DESIGN AND DEVELOPMENT OF REALISTIC FOOD MODELS WITH WELL-CHARACTERISED MICRO AND MACRO-STRUCTURE AND COMPOSITION.

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ABSTRACT

This article presents an EU project, DREAM, started two years ago, that develops realistic, physical and mathematical food models to be used as standards that can be exploited across major food categories. We underline the need for physical models realistic enough to cope with the wide diversity of food products and we detail their selection criteria, keeping in mind that these models should be versatile enough to favour the development of common approaches to risk assessment and nutritional quality for food research and industry. We also summarize the different sources of knowledge (scientific from various disciplines, expert engineers …) that have to be completed, the essential properties to be determined at every structural scale and the scientific models of different phenomena to be integrated. An example of reverse-engineering approach is also proposed to optimise technical pathways in food processing, as aimed to be promoted by DREAM project.

Keywords: model, multi-scale, cellular medium, plant, meat, dairy, cereals, properties, knowledge, integration.

1. INTRODUCTION

The physical and chemical properties of food constituents, their interactions and assemblies in food matrixes influence consumer's health in terms of bioavailability of nutrients, phytochemicals and toxicants as well as microbial food safety and quality. Beside macronutrients delivery, food may provide a wide variety of positively bioactive molecules like peptides in meat or milk products (Meisel, 2004), phytochemicals like polyphenols which have a contribution in preventing cardiovascular diseases (Das and Das, 2007), but also negatively active such as mycotoxins in cereal based products (Visconti et al., 2004). For solid foods, the release of these compounds, and thus their bioaccessibility, is largely affected by the complex multiscale structure of the matrix elaborated during processing. The safety and quality of food depend on its propensity to support microbial growth, spores germination and toxin synthesis. Despite the amount of work on the fate of microorganisms in the food chain (Antwi et al., 2007), the importance of food structure on these phenomena is poorly understood and has not been exploited in food preservation, in food risk assessment as well as in the emerging field of the assessment of food functionality.

For long, food processing was mostly dedicated to product safety, stabilization and scaling-up operations in industry; process engineers applied concepts from chemical engineering and focused on time-temperature diagrams for predicting micro-organisms survival and growth in foods. Nowadays, the consumer's driven demand for products of high sensory and nutritional quality has brought together the interests of process engineers and food scientists on "how to build up the right structures" of foods (Aguilera, 2006). The need for a pluridisciplinary approach is illustrated by the emergence of food material science which considers food as a multi-scale object, with various possible interactions and dynamics (Donald, 2004). Indeed, changes in food product structure resulting from the modification of a single physical variable (moisture, temperature, residence time…) have been largely studied at a single structural level. However, neither changes in state nor their dynamics and spatial distribution have been thoroughly studied yet, and products are frequently analysed after being processed through experimental designs which consider processes as "black boxes". Conversely, strong progresses have been made in modelling food processes (Bimbenet *et al.*, 2007). But still, their extension to the design and processing of real foods encounters limits in the unavailability of material properties, the uncertainty linked to the variability of raw materials, the diversity of conceptual frame of existing models (Rodriguez-Fernandez *et al.*, 2007). As a consequence, the resulting models of food structure modification under processing can be used only over a tiny experimental domain and the links with their end-properties scarcely predicted.

In this context, the DREAM project (http://dream.aaeuropae.org/) aims (i) to propose realistic generalized model foods (GMF) to be used by downstream partners for main properties assessment, and (ii) to integrate the basic knowledge models (BKM) available under various formalisms for designing them (Fig.1). To address the first objective, realistic, physical and mathematical food models (GMF) of the four major food categories (vegetable and fruit products, meat, dairy and bakery products) are developed in four workpackages (WP2-5). In relation with each WP, WP1 fulfills the second objective. WP6 and 7 assess the relevance of GMF and BKM respectively for toxicology, microbiology, nutritional tests (WP6) and for transfer to industry, specially SMEs (WP7).

