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## Modelling and analysis of complex food systems: state of the art and new trends

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24 **Abstract**

25 The aim of this review is twofold. Firstly, we present the state of the art in dynamic modeling  
26 and model-based design, optimization and control of food systems. The need for nonlinear,  
27 dynamic, multi-physics and multi-scale representations of food systems is established.  
28 Current difficulties in building such models are reviewed: incomplete, piecewise available  
29 knowledge, spread out among different disciplines (physics, chemistry, biology, consumer  
30 science) and contributors (scientists, experts, process operators, process managers), scarcity,  
31 uncertainty and high cost of measured data, complexity of phenomena and intricacy of time  
32 and space scales. Secondly, we concentrate on the opportunities offered by the complex  
33 systems science to cope with the difficulties faced by food science and engineering. Newly  
34 developed techniques such as model-based viability analysis, optimization, dynamic Bayesian  
35 networks etc. are shown to be relevant and promising for design and optimization of foods  
36 and food processes based on consumer needs and expectations.

37

38 **Introduction**

39 Food engineering covers a large spectrum of applications that include, but are not limited to:  
40 product engineering, process engineering, control, optimisation and decision support systems.  
41 Some 25 years ago, modelling and simulation of food processing was mostly dedicated to  
42 product preservation with safety considerations, most of the studies focused on time-  
43 temperature diagrams for predicting and limiting residual spores or micro-organisms in foods.  
44 Due to increased process understanding and computing power, applications emerged where

45 other quality attributes were considered: moisture content, colour, viscosity, sometimes food  
46 composition. More recently, food structure was also considered (e.g. viscosity, porosity) and  
47 models became available to represent the evolution of such structure (Theys, Geeraerd & Van  
48 Impe 2009). In parallel, progress in observation and analytical methods (imaging techniques,  
49 magnetic and electronic beams) allowed investigating different structural scales and  
50 interactions between chemical species, mainly between macromolecules and small molecules.  
51 Food starts to be viewed as a complex system, with various possible interactions between key  
52 variables at different scales (from nano scale to macroscopic one) (Baudrit, Sicard, Wuillemin  
53 & Perrot 2010).

54 It is now recognised in most scientific domains that dynamic modelling and computer  
55 simulations are valuable tools for product and process understanding, design, optimisation  
56 and control. The purpose of a mathematical model is to capture relevant features (in a given  
57 context) of a complex object or process, based on existing theoretical understanding of the  
58 phenomena and available measurements. Current industrial applications usually rely on  
59 extremely simplified, stationary models that cannot produce a realistic evaluation of transient  
60 effects on plant performance, quality and safety conditions and environmental impact. The  
61 modelling and simulation research efforts should be directed towards main phenomenological  
62 aspects, coupling different scales, such as heat, mass, momentum, population balance coupled  
63 with chemical reactions.

64 Design of new foods as ‘intelligent’ vectors for target molecules responsible for nutritional or  
65 sensory properties became a major goal for food industry. These target molecules can be  
66 sapid or aroma compounds, micro-nutriments or microorganisms of interest (technological

67 flora used in the fermented products) whose controlled release or digestion satisfies  
68 physiological objectives of bioavailability. E. Windhab suggested in 2004 an integrating  
69 concept (PIECE: Preference, Acceptance Need) taken over by the platform ‘Food for life’,  
70 expressing the need to establish a compromise between all these properties. Up to now, few  
71 studies were able to work in a such a complex design space. Existing reverse engineering  
72 publications focus either on safety or sensory questions. Sustainability and environmental  
73 impact are additional factors to be taken into account.

74 The emerging field of complex systems science, situated at the crossroads of mathematics and  
75 artificial intelligence (cf. the living roadmap for complex system [http://cssociety.org/wiki-](http://cssociety.org/wiki-download_wiki_attachment.php?attId=123)  
76 [download\\_wiki\\_attachment.php?attId=123](http://cssociety.org/wiki-download_wiki_attachment.php?attId=123)), develops methods and tools to comprehend and  
77 describe instable and changing environments, systems that evolve and adapt through internal  
78 and external dynamic interactions and are not predictable within a conventional scientific  
79 framework. Our thesis is that techniques developed in complex systems science are applicable  
80 and useful to tackle difficulties encountered in food systems.

81

## 82 **Understanding and modelling of complex food systems: state of the art**

83 Model-based approaches in food science, technology and engineering have received great  
84 attention during the past three decades (Banga, Balsa-Canto & Alonso, 2008; Datta, 2008;  
85 Sablani, Datta, Rahman & Mujumdar, 2007) and numerous academic works have been  
86 dedicated to modelling and its applications (Bimbenet, Schubert & Trystram, 2007). The  
87 demand for models is now clearly established; as an example, the European Food for Life

88 platform (www.ciaa.be) presents modelling as a key tool for the development of European  
89 food Industries. Compared to chemical engineering, where modelling is now part of virtually  
90 any scientific and technical development, food engineering follows a similar trend, with  
91 considerable (~20 years) delay. In the authors' view, one of the main reasons for this delay is  
92 the increased complexity of food systems, including physical, chemical and biological  
93 phenomena on a wide range of time and space scales (Georgakis, 1995; Perrot, Bonazzi &  
94 Trystram, 1998; Christakos, 2002; Banga et al., 2008).

95

#### 96 *Dynamic models for food systems*

97 This review makes a particular emphasis on dynamic models, able to describe transient  
98 process operation. Typical examples are batch processes, which always operate in transient  
99 state. For continuous processes, optimising start-up, shutdown or recipe change regimes can  
100 be important for reducing costs and environmental impact. On-line control of continuous  
101 processes also require dynamic models for unavoidable disturbance compensation, such as  
102 variations in raw materials (Trystram & Courtois, 1994).

