefore, we consider bread baking as a MBP as well.

275 Mathematically, a MBP (often called as Stefan problem) is related to time-
276 dependent problems (i.e. parabolic type equations) where boundary position must be
277 determined as function of time and space (Crank, 1987). For instance, let us consider
278 the melting of some material; this type of problem can be formulated considering the
279 heat balance equation for each region i.e. solid and liquid regions (not shown for
280 simplicity), and establishing the following interface condition besides temperature
281 continuity condition:

$$282 \quad k_2(T) \frac{\partial T_2}{\partial x} - k_1(T) \frac{\partial T_1}{\partial x} = \lambda \frac{\partial S}{\partial t} \quad (1)$$

283 where subscripts 1 and 2 symbolize solid and liquid regions, respectively. This
284 boundary condition represents the *enthalpy jump* at the temperature of phase transition.
285 Based on a physical approach, a different mathematical formulation is possible by
286 defining an *equivalent* heat capacity per volume unit through the enthalpy definition
287 (Bonacina et al., 1973):

$$288 \quad \tilde{C}(T) = \frac{dH(T)}{dT} = C(T) + \lambda \delta(T - T_f), \quad C(T) = \begin{cases} C_1(T), & T < T_f \\ C_2(T), & T > T_f \end{cases} \quad (2)$$

289 Applying this approach to thermal conductivity, the two-region problem including an
290 interface condition can be solved by only one partial differential equation with
291 equivalent coefficients that include the phase change. For a generalized and unique
292 solution to the problem, smoothed heat capacity and thermal conductivity must be
293 defined: a Delta-type function is used instead of Delta function in order to achieve large
294 but finite values in the phase transition temperature range (Bonacina et al., 1973).

295 So, the mathematical model for bread baking presented in this work is based on
296 the MBP formulation described above. Note that no empirical coefficient to determine

297 the interface position or any imposed additional condition is needed for including the
298 formation and advancing of the evaporation front inside bread in the model.
299 Furthermore, the following assumptions were used to develop the mathematical for
300 bread baking:

301

- 302 • Control volume is homogeneous and continuous; the porous medium concept is
303 included through effective or apparent thermophysical properties.
- 304 • Volume change during baking is neglected (this phenomenon is under study and
305 will be incorporated in the model in a future work).
- 306 • There exists local thermodynamic equilibrium.
- 307 • Heat is transported by conduction from surface to bread core according to Fourier's
308 law, but an effective thermal conductivity is used to incorporate the evaporation-
309 condensation mechanism in heat transfer.
- 310 • Energy from oven ambient to bread surface is transferred by convection and
311 radiation.
- 312 • Only liquid diffusion in the crumb and only vapour diffusion in the crust are
313 assumed to occur (Luikov, 1975).
- 314 • Liquid water migrates from the core towards to the evaporation front under a water
315 content gradient, and liquid water flux is described by Fick's diffusion law.
- 316 • Water evaporates at 100 °C.
- 317 • Water vapour migrates from the evaporation front to bread surface under a water
318 vapour concentration gradient, and mass flux is described by Fick's diffusion law.
- 319 • Water vapour is transferred to oven ambient through convective flux.
- 320 • A smoothed Heaviside function replaces the Delta function for defining equivalent
321 thermophysical properties in the MBP formulation.

322

323 The evaporation-condensation mechanism is incorporated in the model, but only in the
324 heat transfer balance; we neglect its contribution to mass transport since the water
325 content increase at the bread core is not relevant opposite to overall weight loss during
326 baking. In addition, more information is needed to include this mechanism in the mass
327 balance due to its complexity. Following, the heat and mass balance equations and
328 boundary conditions of the SHMT model are presented.

329

330 4.1. Governing equations

331

332 Heat balance equation:

$$333 \rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) \quad (3)$$

334 Mass balance equation:

$$335 \frac{\partial W}{\partial t} = \nabla \cdot (D \nabla W) \quad (4)$$

336 All thermophysical properties are continuous functions including the phase change, and
337 are valid for the entire temperature and water content ranges observed during baking,
338 i.e. both balances consider SHMT in dough, crumb and crust. Description and analysis
339 of thermophysical properties are presented in the second article (Purlis and Salvadori,
340 2008).