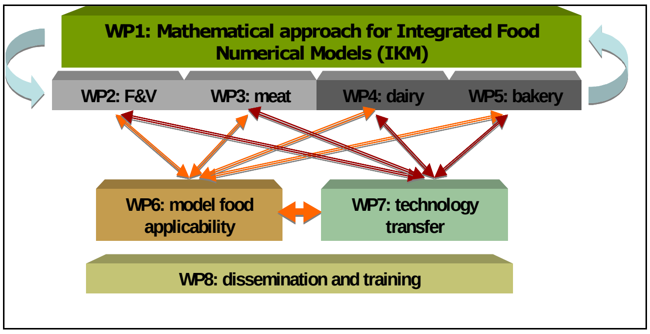


Figure 1: Organization of Dream project

In the following, these works are illustrated by a few examples of the design of GMF (section 2) and BKM building (section 3) after having stated their knowledge background at each step.

2. MODEL FOODS (GMF)

The four major food categories can be envisioned according to generic models of their structure which suggests according to their physical appearance and technical pathway listed in Table 1.

Table 1: first classification of model food structure

	Generic model structure	Example of food product
Raw and semi-processed	Filled cellular solids	Tomato, cabbage, apple
	Protein cellular networks	Pork, poultry, beef
Formulated and processed	Combined gelled/dispersed/ aerated systems	Yoghurts, creams, cheeses, protein based foams
	Open solid foams	Bread, biscuits, snacks

The GMF definition includes the food product, its structural characterization, its processing pathway and the guidelines for determining them. After enhancing their generic feature, in the following, we illustrate those by two examples from Table 1.

2.1 The multi-scale cellular medium

The knowledge gained on the multi-scale structure of these model foods suggests a generic scheme of multi-scale cellular medium with different structural entities, in analogy with cellular solids, the properties of which are modeled from the knowledge of the properties of these entitites (Gibson & Ashby, 1997). The cells (or bubbles in foam, droplets in emulsion) are entrapped in a network of walls or fibres (meat) which may adhere to each other or be separated by an interface. The whole organization, represented in fig.2 as an equivalent effective medium, can be defined by an architecture where the preceding entities may be repeated and associated, according to more or less periodic and isotropic arrangements.

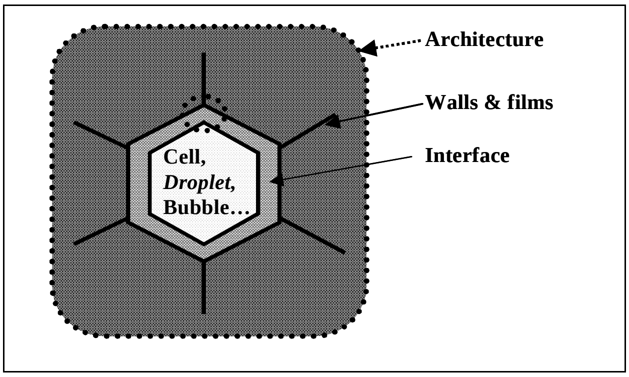


Figure 2: Multi scale cellular representation of model food structure

Depending on the information available and the scale observed, each entity may in turn defined as a cellular medium at a lower scale, which finally allows to achieve the necessary change of scale. Although schematic, this representation is based on all the observations performed by instrumental methods (Microscopies, Nuclear Magnetic Resonance, X-ray tomography) and quantitative inputs may be provided by image analysis. Its interest also relies on the possibility to infer the end-use properties (nutritional, microbiological, toxicological) of the product from the contribution of each structural entity, which in turn depends on the food category considered. For instance, many minor bioactive compounds may be stored close to the interface and released during digestion once the architecture broken down into pieces.

2.2 Application to the plant GMF

Most fruits and vegetables are eaten with limited processing and their microstructure is largely imparted by nature. They are a valuable source of a number of micronutrients, which show interesting activities related with human health. Because of the wide diversity of plant tissues, different models must be developed that are representative of leaf, root and fleshy fruit tissues, in order to relate the composition of fruit and vegetables to their functional and nutritional properties. Data accumulated on their composition, including influence of variety and growing conditions, may cover this area, but these tables give no indication on the actual amount available for physiological activity after absorption in the gut. Moreover, the bioavailability of micronutrients is extremely variable due to their chemical structure and to the plant matrix (Parada and Aguilera, 2007). The micronutrients are largely confined into a cellular structure determined by cell walls (Fig.2), from which they need to be released for absorption.

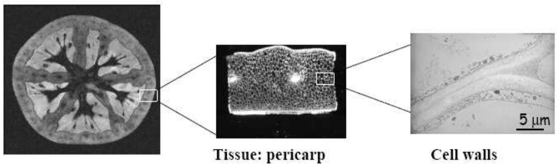


Figure 3: Multi-scale structure of a fleshy fruit selected as model of plant food product (Devaux et al., 2009).

