Articles for

ORAL PRESENTATIONS

SESSION 4-2

Modelling - 2

Central Composite Design and Desirability Approach for Process Optimization: How Use? Case-Studies: *Alicyclobacillus acidoterrestris* in Juices and Lactic Acid Bacteria in Brines

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Abstract. *This paper proposes an overview of process optimization in food microbiology and technology, through Central Composite Design (CCD) and Desirability Approach (DA). Growth/inactivation of* <u>*Alicyclobacillus acidoterrestris*</u> *and Lactic Acid Bacteria (LAB) were used as case-studies.*

Case-study 1. pH (3.5-5.5), cinnamaldehyde (0-80 ppm) and eugenol (0-160 ppm) were combined through a 3 variables/5 levels CCD to point out the optimal conditions for the inhibition of <u>*A. acidoterrestris*</u> *spores in a laboratory medium. The DA pointed out that the effect of cinnamaldehyde could be regarded as strong, as the highest amount prolonged the lag phase of ca. 4 days.*

Case study 2. The growth of some strains of <u>*Lactobacillus plantarum*</u>*, isolated from table olives, was studied in a system containing NaCl (0.0-6%), glucose (0.0-4.0%) and two phenolic compounds (p-coumaric and vanillic acids-0.0-0.4%) with a CCD at 4 variables/5 levels. After 24 h, a significant inhibition of cell count could be achieved through NaCl; however, for a prolonged storage, p-coumaric acid was the strongest variables, able to affect and inhibit LAB growth.*

In conclusion, the combined use of CCD and DA approach is a suitable mean for process optimization, both to design a preserving treatment for juices (as reported for <u>*A. acidoterrestris*</u>*) and study the conditions enhancing the growth of useful microorganisms (like LAB in olive brines).*

Keywords. Design of Experiments, Desirability, *Alicyclobacillus acidoterrestris*, Combined Treatment, Lactic Acid Bacteria.

Introduction

An interesting tool in food microbiology is the Box-Wilson Central Composite Design, usually called Central Composite Design (Bevilacqua, Corbo & Sinigaglia, 2010c).

There are several kinds of Box-Wilson Design (Circumscribed, Inscribed and Face-Centered), depending on the distance of the levels from the average value of each variable; the most used approach in food science is the Circumscribed Design, usually referred to as CCD (Central Composite Design) (Bevilacqua et al., 2010c).

It involves five different levels for each factor and contains a factorial design, added with some combinations containing the central point (i.e. the mean value of each factor) and some star points (i.e. the minimum and the maximum of the range) to allow a good estimation of the curvature of the output (Bevilacqua et al., 2010c).

A CCD is the background for the building of a polynomial equation, reading as follows (Van Boekel & Zwietering, 2007):

$$y = \beta_0 + \sum_{j=1}^{n} \beta_j \cdot X_j + \sum_{j=1}^{n} \sum_{k=j+1}^{n} \beta_{jk} \cdot X_j \cdot X_k + \sum_{j=1}^{n} \beta_{jj} \cdot X_j^{\;2}$$

where $\sum_{j=1}^{n} \beta_j \cdot X_j$ is the individual effect of each factor; $\sum_{j=1}^{n} \sum_{k=j+1}^{n} \beta_{jk} \cdot X_j \cdot X_k$ indicates the interactions amongst the variables; finally, the term $\sum_{j=1}^{n} \beta_{jj} \cdot X_j^{2}$ takes into account a possible non-linear/quadratic effect of some factors.

Generally, the polynomial equation is accompanied by surface response plots, showing the effects of the independent variables on the dependent one. A new approach in the field of CCD for food science and microbiology, is the use of saddlepoint and desirability approach (Bevilacqua, Corbo & Sinigaglia, 2010a; Bevilacqua et al., 2010c; Bevilacqua, Sinigaglia & Corbo, 2010d). A saddlepoint is the point of the maximum or minimum response of the dependent variable; for food science and technology, it assumes a strong practical implication, as it gives the unique combination of the independent variables resulting in the minimum or maximum value of the dependent factor.

Concerning the desirability, it is a prediction profile of the effect of each independent variable on the dependent one and is based on the polynomial equation. From a mathematical point of view, the desirability is a dimensionless parameter and is included in the range 0-1: the value is set to 0 when the output (dependent variable) is completely unacceptable, whereas it is imposed to 1 when the dependent factor is acceptable (desired value or output) (Bevilacqua et al., 2010c). The desirability function can be evaluated as follows:

$$d = \begin{cases} 0, & y \le y_{min} \\ (y-y_{min})/(y_{max}-y_{min}) & y_{min} \le y \le y_{max} \\ 1, & y \ge y_{max} \end{cases}$$

In this equation, y is the output of the process and y_{max} and y_{min} the maximal and the minimal response, respectively. The desirability approach represents a useful tool to point out a good compromise between the optimal response of the process (i.e. the saddle point) and the costs (Bevilacqua et al., 2010c).

This paper reports two case-studies (the optimization of a preserving treatment to inactivate *Alicyclobacillus acidoterrestris* and the evaluation of the condition for the optimal growth of lactic acid bacteria) to show the impact and importance of desirability/saddlepoint approach in food microbiology.