341

342 4.2. Boundary conditions

343

344 The heat arriving to the bread surface by convection and radiation is balanced by
345 conduction inside the bread:

$$346 \quad -k\nabla T = h(T_s - T_\infty) + \varepsilon\sigma(T_s^4 - T_\infty^4) \quad (5)$$

347 The water migrating towards the bread surface is balanced by convective flux:

$$348 \quad -D\rho_s\nabla W = k_g(P_s(T_s) - P_\infty(T_\infty)) \quad (6)$$

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

350 Further discussion about boundary conditions is included in the second paper (Purlis
351 and Salvadori, 2008).

352

353 **5. Conclusions**

354

355 The evaporation-condensation mechanism proposed to explain the rapid heating
356 of porous dough during baking is confirmed through experimental findings.
357 Evaporation-condensation appears as a characteristic mechanism of porous media, and
358 occurs either if the porous structure is closed (dough) or open (crumb) until the
359 temperature has reached 100 °C (i.e. evaporation temperature). Furthermore, the
360 existence of a progressive evaporation front is essential for the bread baking process;
361 the advancing of this interface produces the outer crust which avoids dehydration of the
362 crumb due to structural characteristics that restricts the water vapour diffusion from the
363 bread core to the oven ambient.

364 These two major phenomena are incorporated in a mathematical model to
365 describe the simultaneous heat and mass transfer occurring during baking of bread.
366 Though bread baking is clearly a moving boundary problem, it is the first time that a
367 rigorous MBP formulation is applied to model this process. This approach gives the
368 possibility of handling simple equations with continuous equivalent (and apparent)
369 thermophysical properties, valid for the entire operative range of baking. Besides, no
370 empirical parameters or imposed or fictitious boundary conditions are used to determine

371 the interface position, i.e. the model describes the evaporation front in a natural,
372 unforced way.

373 Finally, the mathematical model presented in this work can be used to study the
374 baking of other products, such as biscuit, cake and other types of bread. As well, this
375 formulation could be implemented for modelling other processes with simultaneous
376 heat and mass transfer and a moving phase change interface, e.g. high-temperature
377 drying, cooking, roasting.

378

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380

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385

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- 441

442 **Figure captions**

443

444 **Figure 1.** Sampling regions for determination of water content distribution in bread
445 during baking. The schema represents the central cross-section (1 cm thickness) in the
446 axial direction of bread.

447

448 **Figure 2.** Temperature variation in bread during baking at 180 °C under natural
449 convection condition. Final locations of thermocouples are given in terms of distance
450 from upper surface along the vertical axis of the middle cross-section of bread. Final
451 height of bread: 5 cm.

452

453 **Figure 3.** Water content (wet basis) variation in bread during baking at 180 °C under
454 natural convection condition. Initial (i.e. unbaked dough) moisture corresponded to
455 39.71%.

456

457 **Figure 4.** Weight loss (relative to initial dough mass) of bread as a function of baking
458 time. (\diamond) 180 °C; (\square) 200 °C; (\triangle) 220 °C. Filled symbols for natural convection and
459 empty symbols for forced convection.

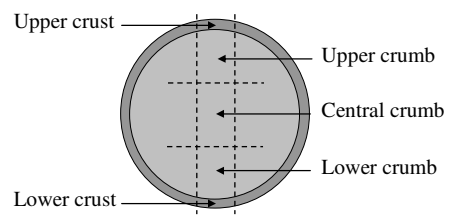
460

461 **Figure 5.** Drying rate of bread as a function of baking time. (\diamond) 180 °C; (\square) 200 °C;
462 (\triangle) 220 °C. Filled symbols for natural convection and empty symbols for forced
463 convection.

464

465 **Figure 6.** Variation of crust thickness during baking. (\diamond) 180 °C; (\square) 200 °C; (\triangle) 220
466 °C. Filled symbols for natural convection and empty symbols for forced convection.

Fig.1



ACCEPTED MANUSCRIPT

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