We thus need to understand how the varying resistance of cell walls to mechanical disruption at the cellular level can be understood and modelled in raw plants, by using tissues with e.g. different histology and cell wall thickness (Fig.3); how processing and in particular thermal processing can change these properties, and create pores through which water-soluble molecules may diffuse, and gaps sufficient for migration of fat droplets and micelles; how this interacts with the form in which the nutrients are present in the food, and in particular their solubility. Carotenoid bioaccessibility from tomatoes is thus modulated by the sequence in which heat and grinding treatments are applied, in link with cell-wall degrading enzymes activities. The model of closed, or fluid-filled, cellular solids (Warner *et al.*, 2000) can be adapted to relate structure-mechanical properties by coping with turgor pressure and determine the various scale elements (cell and cell wall, tissue, organ…) to be used as input parameters.

2.2 The biomimetic meat GMF

Meat products are built of protein networks, a major source of essential amino-acids. Proteins undergo oxidations and conformational changes, especially during cooking, which could decrease their nutritional value. In order to better understand the mechanisms involved in these changes and their related kinetics under processing, whilst getting rid of biological variability, a mimetic model has been developed (Promeyrat et al., 2011). This model is based on a suspension of myofibrillar proteins extracted from 2 pure fiber type muscles (rabbit). Oxidants with various iron concentrations were added to enrich this basic model, then heat treated between 45 to 90°C, 5 to 120mn (Fig. 4). Protein oxidation and denaturation were assessed by measurement of carbonyl groups and protein surface hydrophobicity, respectively. Results show that heat treatment alone do not lead to amino-acids oxidation whereas there is a synergy between oxidants and heat. Comparison of the mimetic model with pork meat for the same iron concentration (Fig.4) underlines the protection by antioxidants in the latter case. Conversely, measurements of protein surface hydrophobicity showed that thermal denaturation occured very rapidly (≤5mn for T ≥75°C) for pork meat as for models.

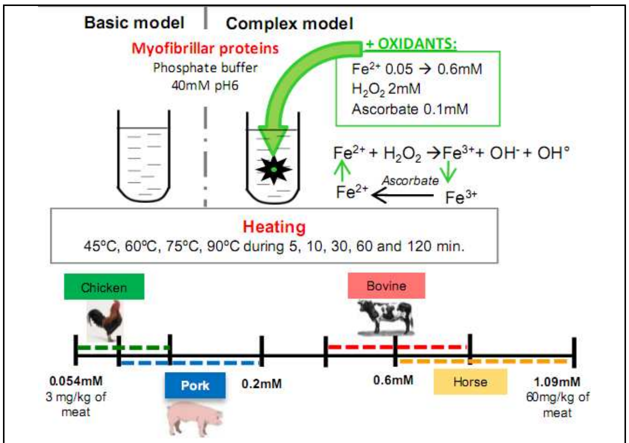


Figure 4: Design and process of meat GMF mimetic and iron content in different animal species (Promeyrat et al., 2011).

The latters will be further complexified by adding antioxydants in order to better mimick real meat products. Results will contribute to determine mathematical models for changes induced by oxidation and thermal denaturation of proteins in meat during cooking.

3. FOOD MODELS

In addition to the limits encountered in modelling food processes, the close interaction between continuous structural changes and transfer mechanisms impairs the complete modeling of coupled physical, chemical and microbiological phenomena. The fragmentation and incompletion of our knowledge require integration of technological know-how in mathematical models (Perrot *et al.*, 2011). In this purpose, the whole food chain system can be viewed as a complex one, like in recent scientific issues in biology. The emerging science of complex systems proposes new ways to understand systems located in turbulent, instable and changing environments, which are not predictable within a conventional scientific framework.. The application of those concepts relies on the tools able to take explicitly into account the fragmented and heterogeneous knowledge available on the dynamics of the process with uncertainty on the global behavior of the system.

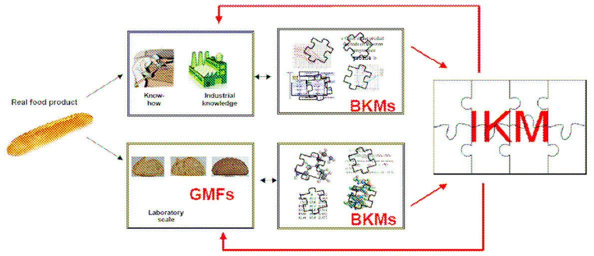


Figure 5: integrating model knowledge (IKM) of food processing; GMF= generalized model foods; BKM = basic knowledge model.