Materials and Methods

Case-study 1: Alicyclobacillus acidoterrestris

Strains. Six *A. acidoterrestris* strains were used throughout this study (γ4, isolated from a spoiled pear juice, and c1, c6, c8, c10 and c24, isolated from soil); the strains belong to the Culture Collection of the Department of Food Science (University of Foggia). Spores were produced as reported by Sinigaglia, Corbo, Altieri, Campaniello, D'Amato & Bevilacqua (2003).

Sample preparation. Experiments were performed in Malt Extract Broth (Oxoid, Milan, Italy), inoculated with ca. 10^3 spores/ml of a cockatil of the six strains. The pH of the medium (3.5-5.5), the amounts of eugenol (0-160 ppm) and cinnamaldehyde (0-80 ppm) (MP Biomedicals, Solon, OH) varied according to a Central Composite Design at 3 variables and 5 levels. The samples were stored at 44°C and analyzed throughout 10 days; alicyclobacilli number was evaluated through absorbance measurement at 420 nm.

Data modeling. Data were modelled through the Gompertz equation, as modified by Zwietering, Jongenburger, Rombouts & Van't Riet (1990) and the prolongation of lag phase, compared to the control (the samples without antimicrobials, pH 4.5) was evaluated (Δλ). Δλ was used as the dependent variable for CCD modeling and evaluation of desirability through the software Statistica for Windows (Statsoft, Tulsa, OK).

Case study 2: Lactic Acid Bacteria

Strains. Three strains of *L. plantarum* (c9, c10 and c15) were used in this study (Bevilacqua, Altieri, Corbo, Sinigaglia & Ouoba, 2010b). The strains stored at -20 °C in MRS broth (Oxoid), added with 33% of sterile glycerol, and grown before each assay in MRS broth, incubated at 37°C for 48 h.

Sample preparation. Growth and glucose metabolism of lactic acid bacteria were determined in the broth reported by Bover-Cid & Holzapfel (1999), added with 1.0% of tyrosine disodium salt (Sigma-Aldrich). The individual and additive effects of glucose (0-4.0%), NaCl (0.0-6.0%) and secondary phenolic compounds (p-coumaric and vanillic acids) (0.0-0.4%) (Sigma-Aldrich) were investigated through a four variables-five levels CCD. The pH of medium was adjusted to 5.3 with HCl 2N and HCl 0.1N and then the medium was autoclaved for 10 minutes at 121°C. The samples were inoculated with approximately 10^3 cfu/ml of a microbial cocktail of the 3 strains, incubated at 37°C and removed periodically over 7 days, in order to evaluate the microbial growth or viability loss.

Cell number evaluation. Viable count of lactic acid bacteria was performed on MRS agar, incubated at 30°C for 2-4 days under anaerobic conditions. Data were modelled as $\log N_t/\log N_0$, where N_0 is the initial inoculum and N_t the viable count after the time t.

pH determination. pH was evaluated through a pH-meter Crison 2001 (Crison, Barcelona, Spain). As the pH decreased, data were modelled through a negative modified Gompertz equation (Zwietering et al., 1990).

Data modeling. Standardized values of cell counts after 24, 48, 96 and 168 h of incubation, as well as the decrease of pH were used as dependent variables for desirability approach.

Results and Discussion

Case study 1: Inactivation of Alicyclobacillus acidoterrestris

The first case-study shows an example of process optimization for the inactivation of an emerging and spoiling microorganism of juices (*A. acidoterrestris*). The desirability approach highlighted the effects of eugenol and cinnamaldehyde; they influenced the growth of alicyclobacilli in the system when their amount was >40 ppm. However, the effect of cinnamaldehyde could be regarded as strong, as the highest amount prolonged the lag phase of ca. 4 days (the desirability value was 0.9); otherwise 160 ppm of eugenol, if used alone, prolonged the lag phase of ca. 1.5 days (figure 1). These data can be used for validation in real systems.

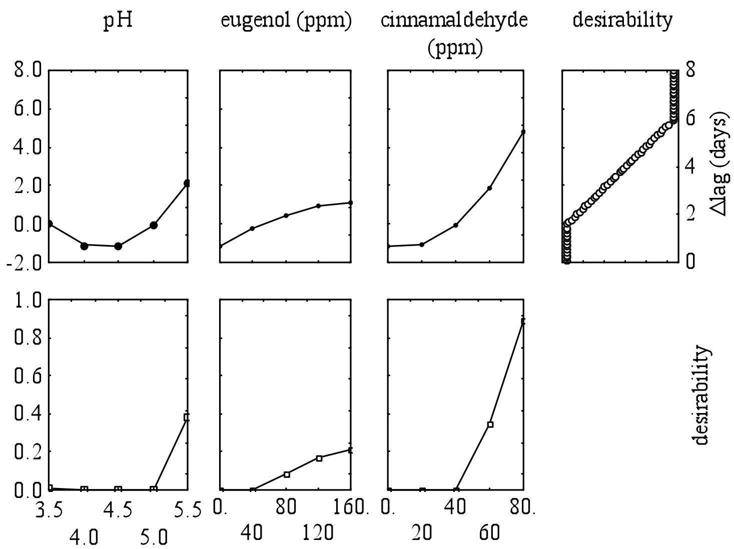

Figure 1. Effects of pH, cinnamaldehyde and eugenol on the prolongation of the lag phase (days). Desirability functions.