103

#### 104 *First principles vs. data-driven models*

105 When modelling approach is primarily guided by the knowledge of the underlying  
106 mechanisms, the resulting model is usually termed as 'first principles' or 'white box'.  
107 Classical examples include heat, mass and momentum transfer, chemical and biochemical  
108 conversions, etc. The scales covered by first principles range from atomic to macroscopic  
109 ones. A lot of innovative work today is dedicated to micro and meso scale. As an example,

110 SAFES (Fito, LeMaguer, Betoret & Fito, 2007) illustrates the use of thermodynamics to  
111 understand the evolution of food during processing. Multiphase approaches viewed as a  
112 general background by Datta (2008) cover similar scales. Available molecular tools become  
113 increasingly relevant for food matrices but the connection with macroscopic scales remains  
114 difficult.

115 In contrast with first principles, empirical ‘data-driven’ or ‘black-box’ models describe  
116 observed tendencies in experimental data by arbitrary mathematical functions such as  
117 polynomials or artificial neural networks (ANN). Quick and easy-to-use when sufficient  
118 experimental data is available, such models also encounter important limitations when applied  
119 to food systems: risk of over-parameterisation, interpretation difficulty, lack of generalisation  
120 ability when food composition or process parameters are changed outside the range of the  
121 initial experimental design (Banga et al., 2008). Last but not least, the number of required  
122 measurements increase exponentially with the number of studied factors.

123 A quite efficient intermediate approach consists in designing a model structure based on first  
124 principles and complete missing information by empirical relationships derived directly from  
125 experimental data. Such models are sometimes called ‘grey box’. A dynamic research field is  
126 the development of artificial intelligence-based approaches (Linko, 1998; Davidson, 1994;  
127 Allais, Perrot, Curt & Trystram, 2007) taking into account the human expert knowledge.  
128 Many applications especially for food quality control (for a review see (Perrot et al., 2006))  
129 were reported, mostly based on the theory of fuzzy sets. Nevertheless, the bottleneck of these  
130 approaches is the difficulty to capture the dynamic of the system using the expert knowledge.  
131 This difficulty was also pointed out by the community of cognitive science (Hoffman,



132 Shadbolt, Burton & Klein, 1995; Farrington-Darby & Wilson, 2006).

133

134 [Figure 1 about here]

135

### 136 *Building of the food models*

137 A typical approach for model development is schematically shown in Figure 1. On the basis  
138 of literature review, previous scientific or expert background and experimental evidence, a  
139 first set of hypothesis, mechanisms, state variables and parameters is defined. Generally, one  
140 space and/or time scale is explicitly taken into account. Other scales are usually lumped into  
141 some apparent or average material properties. Uncertainty is rarely considered. When it is, it  
142 can be taken into account explicitly, e.g. via fuzzy numbers (Ioannou, Mauris, Trystram,  
143 Perrot, 2006) or implicitly by considering statistical distributions of model parameters.  
144 Selected model structure primarily depends on the planned use of the model: hypothesis  
145 testing, simulation, state estimation and software sensors, control design optimisation, etc.  
146 Model parameters are determined from classical experimental designs or from specifically  
147 designed optimal ones (Banga, Balsa-Canto & Alonso, 2008). Once the model is build and its  
148 parameters determined, a range of tools is available for indentifiablity, sensitivity and  
149 uncertainty analysis, both structural and parametric (Walter and Pronzato, 1997). The  
150 outcome of these procedures may be the reconsideration of model hypothesis and structure,  
151 and/or the design of additional experiments to allow reliable parameter identification.

152

### 153 **Limitations of current modelling approaches for food systems**

154 Model-based approaches in food engineering are usually subject to one or more of the  
155 limitations synthesised in the first column of Table 1 (Bimbenet et al., 2007; Baudrit, Hélias  
156 & Perrot, 2009; Fito et al., 2007; Ioannou, Mauris, Trystram, & Perrot, 2006; Perrot et al.,  
157 2006; Van Impe, 1996). Moreover, several of these difficulties often arise simultaneously in  
158 food technology and biotechnology (Van Impe, 1996).

159 [Table 1 about here]

160 In many domains, existing knowledge of food scientists has led to specific models, valid in a  
161 tiny domain, either of composition or of physico-chemical environment. Moreover, their  
162 conceptual framework does not allow easy integration of results coming from other existing  
163 models (Rodriguez-Fernandez, Balsa-Canto, Egea & Banga, 2007). For instance, most  
164 processing aspects are covered by differential equations of heat and mass transfer phenomena  
165 (H&M), whereas microbiological or chemical aspects are mostly described by simple kinetic  
166 equations; coupling those is sometimes possible but not easy or general. Moreover non  
167 homogeneous scales can increase the complexity of the modelling task.

168 Furthermore, experimental data in food science and technology is often limited in amount and  
169 quality. On-line sensors are currently available for technological measurements only, such as  
170 temperature, pressure, velocity, etc. Measurements related directly to food quality (microbial  
171 count, desired or undesired compound concentration, texture...) are still performed by off-line  
172 laboratory analysis and are slow, costly, and labour-intensive. In large projects, a rule of  
173 thumb is that one laboratory analysis is ultimately obtained per full-time equivalent of the  
174 personnel involved in the project and per day. Compared to measurements performed in other  
175 fields (mechanics, electronics and even chemistry), laboratory analysis in food science are

176 subject to significant uncertainty. Differences of  $\pm 0.5$  logarithmic units on replicate microbial  
177 counts, for example, are considered normal, while this represents a factor of 3. In sensory  
178 analysis, 30 or 50% variations between replicates are usual. Testing mechanism hypothesis  
179 and building reliable models based on scarce and uncertain data is obviously a difficult task.  
180 To cope with the bottlenecks bring by the study of food complex systems, some ways of  
181 research appear to be promising (second column in Table 1).

182

### 183 *Co-operation between disciplines*

184 Many scientific fields share the challenge of unifying complex and dissimilar data (Desiere,  
185 German, Watzke, Pfeifer, & Saguy, 2001) and deal with multiple physics models. As shown  
186 by Datta (2008), food structure development is not just a function of current parameters like  
187 temperature and moisture, but of their entire history, when the complex physical structure  
188 develops, changes porosity and transport properties.