Recently, some of these tools (Monte Carlo, Neural and Bayesian Networks, fuzzy logic, expert systems…) have been implemented in various applications, such as immunology (Cohen and Harel, 2007), systems engineering (Beckerman, 2000), bioinformatics (Desiere *et al.*, 2001). In our context, these tools have to be tested for the multiscale dynamic reconstruction of the processes of food models (Fig. 5). Cognitive maps of technical knowledge (know-how) on processing of the selected food models are first to be drawn as illustrated by the conceptual map of cereal food processing (Fig.6). It encompasses process, like mixing, the product, including its control and state variables, from generic to specific and can be used on an electronic knowledge like for Web surfing.

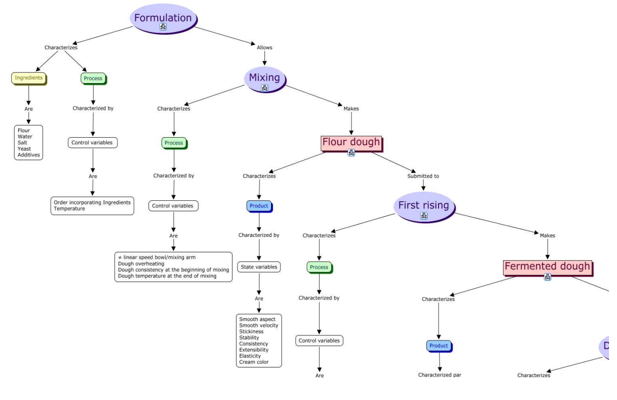


Figure 6: example of a piece of cereal processing knowledge map (from Turbin et al., 2010).

For each model food, available BKMs have to be validated and integrated into a mathematical model (IKM) for multistage dynamic reconstruction of food models (GMFs), which can in turn be implemented for reverse engineering. The following illustrates this approach taking example on two other GMFs from Table 1.

3.1. BKM for structure- properties of open solid foams cereal foods

Open solid foams can be considered as valuable models for most cereal and bakery foods since their physical properties can be determined from (1) the intrinsic properties of the solid phase, (2) product density and (3) cellular structure. The contribution of product density can be derived from Gibson and Ashby's model (1997) for cellular solids, at least for mechanical properties, but the contribution of other factors is poorly known. Recently numerical finite element models (FEM) of solid foams have allowed assessing the effect of cellular structure described by images from X-ray tomography on product texture (Guessasma *et al.*, 2008). Besides extending Gibson & Ashby's model, these numerical simulations have shown that the more heterogeneous the cellular structure, the stiffer the foam, due to the regularity of cell wall size (Fig. 7). This result may have some implications on the texture (firmness) of bakery products, regarding the large range of crumb grain.

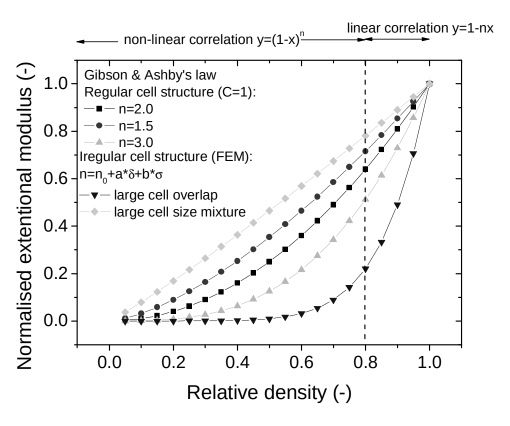


Figure 7: Examples of FEM simulation of solid foam modulus against relative density for various cell structure (from Guessama et al., 2011)

Besides, FEM may be also apply to model the mechanical behavior of the solid phase of the foam, envisioned as a composite of starch and gluten (and other components), and the properties of which depend on composition and morphology (Fig. 3). Mechanical properties of such composite materials can then be used as inputs to compute the solid foam properties, which allows achieving the change of scale. For vitreous brittle products, the lack of adhesion between starch and proteins has been shown of great importance on composite behavior and its fragility, promoting rupture at phase interface (Chanvrier et al., 2006). Indeed, the fracture properties and water dynamics in the matrix have to be determined because they govern the sensory quality, the stability and also the digestibility, through the delivery of small molecular weight components in the gastrointestinal tract and thus envision their de-structuration during mastication.