Case study 2: Lactic Acid Bacteria

The second case-study focuses on the individuation of the conditions for an optimal growth of LAB in olive brines. Figure 2 shows the desirability approach for the growth of LAB in presence of glucose, NaCl, *p*-coumaric and vanillic acids after 24 h. The graphs was obtained by imposing a value of 0.5 to desirability when the standardized cell count ($logN_t/logN_0$) was 1 (neither growth nor survival). The increase of glucose, NaCl, as well as phenolic compounds in the medium exerted a negative effect on LAB growth and determined a decrease of the cell count; what it is important to underline is that as single factor, none of the independent variable reduced the standardized value of cell count to values lower than 1, thus suggesting that LAB were able to grow in the most of the combinations of CCD. Only the highest amount of NaCl (6%) exerted a strong effect on LAB population (as one could infer form the standardized value of cell count of ca. 1).

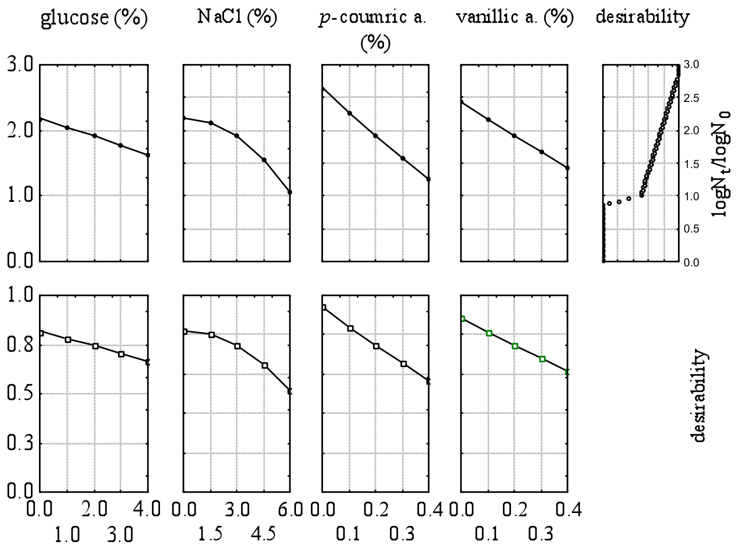

Figure 2. Effects of glucose, NaCl, *p*-coumaric and vanillic acids on the growth of lactic acid bacteria after 24 h. Desirability functions.

The use of the desirability approach for cell counts after 48, 96 and 168 h revealed that *p*-coumaric acid was the dependent variable acting in a strong way on cell viability, able to reduce lactic population significantly. As an example, figure 3 shows the desirability approach referred to cell numbers after 48 h.

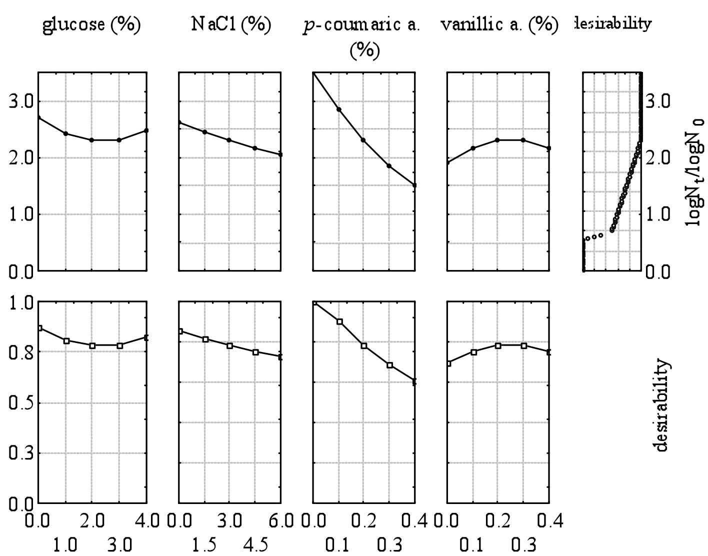

Figure 3. Effects of glucose, NaCl, *p*-coumaric and vanillic acids on the growth of lactic acid bacteria after 48 h. Desirability functions.

Concerning the decrease of pH, statistical analysis revealed that it was affected in a strong way by *p*-coumaric acid; moreover, the desirability approach, as well as the building of a surface response plot, pointed out a critical threshold of the concentration of *p*-coumaric acid of 0.2%, after which LAB did not cause the acidification of the medium (data not shown).

Conclusions

The desirability approach is an useful tool in food microbiology, as it offers a kind of summary and an overview of the influence of each factor of CCD, both as single element and combined with the other variables. Moreover, it points out some practical conclusions concerning the optimization of a preserving treatment/microbial growth.

The two case studies showed that the use of desirability approach allowed the estimation of the conditions (i.e. exact values of active compounds) resulting in the inhibition/inactivation of *A. acidoterrestris* and the individuation of the most important variable (i.e. *p*-coumaric acid) that could affect LAB in brines.

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Modeling and Simulation of Drying Phenomena and Rheological Behaviour of Potatoes

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Abstract. *Some food products are characterized by high moisture contents. A considerable moisture removal could be induced during drying processes. As a consequence of the moisture,, an important changes in the pore product size complicates the analysis of heat and mass transfers.*

This work gives a mathematical formulation of transfer phenomena (heat, mass and momentum) in cube-shape potato samples. The model describes the drying process of a deformable media and takes into account the effect of the deformation on the transport of mass and energy.