189 One of the research streams is related to the development of reliable models integrating  
190 different sources and format of knowledge is so-called knowledge integration. The principle  
191 is to deal with the different pieces of the puzzle of knowledge represented under different  
192 formalisms: data, models, expertise. One of the problems that must be addressed (Stuurstraat  
193 & Tolman, 1999) is how to cope with the conflicting requirements of each particular  
194 subsystem, optimized for its own knowledge domain. No easy solutions are available by now.  
195 The key point is the ability to cope with knowledge of different nature, at different scales,  
196 expressed in different formalisms (conservation laws and human rules of expertise for  
197 example) and to be able to take them into account in a unified manner. Nevertheless, this

198 issue is a key for the future, enabling us to exploit the different sources of knowledge that we  
199 are developing in our laboratories today. Interactions between various fields of science was  
200 pointed out in connection with environmental and natural resource issues (Christakos, 2002)  
201 biological issues (Olivier et al., 2010), nutrition (McLachlan & Garrett, 2008) etc.

202

### 203 *Uncertainty*

204 Another key issue in food processes is the management of the uncertainty. Explicit integration  
205 of uncertainty has become crucial in industrial applications and consequently in decision  
206 making processes (Baudrit, Dubois & Guyonnet, 2006). In food processes, few contributions  
207 are available including uncertainty on model parameters or on model structure itself (Perrot et  
208 al., 2006; Petermeier et al., 2002). However, taking into account the complexity of  
209 microbiological and/or physicochemical transformations in food processes, available  
210 knowledge is often tainted with vagueness, imprecision and incompleteness. Furthermore, for  
211 use in industrial applications, models and especially mechanistic models should be studied  
212 upon their sensitivity to this uncertainty (Bimbenet et al., 2007; Banga, et al., 2008).

213

### 214 *Computing power*

215 Computationally demanding tasks are increasingly used in food processes. These include for  
216 example simulation of spatially distributed models, stochastic migration of molecules to  
217 determine diffusion and partition properties in complex media (Vitrac & Hayert 2007),  
218 mathematical viability calculations (Sicard et al. 2009), dynamic optimisation (Banga, J.R.,  
219 Balsa-Canto, Moles & Alonso 2003), global sensitivity analysis etc. These tasks require new

220 calculation methods on computer grids to be tested and implemented (Reuillon, Chuffart,  
221 Leclaire, Faure & Hill 2010).

222

223 *A representative example: modelling of a cheese-making process*

224 To illustrate previous considerations, consider the case of the modelling and simulation of a  
225 cheese making process. The quality of soft mould cheese depends on environmental factors  
226 during ripening (relative humidity, temperature, gas composition) and on interactions between  
227 inoculated micro-organisms and curd substrates. The concentrations of these substrates is  
228 subject to variations in milk quality and cheese-making conditions (Helias, Mirade & Corrieu,  
229 2007). Over the last 10 years, more than 112 studies (FSTA and ISI web of sciences sources)  
230 have been carried out to understand this process in a microbial, physicochemical, biochemical  
231 and sensory points of view. About 52% of those models were empirical. For example Bonaiti,  
232 Leclerc-Perlat, Latrille and Corrieu (2004) developed a RSM approach to predict the pH and  
233 substrate evolution versus time for a soft cheese. Sihufe et al. (2010) used the principal  
234 component analysis to predict the optimal ripening time, while Jimenez-Marquez, Thibault  
235 and Lacroix (2005) have proposed a neural network to predict the ripening state of a cheese.  
236 Nearly 46% of the studies fell into the first principles category. 44% were mechanistic  
237 approaches based on mass transfer laws, e.g. for syneresis prediction (Helias et al., 2007;  
238 Tijsskens & De Baerdemaeker, 2004), sometimes combined with microbial growth laws (Riahi  
239 et al., 2007; Guillier, Stahl, Hezard, Notz & Briandet, 2008). In the remaining 2% of the  
240 publications, expert systems were developed.

241 Most of the analysed publications were focused on one specific phenomenon, were limited to  
242 the experimentally explored domain without any generalisation ability and without taking into  
243 account the inherent uncertainty. For example the mass loss model presented in (Helias et al.,  
244 2007) is developed under the hypothesis of average water and convective heat transfer  
245 coefficients fixed for air velocity upper than  $0.2 \text{ m.s}^{-1}$  while for some ripening chamber in the  
246 industry this velocity is lower than  $0.2 \text{ m.s}^{-1}$ . Water activity is also supposed to be constant  
247 while it is true in some specific configurations of the process. Integrating other type of  
248 information, such as expert knowledge or dealing explicitly with the uncertainty of the  
249 process could have enhanced the results. Each of those studies, constitute a part of the puzzle  
250 of knowledge that were built to understand the cheese making process but are not sufficient,  
251 taken alone, (1) to understand it in its global behaviour including all the scales and (2) to use  
252 it in decision making systems.

253 Some recent studies have nevertheless proposed approaches for modelling the links between  
254 different scales and different type of knowledge, including uncertainty (Arguelles, Castello,  
255 Sanz & Fito, 2007; Baudrit, Sicard, Wuillemin & Perrot, 2010; Thomopoulos, Charnomordic,  
256 Cuq & Abecassis, 2009). Quite a few such integrating approaches are available up to now.  
257 Knowledge is still missing to model complex processes such as cheese making. Considerable  
258 experimental effort, large databases and progress in microbial physiology are needed to  
259 understand numerous variables relevant for cheese making and their interactions.

260

261

262

263 **New opportunities: Complex system science for food engineering**

264

265 It follows from previous considerations that remarkable opportunities are now open for  
266 theories and techniques developed in the field of complex systems science, to be applied and  
267 adapted to food science and technology. The rest of this review will concentrate on  
268 knowledge integration, management of the uncertainty and model analysis for reverse  
269 engineering purposes.