By extending the use of numerical methods and improving experimental ones, it will be possible to better cope with the changes of composition (dietary fibres, fatty acids, enzymes…) at different structural levels during processing from the divided solid medium (flour), through mechanical and thermal actions, to a continuous matrix with multi-scale porosity.

Finally, numerical models are now available for simulating most cereal processes, except mixing. This lack is illustrated by the limitation of the SAFES approach which ignores the flow operations (kneading, shaping) when applied to bread making (Segui *et al.*, 2007). It evidences the need for integrating know-how either by a probabilistic approach or qualitative physics (Ndiaye *et al.*, 2009).

3.2. BKM for process-properties and integration of expertise

Cheese manufacturing is certainly one of the most representative areas of food industry in Europe. In spite of this industrial importance, soft cheese like Camembert is an ecosystem and a bioreactor difficult to assess in its entirety. Despite extensive research conducted on this product, knowledge remains fragmentary and incomplete and no model provides a comprehensive representation of the process. In this context, Dynamic Bayesian Networks (DBN) have been used to model the network of interactions occuring at different scales and reconstruct its dynamics (Baudrit et al., 2010). The concept of DBNs provides a practical mathematical formalism that enables to describe dynamical complex systems tainted with uncertainty. DBNs are an extension of classical Bayesian networks that rely on probabilistic graphical models in which nodes representing random variables are indexed by time. They are very useful tools for combining expert knowledge with data at different levels of knowledge, where the structure can be explicitly built on the basis of expert knowledge and conditional probability, quantifying dependence between variables, can be automatically learned without *a priori* knowledge on the basis of a dataset. From operational and scientific knowledge, Baudrit *et al*. (2010) defined the structure of a DBN providing a qualitative representation of the coupled dynamics of microorganism behaviour (*Kluyveromyces marxianus* (Km), *Geotrichum candidum* (Gc), *Brevibacterium aurantiacum* (Ba) with their substrate consumptions (lactose (lo), lactate (la)) influenced by temperature (T) and involving the sensory changes (Odour, Under-rind, Coat, Colour and Humidity) of cheese during ripening (Fig.8).

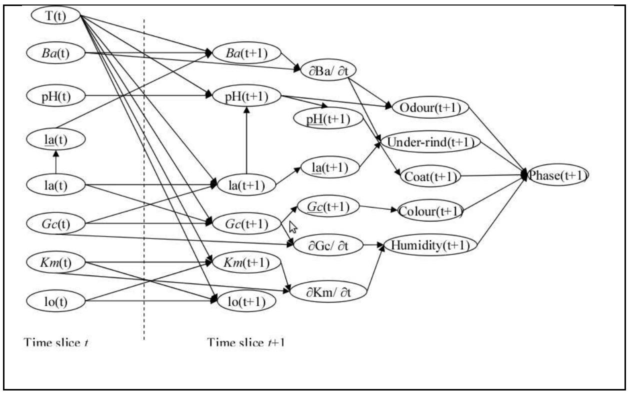


Figure 8: Dynamic Bayesian network representing the coupled dynamics of micro-organism growth with their substrate consumptions influenced by temperature and involving the sensory changes of cheese during the ripening process (from Baudrit et al., 2010).

After the learning step to define conditional probability distributions from experimental trials with various temperature and humidity, DBNs inferences can be carried out in order to simulate the behaviour of microbial activities associated with sensory development, for instance the beliefs of the possible trajectories of the yeast *Km* during ripening at 8°C (Fig.9a). This figure means, for instance, that at the 27th day of ripening, the concentration of Km has a probability of 39% to be ≈ 10^7cfu/g FC and that it cannot be lower than 3.10^5. In addition the mean evolution of *Km* (Fig.9b) as well as the modal evolution of odor properties(Fig.9c) could be estimated by DBN simulations and compared to experimental data.

