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The virtual food system: Innovative models and experiential feedback in technologies for winemaking, the cereals chain, food packaging and eco-designed starter production

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A B S T R A C T

This article presents an overview of five use-cases that illustrate food-system modeling approaches, most of them combining quantitative and qualitative methods. The cases deal with issues as diverse as: the modeling of winemaking fermentation; the choice of a food packaging material; the design of solid foam cereal products; argumentation modeling to support multistakeholder decision-making, and the control of freeze-drying for eco-design purposes. They tackle several challenges to modeling and knowledge engineering in food systems: capitalizing data and knowledge; structuring a shared vocabulary and domain knowledge in an ontology; formalizing viewpoints and contradictions from food-related debates; supporting multi-criteria decision-making.

1. Introduction

This article aims to demonstrate how abstraction—as tackled by mathematical as well as computer science approaches (e.g. knowledge representation, decision support, etc.)—can prove highly beneficial for dealing with issues as concrete as those found in food technologies. Indeed, food processes are complex for various reasons, some of which are recalled here:

– numerous criteria are used to describe food properties;
– numerous food-process parameters of impact food properties;
– these parameters are non-independent, and can be quantitative or qualitative;
– they are difficult to measure online due to sensors limitations;
– they can be very complicated to mathematically model because their dynamics are usually nonlinear and they are over-parameterized (quantitative case);
– parameter values are consequently often ill-known, missing, imprecise or uncertain.

These scientific barriers make food processes a challenge for modeling or data engineering approaches.

Five successful attempts are presented in this paper, most of them combining quantitative and qualitative approaches. They deal,

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respectively, with the modeling of winemaking fermentation to control wine characteristics (Section 2), the design and choice of a packaging material for a given food product (Section 3), the design of solid foam cereal products (Section 4), argumentation models to support decision-making among multiple food-chain stakeholders (Section 5), and the control of freeze-drying for both reduction of energy efficiency and bacterial quality objectives (Section 6). The last two sections feature specificities in the type of approach, as Section 5 proposes a purely qualitative approach whereas Section 6 presents a systemic approach with eco-design purposes.

These studies illustrate how to:

- capitalize data and knowledge (Section 2, 3 and 4);
- structure a shared vocabulary and domain knowledge in an ontology (Section 2 and 6);
- formalize viewpoints and contradictions in a debate (Section 5);
- support multi-criteria decision-making (Sections 3, 5 and 6).

Focused on models and experience developed within the "Science for Food and Bioproduct Engineering" (CEPIA) Division of the French INRA research institute, the typology of problems covered by the experiences presented in the paper is illustrative of the type of issues that one can face in the food industry. Launched by the CEPIA Division, a similar initiative at the European level is currently pursued in the COST Action "FoodMC" (www.inra.fr/foodmc).

In winemaking (Section 2), the most important fermentative aromas were successfully described using mathematical modeling. In these processes, several state variables were estimated online thanks to sensors developed at the INRA. Moreover, an integrated methodology was proposed for process control coupling models from online sensors, databases and ontologies.

In the field of food packaging (Section 3), mathematical models were used to describe the evolution of atmosphere inside the packaging headspace based on packaging and food characteristics. These models are used to study food transformation and to help improve packaging design. Packaging improvements were obtained by coupling models with multicriteria optimization.

Qualitative models can be seen as a flexible alternative when there is insufficient information to develop a mathematical model. These kinds of models integrate available scientific knowledge and experts' know-how in process description. Here, knowledge-based models were used through qualitative reasoning and phenomenological modeling for the design of solid foam cereal products (Section 4), where they enabled prediction and learning of cereal food texture and rheology.

That said, food technologies are not limited to process modeling. Food systems involve various stakeholders, each with their own objectives, priorities, interests, etc. Qualitative models, in particular computer science approaches, offer a relevant approach to represent stakeholders' knowledge and their logics behind their reasoning. This paper develops an example presenting an argumentation approach to express a debate concerning breadmaking recommendations and support decisionmaking (Section 5).