270

271 *Knowledge integration*

272 Knowledge integration has been reported in several application fields, including food science.  
273 Quintas, Guimaraes, Baylina, Brandao & Silva (2007) studied complex caramelisation  
274 reactions. Alternative reaction pathways have been suggested, each described by a different  
275 set of differential equations. Automatic model selection was performed based on parameter  
276 identification results. Allais, Perrot, Curt & Trystram (2007) illustrate how mechanical laws  
277 can be coupled with an expert knowledge database to better comprehend a sponge finger  
278 batter process. Hadyanto et al. (2007) applied similar ideas to quality prediction of bakery  
279 products.

280 A Systematic Approach for Food Engineering Systems (SAFES) based on the theoretical  
281 framework of irreversible thermodynamics has been proposed by Fito, Le Maguer, Betoret &  
282 Fito (2007). The principle is to define a simplified and unifying space of structural features,  
283 called 'structured phases and components'. These features are grouped in a composition  
284 matrix and are time dependant. The approach has been applied to different processes, e.g.

285 prediction of the change in protein conformation during ripening (Arguellese et al., 2007). A  
286 central hypothesis is the identifiability of the resulting model. This hypothesis is not always  
287 satisfied, however, when establishing relationships between food composition and structure,  
288 in realistic foods.

289 The contribution presented by Thomopoulos et al. (2009) concentrates on durum wheat chain  
290 analysis. The developed information system allows the integration of experimental data,  
291 expert knowledge representation and compilation as well as reasoning mechanisms, including  
292 the decision tree learning method. The principle is to encode the existing knowledge about a  
293 given food chain in a unified language. The uncertainty pertaining to the expert knowledge is  
294 taken into account in the form of fuzzy sets. The information system can be used in assisting  
295 decision makers but can not handle numeric approaches, like model based optimal control.

296 As a last example, Baudrit et al. (2010) have shown that by introducing expert knowledge, a  
297 good prediction on the microbial and physicochemical kinetics during the ripening of a  
298 camembert type cheese was possible, based on limited experimental data set. The theoretical  
299 framework used here is that of Dynamic Bayesian Networks (DBNs) proposed by Murphy  
300 (2002). DBNs are classical Bayesian networks (Pearl, 1988) in which nodes representing  
301 random variables are indexed by time (equation 1). In the considered example, the average  
302 adequacy rate in predicting microscopic and macroscopic scales was of 85%, on a test data  
303 basis of 80 measurements.

304

305

$$P(X(1), \dots, X(\tau)) = \prod_{t=1}^{\tau} \prod_{i=1}^N P(X_i(t) | Pa(X_i(t))) \quad (1)$$



306 where  $X(t) = \{X_1(t), \dots, X_N(t)\}$  and  $Pa(X_i(t))$  denotes the parents of  $X_i(t)$  in the graphical  
307 structure of the DBN. This probability represents the beliefs about possible trajectories of the  
308 dynamic process  $X(t)$ . Figure 2 illustrates a DBN representing a network applied on the  
309 example of cheese ripening.

310

311 [Figure 2 about here]

312

### 313 *Management of the uncertainty*

314 Uncertainty, as explained in detail by Datta (2008), is usually of significant concern in food  
315 processing, perhaps more than in other domains. Uncertainties are often captured within a  
316 probabilistic framework. It is particularly true in food engineering for risk assessment (Aziza,  
317 Mettler, Daudin & Sanaa, 2006). Generally, uncertainty pertaining to the parameters of  
318 mathematical models representing physical or biological processes can be described by a  
319 single probability distribution. However, this method requires substantial knowledge to  
320 determine the probability law associated with each parameter. It is more and more  
321 acknowledged that uncertainty concerning model parameters has two origins (Ferson &  
322 Ginsburg, 1996):

323 It may arise from randomness (often referred to as ‘stochastic uncertainty’) due to natural  
324 variability of observations resulting from heterogeneity or the fluctuations of a quantity over  
325 time.

326 Alternatively, uncertainty may be caused by imprecision (often referred to as ‘epistemic  
327 uncertainty’) due to a lack of information. This lack of knowledge may arise from a partial

328 lack of data or because experts provide imprecise information. For example, it is quite  
329 common for experts to estimate the numerical values of parameters in the form of confidence  
330 intervals according to their experience and intuition.

331 The uncertainty affecting model parameters is thus due both to randomness and incomplete  
332 knowledge. This is typically the case in presence of several, heterogeneous sources of  
333 knowledge, such as statistical data and expert opinions. The most commonly used theory for  
334 distinguishing incompleteness from randomness is the imprecise probabilities calculus  
335 developed at length by Peter Walley (1991). In this theory, sets of probability distributions  
336 capture the notion of partial lack of probabilistic information. While information regarding  
337 variability is best conveyed using probability distributions, information regarding imprecision  
338 is more accurately represented by families of probability distributions. Examples of tools to  
339 encode probability families include probability boxes (Ferson & Ginsburg, 1996), possibility  
340 distributions (also called fuzzy intervals) (Dubois, Nguyen & Prade, 2000) or belief functions  
341 introduced by Dempster (Dempster, 1967) and elaborated further by Shafer (Shafer, 1976)  
342 and Smets (Smets & Kennes, 1994) make it possible to encode such families.

343

344 [Table 2 about here]

345 As an illustration, consider mass loss model during a ripening process, developed by Baudrit,  
346 Hélias & Perrot (2009). The idea of this contribution is to take into account the imprecise  
347 nature of available information about the heat and water transfer coefficients and to jointly  
348 propagate variability and imprecision to the estimation of cheese mass loss through the  
349 ripening process. In order to do this, the most faithfully available knowledge and the

350 associated form of uncertainty was implemented (Table 2). For the measurements, spatial  
351 variations of humidity and temperature due to climate control were taken into account. Due to  
352 low airflow velocity inside ripening chambers, imprecision about the heat and mass transfer  
353 coefficients reported in the literature was incorporated and represented by means of a  
354 possibility distribution. The joint propagation of these uncertainties, coupling random  
355 sampling with interval calculus, has led the authors to provide key information for improving  
356 the control of the mass loss of cheeses under industrial conditions. A further step forward  
357 would be the integration of the uncertainty as part of the model equations.