The model is implemented in a finite element solver. The Arbitrary Lagrange-Eulerian (ALE) formulation was used to solve the problem with moving boundaries.

The simulation allows the derivation of the time and space evolutions of temperature, moisture, deformation, stress and strain of potato during convective drying. The spatiotemporal variations of moisture content and temperature reflect product drying behaviour very satisfactorily, well known in literature. Tensional stresses were recorded at the product surface and were equilibrated by compressive stresses in the inner of the product. The evolutions of both stresses depend on the moisture gradient.

Keywords. Food drying, modeling, heat and mass transfers, rheological behaviour, simulation.

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An artificial intelligence-based approach for arbitration in food chains

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Abstract. *Food chain analysis is a highly complex procedure since it relies on numerous criteria of various types: environmental, economical, functional, sanitary, etc. Quality objectives imply different stakeholders, technicians, managers, professional organizations, end-users, public collectivities, etc. Since the goals of the implied stakeholders may be divergent, decision-making raises arbitration issues. Arbitration can be done through a compromise – a solution that satisfies, at least partially, all the actors – or favor some of the actors, depending on the decision-maker's priorities.*

Several questions are open to support arbitration in food chains: what kind of representation and reasoning model is suitable to allow for contradictory viewpoints ? How can stakeholders' divergent priorities be taken into account ? How can the conflicts be solved to achieve a tradeoff within a decision-support system ?

This paper proposes an artificial intelligence-based approach to formalize available knowledge as elements for decision-making. It develops an argumentation-based approach to support decision in food chains and presents an analysis of a case study concerning risks/benefits within the wheat to bread chain. It concerns the controversy about the possible change in the ash content of the flour used for commonly consumed French bread, and implies several stakeholders of the chain.

Keywords. Decision-making, quality construction in food chains, sustainability, benefits and risks analysis, knowledge representation, reasoning, argumentation, decision-support.

Introduction

Food quality assessment relies on criteria classically grouped into four main types: nutritional, sensorial, service or practicity and sanitary quality. These can be supplemented by other emerging concerns such as environmental quality, economic quality, etc. However, all of these aspects of quality and their various components are not always compatible and their simultaneous improvement is a problem that has no simple solution. Moreover the importance attached to the different involved criteria varies among several stakeholders.

A tradeoff between nutritional, organoleptic and sanitary quality has been built in an empirical way within agri-food chains, with progressive control of transformation processes. With the emergence of new concerns and requests, consumers are becoming more receptive to these new problems and new tools are needed to meet emerging needs by adapting, innovating, optimizing decision schemes within agri-food chains.

This paper proposes an artificial intelligence-based approach to allow the formalization of available knowledge as elements for decision-making, based on an argumentative decision system. Very few studies deal with the advantages of argumentative methods as explanation elements for decision support (Amgoud and Prade, 2009), which is the question considered here. The paper presents an analysis of a case study concerning risk/benefit evaluation within the wheat to bread chain, according to recommendations for more whole-grain products given by the PNNS public health policy in France. It gives a brief overview of the results obtained in (Bourguet, 2010) through a simplified version of the model and an extract from the data.

Materials and Methods

Information sources

Several kinds of information sources were used in this study. They include, from the most to the least formal ones:

1. scientific peer-reviewed articles;
2. technical reports or information published on websites;
3. scientific conferences and research project meetings;
4. expert knowledge obtained through interviews.

For the considered case study concerning the position of the bread chain regarding the PNNS recommendations, we used the following sources. The scientific peer-reviewed articles we analyzed include Bourre et al. (2008), Slavin & Green (2007), Dubuisson-Quellier (2006), Ginon et al. (2009).

We also analyzed several scientific conference proceedings, and examined numerous technical reports available on official websites concerning the PNNS public health policy (PNNS statutory documents, 2005; PNNS website, 2005), the Healthgrain European project (Dean et al., 2007; Healthgrain, 2009), French projects and symposiums concerning sanitary, nutritional, sensorial and technological qualities of breads (Dinabio, 2008; Cadinno, 2008; Aquanup, 2009; FCN, 2009).

Finally, several interviews were conducted to collect expert knowledge from domain specialists covering various aspects of the bread chain, from health and organoleptic concerns to millers' and bakers' technological or economic concerns.

Argumentation models

Argumentation is a reasoning model based on the construction and evaluation of interacting arguments. Most of the existing models are grounded on the abstract argumentation framework proposed in Dung (1995). In this framework, an argumentation system is defined by a set of arguments *A*, and an attack relation between arguments *R*. Sets of arguments that « make sense » together are then computed, called *extensions*.

Thereafter, ensuing studies enriched Dung's model with complementary features, such as the consideration of preferences among arguments, expressing that some arguments may be stronger than others, or the consideration of contexts (see Bourguet et al., 2010 for a comparison of models).

Classically, the argumentation process follows three main steps : 1) constructing arguments and counter-arguments, 2) evaluating the acceptability of the different arguments, and 3) concluding.

Results

Argument Inventory and Formalization

In this case study, policy decision consists of global recommendations aimed at changing the type of flour used in the common French baguette bread sold in bakeries and retailed in institutional or school catering. The PNNS recommends to develop the consumption of breads made with more whole wheat flour, such as 80-type flour, instead of the 65-type currently used (i.e., containing 0.80 g of minerals per 100 g of flour on a dry basis, instead of 0.65 g per 100 g). The recommendations are mainly supported by nutritional arguments, related to increasing fibers, and buttressed by economic arguments related to increasing yield of raw material extraction (wheat).