Finally, we present an eco-design approach applied for the production of stabilized lactic acid bacteria (Section 6). Life-cycle assessment (LCA) was used to quantify the system's global environmental impacts, providing opportunities for system eco-design and innovation. At unit operation level, bacterial quality and energy consumptions were simulated during freeze-drying, allowing eco-reasoned process control. Knowledge formalization in an ontology served to move towards a multicriteria analysis combining process conditions, product quality and environmental impact at both unit-operation and whole-system level.

As a synthesis, we propose a summary of the issues, methods and results presented in the paper, before concluding with feedback in the form of a global table.

2. Winemaking fermentation: from online monitoring to modeling and information system for data sharing

Alcoholic fermentation, a key step of the winemaking process, is likely to change considerably in the future. Indeed, winemakers increasingly recognize the need for tools controlling fermentation according to the type of wine desired and the characteristics of the grape must. The main objective is to control the bioconversion of sugar into ethanol and CO_2, but the ability to directly control wine characteristics would be a major step forward. Even though wine quality is notoriously difficult to predict (Francis & Newton, 2005; Swiegers, Bartowsky, Henschke, & Pretorius, 2005), some "quality marker molecules" have been identified. Among these markers, fermentative aromas—generated by yeast secondary metabolism—are the most abundant and help shape the fruity flavor.

To tackle these challenges, we developed innovative systems for online monitoring of the kinetics of (i) the alcoholic fermentation and (ii) the major fermentative aromas. The monitoring of alcoholic fermentation is based on measuring CO_2 release. In parallel, we developed an online GC (gas chromatography) system to monitor the synthesis of the main higher alcohols and esters (Morakul et al., 2011; Mouret, Morakul, Nicolle, Athes, & Sablayrolles, 2012). These online monitoring devices allow precise determination of the chronology of synthesis of some key compounds in alcoholic fermentation. The high acquisition frequency makes it possible to calculate the kinetic parameters of synthesis of these molecules, i.e. instantaneous production rate and production yields. These kinetic data are of primary importance for a better understanding of yeast metabolism, but they also have practical interest—instantaneous CO_2 production rate, for instance, is directly proportional to the energy required for temperature control in fermentation tanks (Colombie, Malherbe, & Sablayrolles, 2007; Goelzer, Charnomordic, Colombié, Fromion, & Sablayrolles, 2009). The online data collected were used to build a model predicting the fermentation kinetics (Malherbe, Fromion, Hilgert, & Sablayrolles, 2004), gas-liquid ratio (Morakul et al., 2011) and production kinetics of five fermentative aromas (Mouret, Farines, Sablayrolles, & Trelea, 2015). These data were also used to implement an information system called ALFIS (alcoholic fermentation information system) that allows the acquisition, annotation and consultation of online and offline measurements and provides a rich digital resource for sharing data across technologies and disciplines.

Using 125 fermentations corresponding to 49 natural and synthetic musts and 20 strains, we built a dynamic model—consisting of ordinary differential equations—to predict the main reaction of the fermentation (Malherbe et al., 2004). This model (called MOMAF, for "modeling of the main reaction of alcoholic fermentation") predicts cell growth, fermentation rate and sugar consumption (proportional to ethanol and CO_2 production) from two main fermentation parameters: temperature (including non-isothermal profiles, which are widely used in the industry) and nitrogen additions. This explanatory model is based on physiological considerations and takes into account the main phenomena directly affecting kinetics in enological conditions, including the effects of: (i) nitrogen in yeast synthesis (growth phase) and activation of metabolism (stationary phase); (ii) the transport of sugar into yeast cells; (iii) ethanol inhibition; and (iv) temperature. The results obtained were very satisfactory: mean error between experimental and simulated data was lower than 5% (Malherbe et al., 2004). MOMAF was licensed to a private company and is currently marketed as a simulation software. The model was then completed with a thermal model (Colombie et al., 2007) evaluating the power required to cool the tank during the winemaking process (as fermentation is a very exothermic process). This model opens up new perspectives for the control of alcoholic fermentation, for example to optimize the fermentation duration, tanks scheduling, energy consumption peaks and total energy required.

The next challenge in the modeling of enological fermentation was