358

### 359 **Analysis of the models for reverse engineering purposes applied to complex food systems**

360

#### 361 *Model based optimization for identification and control*

362 Model-based optimization is usually implemented for three major areas in food technology  
363 (Banga et al. 2008): optimal identification of model parameters, building reduced-ordered  
364 models for faster simulation and selection of optimal operating policies (model predictive  
365 control). A worked-out example in the first category is given by Balsa-Canto, Rodriguez-  
366 Fernandez & Banga (2007), where the identification of kinetic parameters for thermal  
367 degradation of microorganisms is considered. Authors show how well-designed time-varying  
368 experiments can achieve an accurate and robust identification of model parameters, with a  
369 reduced experimental effort. In modelling of fermentation kinetics, optimal experimental  
370 design was applied by Bernaerts, Versyck, & Van Impe (2000), Smets, Versyck, Van Impe  
371 (2002), with similar conclusions.

372 A comprehensive review of optimal control for food processes was provided by Garcia,  
373 Balsa-Canto, Alonso & Banga (2006). Global optimisation methods like evolutionary  
374 algorithms, scatter search and particle swarm optimisation ensure robust convergence towards  
375 optimal control profile despite the presence of constraints and local optima. An interesting  
376 contribution can be found applied to the alcoholic fermentation of a beer production process  
377 (Trelea, Titica & Corrieu, 2004). The results demonstrate the possibility of obtaining various  
378 desired final aroma profiles and reducing the total process time using dynamic optimization of  
379 three control variables: temperature, top pressure and initial yeast concentration in the tank.  
380 Applied to the alcoholic fermentation, it has led to the reduction of the production cost  
381 (reducing the process residence time from 121 hours to 95 hours) for an existing sort of beer  
382 without altering its aroma profile (figure 3). Compared to classical sequential quadratic  
383 programming optimisation (SQP), PSO optimisation, as well as other stochastic search  
384 algorithms, require much less conditions on the dynamic model, objective function and  
385 constraints (continuity, derivability) and can thus be applied to almost any existing process  
386 model without further reformulation.

387 [Figure 3 about here]

388

389 *Viability theory for decision help or control purposes*

390 Given the dynamics of a complex process, a ‘viable’ control is sequences of actions driving  
391 the process along admissible evolutions. Admissible evolutions are such that the industrial  
392 production constraints are satisfied and the consumer expectations, expressed as targets, are  
393 reached. The main purpose of the viability theory is to explain the evolution of a system

394 (model exploration), determined by given non deterministic dynamics and viability  
395 constraints, to reveal the concealed feedbacks which allow the system to be regulated and  
396 provide selection mechanisms for implementing them. Cost function can also be associated to  
397 trajectories in the state space. The aim is to reach a target with an optimal trajectory (minimal  
398 cost). If we denote  $S_F(x)$ , the set of evolutions governed by the controlled dynamical system  
399  $x'(t)=f(x(t),u(t))$ , the viability kernel is defined by (Equation 2):

$$400 \quad Viab_F(K) := \{x \in K \mid \exists x(\cdot) \in S_F(x), \forall t > 0, x(t) \in K\} \quad (2)$$

401 This is a variant of the viability problem called capture basin. Numerical schemes to solve  
402 `viability' or `capture' problems were first proposed by Saint Pierre (1994).

403 As in model-based optimizations methods, an optimal control can be calculated on the basis  
404 of the dynamic model. The advantage of the viability approach compared to the previous one  
405 is that the exact calculus of the frontier of the admissible evolutions is included in the viability  
406 scheme (Martin, 2004). It is also possible, by evaluation of the distance of each evolution to  
407 the calculated frontier at each time step, to quantify the robustness of each control trajectory  
408 in the state space (Alvarez, Martin & Mesmoudi, 2010). Indeed, nearer is the evolution to the  
409 frontier of the tube, less robust is the selected viable trajectory. Nevertheless viability suffers  
410 from the curse of dimensionality, with a need for an exhaustive search in the state space, in  
411 contrast to stochastic calculus. Such a bottleneck is in pass to be solved with research led in  
412 computer science and increased availability of powerful computer systems (Reuillon, et al.,  
413 2010).

414 .

415

416 A pioneering application of viability theory to food processes was the optimisation of  
417 Camembert cheese mass loss during ripening, while preserving an equilibrate growth of  
418 ripening microorganisms (expressed using the expert knowledge). The control variables taken  
419 into account in the algorithms were the relative humidity and the temperature of the ambient  
420 air of the ripening chamber (Sicard et al. 2009). In this study, the computation was achieved  
421 by the distribution of the algorithm on a cluster composed of 200 CPU (Central Processing  
422 Units). An example of viability kernel calculated for 12 days of ripening is presented figure 4.  
423 The distance of the determined viable trajectory to the boundary (frontier) of the viability tube  
424 is shown. An optimal ripening control trajectory calculated using the viability algorithm was  
425 implemented and validated experimentally. The gain in ripening time with a trajectory  
426 selected in the viability kernel for a given quality of the cheese, was of 5 days, to be compared  
427 with the residence time in the ripening chamber of around 12 days for a standard control  
428 policy (92% relative humidity and 12°C).

429

430

[Figure 4 about here]

431

432 Finally, both optimal control and viability theory are relevant approaches for reverse  
433 engineering purposes and can integrate global requirements encountered in food industry  
434 (nutritional, organoleptic, economical, technical, environmental, etc...). Nevertheless, their  
435 main limitation is the availability of dynamic models sufficiently representative of the  
436 complex phenomena involved in food processes.