Two alternatives can be pointed out : change common bread to 80-type flour (denoted by T80) or keep 65-type flour (denoted by T65). Table 1 lists the PNNS arguments, which take into account different concerns (Nutrition, Technology, Economy), pursue several goals (%Fibers, %Micronutrients, Process Skills, Costs) and is in favor of the T80 option.

Table 1. Part of PNNS argumentation.

	Stakeh.	Reason	Action	Concern(s)	Goal(s)
1	PNNS	"Using 80-type flour (T80) instead of 65-type flour (T65) for global breadmaking is relevant."	$\curvearrowright$ T80	Nutrition	$\nearrow$ Fibers $\nearrow$ Micronutrients (μnut.)
2	PNNS	"T80 reduces costs due to an increased milling yield."	$\curvearrowright$ T80	Technology Economy	$\searrow$ Process Skills $\searrow$ Costs
3	PNNS	"High-fiber diet reduces the public health costs."	$\curvearrowright$ T80	Economy	$\searrow$ Costs
4	PNNS	"Raising the daily T65 consumption involves increasing salt intake in the diet."	$\curvearrowright$ T80	Nutrition	$\searrow$ Salt

However, these arguments are hampered by other viewpoints and strong reserves on behalf of the concerned wheat processing stakeholders. For instance, baker and miller professionals are apprehensive about possible impacts on their core activities. The French milling profession is pushing for a reconsideration of the PNNS recommendations. A scientific report investigating nutritional impacts of 80-type flour was used. In Table 2, we list arguments from millers' profession, which take into account new concerns and support the conservative option (Action = T65) or a reconsideration of the recommendation (D. for "debranning", O. for "organic").

Table 2. Part of millers' argumentation.

	Stakeh.	Reason	Action	Concern(s)	Goal(s)
1	Millers	"Raising the flour extraction rate causes an increase in flour contaminants."	⟲ T65	Sanitary	↘ Mycotoxins ↘ Pesticide Residues
2	Millers	"Wheat pretreatments (such as debranning) could decrease mycotoxins."	↷ T80 & D.	Sanitary Technology	↘ Mycotoxins ↗ Process Skills
3	Millers	"Wheat pretreatments increase process costs."	⟲ T65	Economy	↘ Costs
4	Millers	"Making organic bread allows to avoid pesticide residues."	↷ T80 & O.	Sanitary Economy	↘ Pesticides Residues ↗ Segmented Supply
5	Millers	"Raising flour extraction rate causes a rise in phytic acid."	⟲ T65	Nutrition	↘ Phytic Acid

Other arguments, in particular from miller and baker professionals, are not presented here for space reasons.

Argumentation-based decision model

We propose an extended decision framework, which takes into account a set of arguments *A*, a set of concerns *C*, a set of actions *D* (for « Decisions »), a set of (ordered) goals *G*, defined as follows.

***Definition 1**:* An extended argumentation-based decision framework is a tuple $(A,C,D,G,\geq,\alpha,\gamma)$ where:

- $C = \{c_1, \dots, c_n\}$ is a set of concerns;
- *A* is a set of arguments, divided into several subsets $A_1, \dots, A_n$ of arguments that are expressed in the concerns $c_1, \dots, c_n$ respectively;
- *D* is a set of mutually exclusive actions;
- *G* is a set of goals;
- $\geq = \{\geq_1, \dots, \geq_n\}$ is a set of (preorder) relations on G. Each $\geq_i$ defines a preference ordering of the goals G, that applies for the concern c_i;
- α is a function: A → D that associates each argument with an action;
- γ is a function: A → G that associates each argument with a goal.

Based on this definition, the attack relation R is then computed in the following way: for a given concern, an argument *a* attacks an argument *b* if and only if their actions are mutually exclusive and the goal of *b* is not preferred to the goal of *a*. This is formalized by Definition 2.

***Definition 2**:* Given an extended argumentation-based decision framework $(A,C,D,G,\geq,\alpha,\gamma)$,

$R = \{R_1, \ldots, R_n\}$ is a set of attack relations, respectively defined on $A_1, \ldots, A_n$ such that:

$$\forall (a,b) \in A_i^2, [(a,b) \in R_i] \Leftrightarrow [\alpha(a) \neq \alpha(b) \text{ and } (\gamma(b),\gamma(a)) \notin >_i].$$

For each concern, arguments and attacks are now defined and can be evaluated as in a classical Dung's system.

Case study output: an illustration

To use the proposed model, the following steps are successively performed:

1. Obtain a representation of all arguments, with their associated stakeholders, concerns, goals and actions.
2. Define preference relations between goals for each concern, according to their prioritizations.
3. Deduce the attack relation between arguments.
4. Compute the decisional resolution which leads to recommending one or several actions.

In this example, we propose to deal with sanitary concerns. Different preferences and the corresponding output recommendations are summarized in Table 3. The two recommendations "debranning wheat flour" (T80 & D.) and "organic bread" (T80 & O.) can be aggregated into a single recommendation "debranning and organic bread" (T80 & D.O.) since both actions are compatible. In the economic concern, this output can be counterbalanced. For instance, none of these actions is recommended when reducing costs and increasing benefits are preferred.