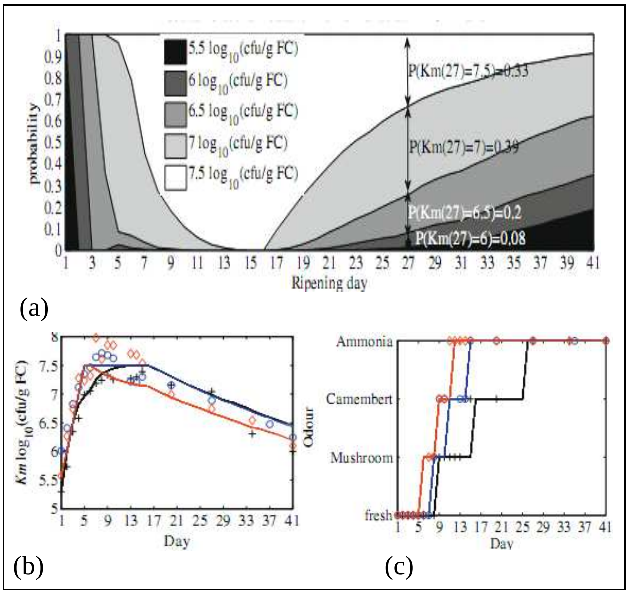
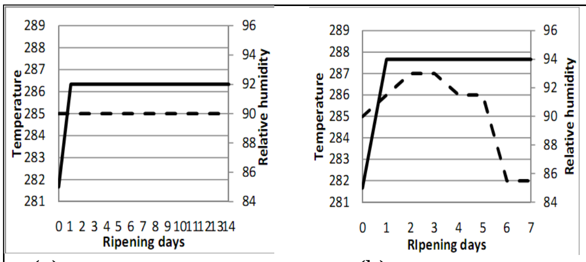


Figure 9: DBN results of (a) Km(t) probability distribution at 8°C, predictive evolutions of (b) Km microbial growth and (c) odour, versus experimental data for ripening performed at T= 8 (+), 12 (o) and 16°C (◊), RH=98%.

The model was thus shown to be able of (1) coupling and integrating heterogeneous knowledge at different scales; (2) predicting the evolution of microbial activities and sensory properties with an overall average adequacy rate of about 85% to experimental data.

3.3. Example of an IKM used for reverse engineering

Following the same practical application, a model of cheese mass loss (Helias et al., 2007) has been considered for optimizing the ripening process. In this purpose, a viability kernel representing a compromise between production costs and ripened cheese quality was computed (Sicard et al., 2009). Viability theory aims at controlling a dynamical system, here cheese during ripening, in order to maintain it in a given set of evolutions, namely the viability kernel. The viability kernel was defined by associating a target on cheese mass at the end of ripening (≈280g) and constraints on microorganisms respiration. It was then computed thanks to the classical heat&mass transfer model, proposed by Helias et al. (2007) that predicts cheese mass, surface temperature and the respiration of the microorganisms. Meanwhile, the cost trajectories, involving the number of control variations and the ripening time are computed to define the compromise between cheese quality and energy consumption saving (Sicard et al., 2009). Then, optimal trajectories, lowering cost, were found; among those, one reached the mass target after 8 days ripening, and the results of its control variations are presented in Fig. 10a, to be compared to the conventional control performed for 12 days ripening (Fig. 10b), without quality loss. Whilst setting a higher humidity (94%), it imposes a daily change of temperature between 14 and 9°C. These controls have been applied to real ripening chambers; the analysis of processed cheese gave sensory results very close to those obtained under classical conditions (12°C, 92%).



(a) (b)

Figure 10: Control (T(K) ---, RH(%) —) of ripening chambers, (a) conventional in industry and (b) optimal computed applying viability approach.

This is an example of the application of the reverse engineering approach to a single food processing operation.

4. CONCLUSION

Food engineering deals with complex systems in which knowledge is incomplete and which depend on many interacting factors. The needed information is not fully available from literature and partly relies on technological expertise. Managing such systems is a real challenge, that can be addressed by Knoweldge Engineering. In order to design Model Foods, we have presented some of its recent applications to build Food Models by describing some tools involved in the EU-Dream project. Dream's goals will be achieved by integrating these models, in order to build an integrated mathematical model (IKM) for multistage dynamic reconstruction of foods which can in turn be implemented for reverse engineering. The application of such approach opens prospects for the virtual design of food products, which will be of help for the sustainable production of high quality foods.

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Caroline Sautot, holds a Master of Science in Biotechnology and a Master in Project Management. She has 5 years experience in the setting up and management of large collaborative research projects. Currently, she manages several FP7 collaborative research projects including the DREAM project.

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