437

438 **Conclusion**

439 The paper reviews current trends in modelling, design and control of foods and manufacturing  
440 processes, by pointing out modern promising approaches to tackle complexity, uncertainty,  
441 lack of complete first principles understanding and of reliable data and its high cost.  
442 Considerable opportunities are now open to capture and manage the complex dynamics of  
443 food systems, coupling different scales and reduce the associated uncertainty. Tight  
444 collaboration with various disciplines is needed to unify complex and dissimilar data and  
445 knowledge. Fundamental tools developed in complex systems science appear to be able to  
446 deal with the identified bottlenecks:

- 447 • Develop high-dimension models, integrating all relevant time and space scales,  
448 without reduction.
- 449 • Develop approaches for decision making and reverse engineering, integrating various  
450 sources of information and associated uncertainty.

451 Key issues towards these goals are knowledge integration, unifying mathematical formalisms,  
452 uncertainty representation and management, optimal control, viability and increased  
453 computing power. Complex system science provides appealing research directions for these  
454 issues and has proven some efficiency to tackle such complex problems as multiscale  
455 reconstruction in embryogenesis (Olivier et al., 2010). Nevertheless, it is obvious that further  
456 interdisciplinary work is required at the frontier of complex system science, which is on its  
457 own at the boundary of mathematics, physics and computer science, and food science. A  
458 generic structure for this modelling approach could lead in the future to intelligent systems

459 able to guide the user in defining a model, coupling different mathematical tools and solving  
460 the problem by bringing together available knowledge, irrespective of its format and scale.

461

## 462 **Selected publications**

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729 List of figures

730

731 Figure 1: A typical approach for model development in food engineering

732

733 Figure 2: An example of DBN applied to cheese ripening presented in Baudrit, Sicard,  
734 Wuillemin & Perrot (2010), with  $l_a$ ,  $G_c$  and  $B_a$  microorganisms concentrations,  $l_a$  and  $l_o$   
735 substrate and product concentration,  $T$  temperature of the ripening cell, colour, coat,  
736 humidity, odour and under-rind macroscopic sensory evolutions.

737

738 Figure 3: Fermentation time reduction of an existing beer without changing the final aroma  
739 profile. Top: aroma concentrations at the end of the alcoholic fermentation. Bottom: operating  
740 conditions for the alcoholic fermentation process.

741

742 Figure 4: An example of viability tube for 12 days of a cheese ripening process. Distance  
743 square map for each point is presented in colour: from blue near the boundary of the viable  
744 tube, to red at the heart of the tube. 3 dimensions are taken into account for the calculus of the  
745 viable state: mass, respiration rate of the microorganisms and temperature of the surface of the  
746 cheese.

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752 List of tables

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754 Table 1: Difficulties for the development and analysis of the models in food engineering  
755 (column 1) and possible solutions (column 2).

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757 Table 2: Type of uncertainties propagated in a mechanistic model of cheese mass loss during  
758 a ripening process.