Table 3. Different preference scenarii and associated outputs in the sanitary concern.

Preferences	Recommended Action(s)
$\searrow$ Mycotoxins $\geq$ $\searrow$ Pesticide Residues	$\circlearrowright$ T65, $\curvearrowright$ T80 & D.
$\searrow$ Pesticide Residues $\geq$ $\searrow$ Mycotoxins	$\curvearrowright$ T80 & O.
$\searrow$ Mycotoxins $\approx$ $\searrow$ Pesticide Residues	$\circlearrowright$ T65, $\curvearrowright$ T80 & D., $\curvearrowright$ T80 & O.

Conclusions

As with any policy action, decision makers rely on arguments from relevant concerns (health, economy, service, etc.) to recommend a decision with positive impacts. Thereby in the PNNS public policy, preferential concerns are health and nutrition, nevertheless secondary concerns such as processing, economy or hedonism also appear in several assessments. The approach described in this paper consists first in formalizing real world arguments and secondly in proposing an extended argumentation-based decision framework. The case study represents an original approach in the A.I. field and an introspective approach in the agrifood chain field.

Future trends in decision support tools involving argumentation methods should be a relevant way to help the stakeholders eliciting and formalizing arguments, which would make them more involved in the decision process and would facilitate interactions between all the stakeholders. Such a decision support system can also be of interest to target a food product for a given (and not a global) segment of consumers. More generally, arbitration-driven argumentation is a promising approach to help humans make well balanced decisions, considering for instance the three pillars of the sustainability concept (social, environmental and economic).

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Knowledge Engineering, a useful tool for integrating food chain

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Abstract. *Issued from cognitive sciences, computer sciences and applied mathematics, Knowledge (K) Engineering encompasses modelling and can be roughly defined by three steps: acquisition of available K, representation of acquired K and computational use of represented K for simulation, validation and optimisation purposes. These different steps are illustrated for various applications to food industry like the durum wheat chain, dough mixing for breadmaking, cheese ripening, based on specific approaches like decision trees and conceptual graphs, qualitative reasoning, Bayesian networks and optimisation under uncertainty and multi-criteria flexible querying, respectively. The application of such approaches opens prospects for the virtual design of food products which will be of help for the sustainable production of high quality foods.*

Keywords: bread, cheese, complex system, durum wheat, modeling, multi-disciplinary, multi-scale.

Introduction

Foods are now developped in response to new demands of consumers, concerned by environmental and nutritional issues. An evolution of the know how in food industry is needed, to improve the qualification of the staff and upgrade the technological level of production lines. However, on the scientific side, during food processing, the close interaction between continuous structural changes and transfer mechanisms impairs the complete modeling of coupled physical, chemical and microbiological phenomena. So, despite the increase of scientific papers and the progresses in understanding multi-scale food structural changes, the knowledge is fragmented and incomplete. The whole food processing chain can be viewed like a complex system, like biological ones. We propose to implement tools able to take explicitly into account the fragmented and heterogeneous knowledge available on the dynamics of the process, with uncertainty on the behaviour of the system. Recently, some of these tools (Monte Carlo, Neural and Bayesian Networks, fuzzy logic, expert systems...) have been implemented in various fields, like immunology for instance (Cohen and Harel, 2007). In the frame of the EU-project Dream, these tools are tested for the multiscale dynamic reconstruction of the processes of Generic Model Foods (GMF) by an Integrated Knowledge Model (IKM). GMF are realistic foods, representative of a whole class of foods through variations of process and composition. Cognitive maps of know-how on GMF processing are drawn and integrated with the Basic Knowledge Models (BKM). BKM are the models currently set in food engineering, based on physical laws, chemical kinetics… but also available from expert's rules (know-how), thus to be formalized. The purpose of Knowledge Engineering is to build this IKM and this paper illustrates how it can be applied to the management of food chain processing through the following examples: durum wheat chain, breadmaking, cheese ripening, presented in this order of decreasing sizes of knowledge grain and domain scale, so that the relevant tools may also be described briefly.

Decision support system to manage the durum wheat chain

The need for food security has triggered the development of tools combining models with databases in the area of predictive microbiology like Sym'Previus (Haemmerlé et al., 2007) but, there is no tool available to manage a whole food chain until food products, integrating heterogeneous information sources on nutritional, sensory and technological aspects. Noting the basic role of cereals in the food of mankind, the management of durum wheat products has recently been addressed, taking into account experimental data from literature, and expert statements describing commonly admitted mechanisms in a qualitative way (Thomopoulos et al., 2009). Since this approach is not based on predetermined models, a specific learning technique has been used, namely decision trees.