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Figure 1

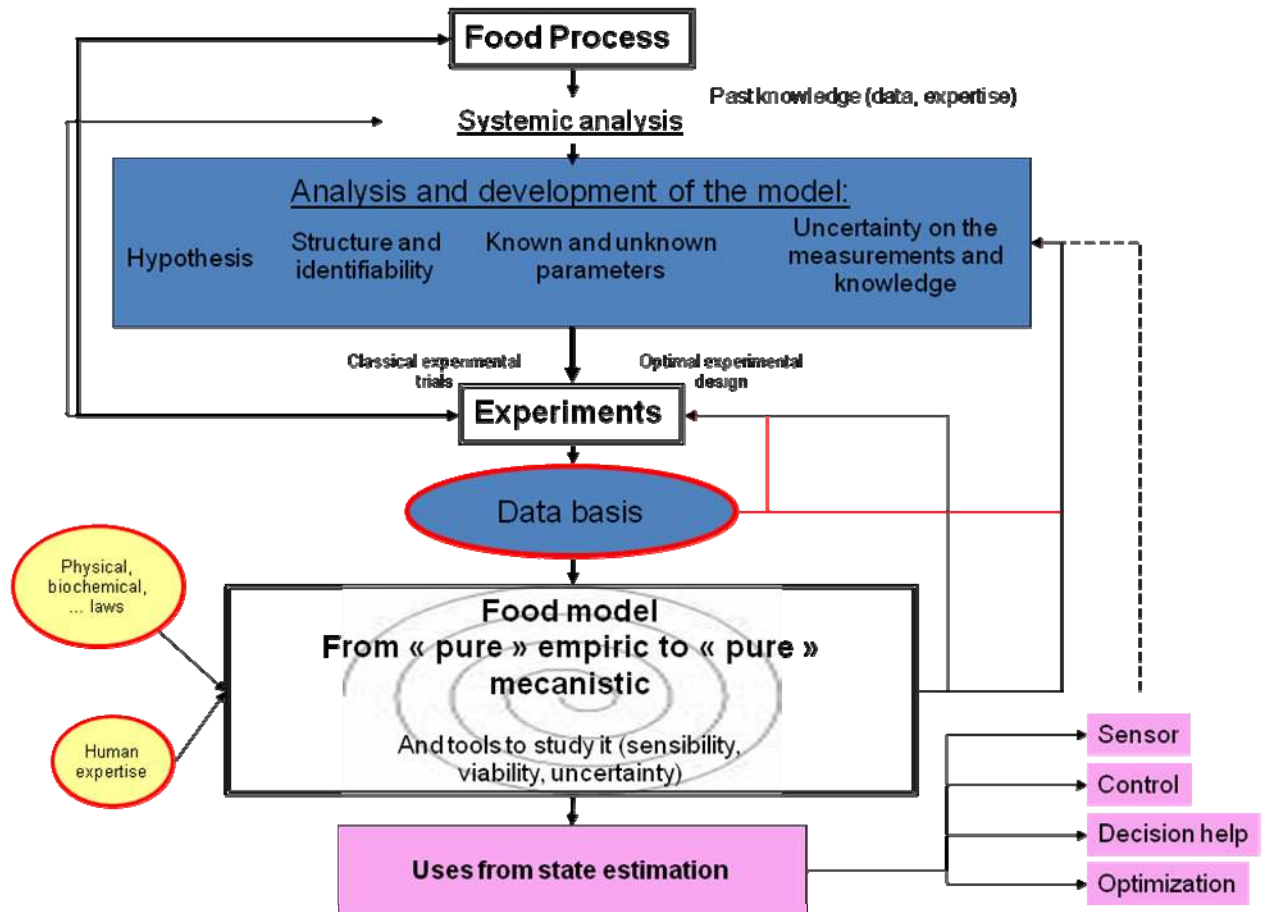


Figure 1: A typical approach for model development in food engineering

Figure 2

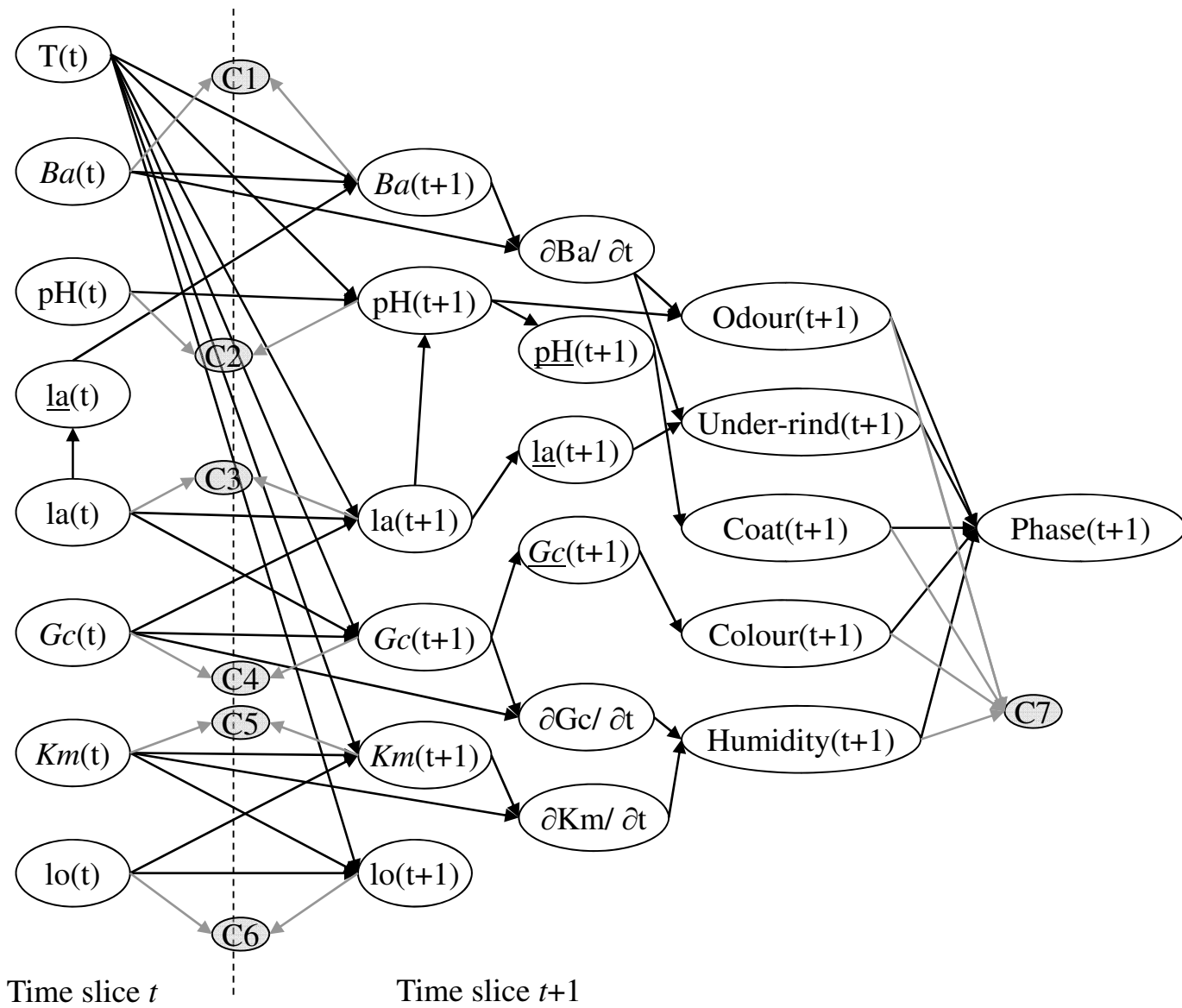


Figure 2: An example of DBN applied to cheese ripening presented in Baudrit, Sicard, Wullemin & Perrot (2010), with  $la$ ,  $Gc$  and  $Ba$  microorganisms concentrations,  $la$  and  $lo$  substrate and product concentration,  $T$  temperature of the ripening cell, colour, coat, humidity, odour and under-rind macroscopic sensory evolutions



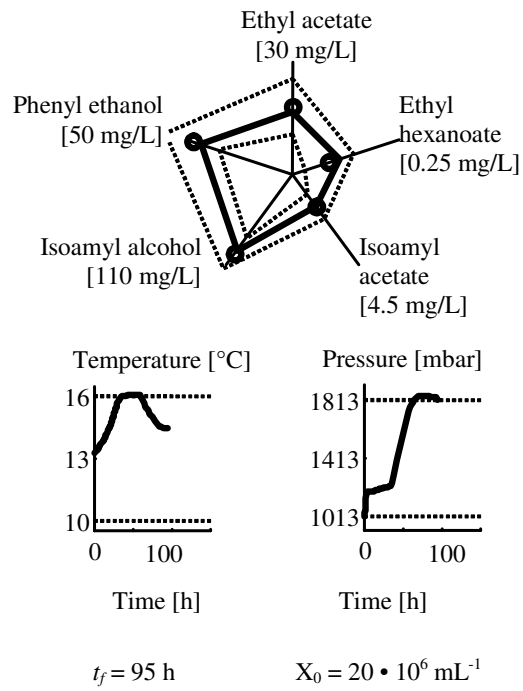


Figure 3: Fermentation time reduction of an existing beer without changing the final aroma profile. Top: aroma concentrations at the end of the alcoholic fermentation. Bottom: operating conditions for the alcoholic fermentation process.