We have to build a system to handle disparate information presented under various forms (quantitative, descriptive…) and referring to very different domains (processing operations, product quality…). These issues may be addressed by tools for the representation of expert knowledge like the **conceptual graph** model and rules. The latter well illustrate the link "If…then…" , like for instance: "Drying a pasta product in which peroxydase is active will yield a pasta with brown color". Here "drying" is a unit operation and "color" a qualitative variable. These rules can be applied either in forward chaining in order to predict an output result in terms of quality, or in backward chaining to determine the possible conditions that can lead to the expected properties (reverse engineering). The management of the food chain is performed using **decision trees**, envisioned as a collection of rules implementing its different variables. In the decision tree, leaves represent the average value (for a continuous variable) or class (for a symbolic variable), whereas the branches represent the conjunction of inputs that lead to this classification (or value). After the trees have been learnt from the data set, we will use them in their predictive form in order to predict the classification, or average value, from input parameters. The knowledge management system involved 29 unit operations of the durum wheat chain and 56 quality variables characterizing the various families of products (couscous, pasta…). Among those, let us examine the impact of the "cooking in water" operation on the "vitamin content" quality, for which 145 experimental results have been reported from 11 references. Once the most discriminating parameters determined (here type of vitamin), a family of decision trees is generated on the basis of vitamin initial composition and previous processing steps (Fig.1). It provides the average value of "vitamin decrease" (%) as terminal leaves, the box plot below indicates the distribution of this variable around the average value.

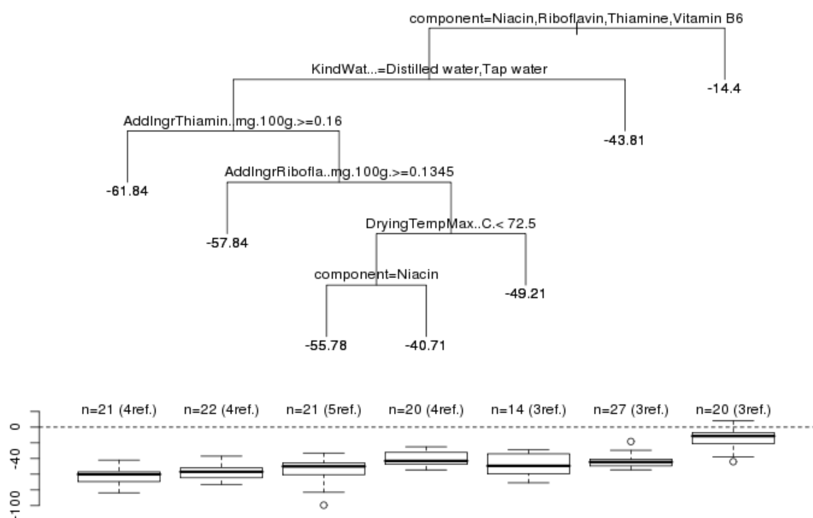


Figure 1: Example of descriptive decision tree learnt from the "cooking in water" data set.

There is a synergy between expert knowledge and experimental data because they complete each other in two ways: (1) a confrontation of both is performed by testing the expert rules using a confidence rate; exceptions to the rule may be identified in order to build new rules (Thomopoulos, 2008); (2) an interactive procedure is proposed (Johnson et al., 2010) to improve the decision tree results through adequate knowledge elicitation.

Formalization of expert knowledge in French breadmaking

French breadmaking has long been a traditional activity relying on craftsman's skills and tacit knowledge. Today, part of know-how is automated and it is also an industrial activity, favoured by the work of breeders and geneticists for stable wheats, involving the risk of supply uniformity and economic dependance for the craft. In addition, causal relations between the physico-chemical ingredients, and sensory and nutritional characteristics of bread according to the process sequence (mixing, proofing ...) remain ill known. The elicitation of tacit knowledge requires a scientific analysis of the processes, but also a knowledge survey from its different actors. A common formalization of these two components allows to build a comprehensive knowledge base, to evidence current practices and investigate future ones. The scientific objectives were to make knowledge emerging on accessible scientific issues and to develop a formal tool for representing it algebraically.

We developed a Q-algebra for writing each set of rules evaluating a characteristic of dough as a **qualitative function.** It has been used to model the states of the dough (1) after 1st mixing and (2) after texturing operations (Ndiaye et al., 2009). The state of the dough (1) is influenced by ingredients characteristics (%flour, water, protein content…). Dough state (2) is defined by 8 criteria, from smoothing velocity to smooth aspect (Fig.2); it is influenced by its consistency (w) at texturing start, by the target temperature at mixing end (x), and by the mixer settings: the difference in linear velocity between the arm and bowl (y) and the expected heat dissipated during texturing (z). These criteria were selected thanks to a glossary on breadmaking available on the Web (Roussel et al., 2010). The functional writing of the set of expert rules allows to calculate the state of a dough according to the state of the inputs of the operation and its settings (Ndiaye et al., 2009). The qualitative determination of the function corresponding to a set of rules is one of the main difficulties of this formalization, a purpose for which an algorithm for automatic determination of qualitative functions is being developped. Once implemeted in the KBS, it allows to determine the states of the inputs of the processing operation (Fig.2).

(a) (b)

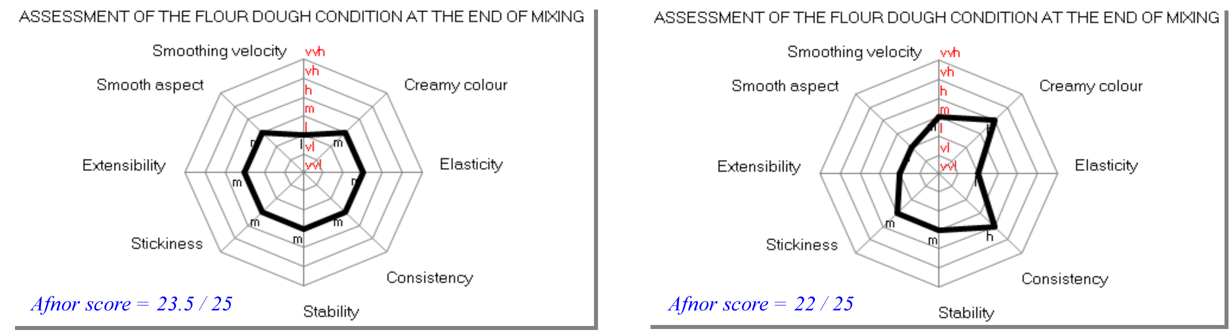


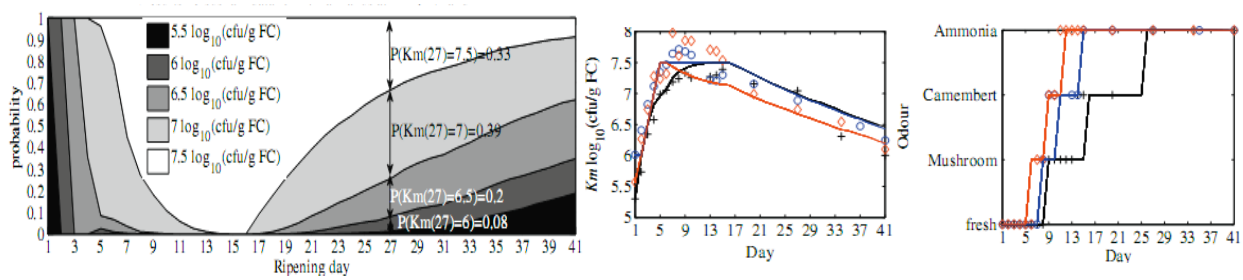
Figure 2: Examples of the KBS outputs: predictions of dough state at the end of texturing, starting from a standard consistency (350 ≤ w≤ 450 UB), a standard target temperature (22 ≤ x ≤ 25 °C), an average difference of velocity y and a heat dissipation z (a) medium and (b) low. Scale ranges from vvh (very excessive) to vvl (very insufficient).

Qualitative algebra is also useful to prospect expert's reasoning in order to build KBS (Kansou et al., 2008), which, in the near future, can be also used to determine the settings of the operation, and the dough composition, that achieve a desired state of dough (reverse engineering) like for the design of composite materials (Michaud et al., 2009).

Modelisation and optimisation of the cheese ripening process

After breadmaking, cheese manufacturing is certainly the most representative area of food industry in France, processing half of milk produced there. In spite of this importance and extensive research, soft cheese like Camembert is an ecosystem and a bioreactor still difficult to assess completely; knowledge remains fragmentary and incomplete and no model provides a comprehensive representation of the process. In this context, we have used **Dynamic Bayesian networks** (DBN) to model the network of interactions occuring at different scales and reconstruct its dynamics (Baudrit et al., 2010). A model of cheese mass loss (Helias et al., 2007) was then 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).

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 marxianu*s Km,…) 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. 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.3 means, for instance, that at the 27th ripening day, Km concentration has a probability of 39% to be $\approx 10^7$cfu/g FC and cannot be lower than 3.10^5.



(a) (b) (c)

Figure 3: 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%.

From DBNs simulations, *Km* mean evolution (Fig.3b), as well as the modal evolution of odour properties(Fig.3c), may be estimated and compared to experimental data. 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.

Viability theory aims at controlling a dynamical system in order to maintain it in a given set of evolutions, namely the **viability kernel**. In the case of cheese ripening, the viability kernel was defined by associating a target on cheese mass at the end of ripening ($\approx$280g) and constraints on microorganisms respiration. It was then computed thanks to a classical heat&mass transfers

(a) (b)

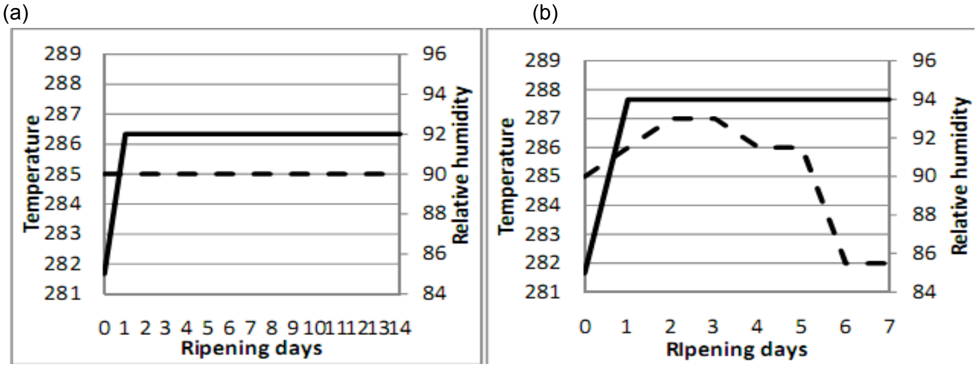


Figure 4: Control (T(K) ---, RH(%) ——) of ripening chambers, (a) conventional in industry and (b) optimal computed applying viability approach.

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). Among the optimal trajectories lowering cost without quality loss, one reached the mass target after 8 days ripening, and the results of its control variations are presented in Fig. 4b, to be compared to the conventional control performed for 12 days ripening (Fig. 4a). 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%). This is an example of application of reverse engineering to a single food processing operation.

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