Figure 4

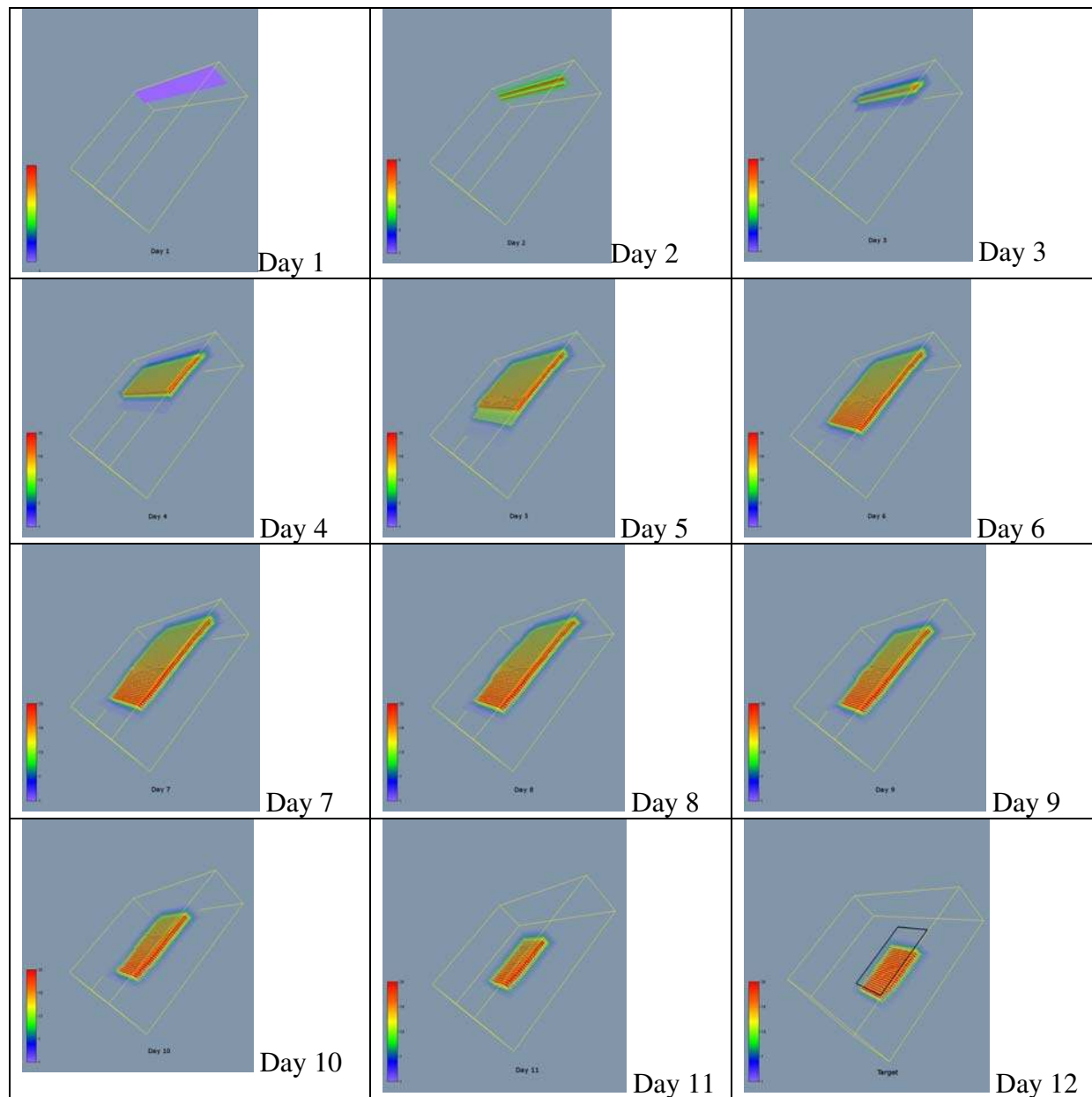


Figure 4: An example of viability tube for 12 days of a cheese ripening process. Distance square map for each point is presented in colour: from blue near the boundary of the viable tube, to red at the heart of the tube. 3 dimensions are taken into account for the calculus of the viable state: mass, respiration rate of the microorganisms and temperature of the surface of the cheese.

Table 1: Difficulties for the development and analysis of the models in food engineering (column 1) and possible solutions (column 2).

<b>Difficulties</b>	<b>Possible solutions</b>
Diversity of the mechanisms (physicochemical reactions, microbial reactions)	<i>Multidisciplinary research team</i> <i>Knowledge integration through appropriate formalisms</i>
Different and non homogeneous scales for variables and different type of knowledge	<i>Unifying mathematical formalisms</i>
Non linear connections between the variables Time scale coupled with space scale	<i>Adapted formalisms</i> <i>Increased computing power</i>
Uncertainty on the measurements and inconsistency in data	<i>Formalisms able to cope with epistemic and stochastic uncertainties</i>
Empiricism and fragmented knowledge Cost and duration of experiments	<i>Co-operation between scientists and experts from different disciplines</i> <i>Modular modelling approach, able to integrate building blocks of different nature</i>

Table 2: Type of uncertainties propagated in a mechanistic model of cheese mass loss during a ripening process.

		Sources of information	Character of knowledge	Mode of representation
Input variables	Respiration rates $r_{O_2}, r_{CO_2}$	Measurements	Precise	Fixed values
	Climate control $R_h(t), T_{\infty}(t)$	Measurements	Spatial variability	Probability distribution
Model parameters	Transfer coefficients $h, k$	Expert opinion + literature	Imprecise	Fuzzy sets
	Literature physical constants $\sigma, \lambda, \alpha, w_{CO_2}, w_{O_2}, \varepsilon, s, C, a_w$	Literature	Precise	Fixed value