Multi-Criteria Reverse Engineering for Food: Genesis and Ongoing Advances

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REVIEW ARTICLE

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Multi-Criteria Reverse Engineering for Food: Genesis and Ongoing Advances

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Abstract

Multi-criteria reverse engineering (MRE) has arisen from the cross-fertilization of advances in mathematics and shifts in social demand. MRE, thus, marks a progressive switch (a) from empirical to formal approaches able to simultaneously factor in diverse parameters, such as environment, economics, and health; (b) from mono-criterion optimization to multi-criteria decision analysis; (c) from forward engineering, observing the results of process conditions, to reverse engineering, selecting the right process conditions for a target output. The food sector has been slow to adopt reverse engineering, but interest is surging now that the industry is looking to shift production towards personalized food. MRE has followed a heterogeneous development trajectory and found applications in different disciplines. The scope of this review spans MRE applications in the food sector covering food packaging and food consumption and focuses on demonstrating potentialities of MRE in a complex field like food. We explain how MRE enables the development of sustainable processes, looking at similar approaches used in sectors other than food. Building on this extensive review, we sketch out some guidelines on approaches to be used in future MRE applications in food, working up from the problem statement.

Keywords Multi-criteria quality design · Reverse engineering · Food eco-packaging · Food sensory perception · Multi-criteria food performance

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Introduction

The design and development of sustainable processes and products that integrate technical and economic criteria, satisfy customer demand, and safeguard ecosystems is a major challenge in the wider context of global change (climate change, energy scarcity, rising energy prices, and so on) [1].

In this context, evaluating product quality, from production to consumption and even afterwards to waste management, is a complex process that has historically relied on numerous criteria (nutritional, sensory, practical, and health–hygiene qualities) that are now further completed by emerging concerns, such as environmental impact and economic value. However, these many aspects of quality and shelf life and their various components are not always compatible, and improving them all simultaneously is a problem that has no obvious solution and sometimes no solution at all when contradictory objectives clash, thus posing challenges for decision-making to determine the best trade-offs [2]. In addition, there is growing demand in Global North countries for functional foods, i.e., foods that deliver additional or

enhanced benefits over and above their basic nutritional value. In this context, reverse engineering is a technique for selecting the right process conditions for the design or redesign of foods, food processes, and food-related systems—typically packaging—which we collapse together under the umbrella term "food design." It thus has driven a switch from forward engineering, observing the results of process conditions, to selecting the right process conditions for a target output. Handling this growing complexity requires numerical and computational approaches, which has ultimately led to the emergence of multi-criteria reverse engineering (MRE). Food design has thus switched (a) from empirical to formal approaches factoring in numerous diverse parameters, and conjointly, (b) from mono-criterion optimization to multi-criteria decision analysis, and (c) from studies on the direct effects of processing on end product properties to reverse approaches that start out from food requirements to design or redesign process and product. Furthermore, changes in food requirements driven by the interests of some consumer segments can dynamically impact all consumer segments (less informed or educated sectors, lower-income sectors, etc.). Such effects have been explored in some food-related socio-economic approaches [3–6].

While "reverse engineering" is applicable in various fields, it generally refers to the process that consists in designing manufacturing conditions according to desired end product properties (and not the contrary). In this paper, the end product is not considered to be an existing food product we try to find the way to reproduce, but a virtual ideal one that would have expected properties. The objective is, thus, to find the way to best obtain it, through modeling and simulation. As for "multicriteria reverse engineering" (MRE), the term denotes a reverse engineering process which allows the designer to consider several criteria simultaneously in the desired end product properties, which increases the complexity of the problem. Hence, MRE is an approach to design innovative product manufacturing and to accurately define the problem to be solved, but it is not bound to any restrictive problem-solving model or tool. On the contrary, it may gain from many. This is what the paper aims to illustrate.

This review is not intended exclusively as a comprehensive review but as a primer on the MRE concept in the food sector. Indeed, MRE offers a way to explore a new trend in food processing and food science and to push further ahead in the development of new food. This paper explains and illustrates how MRE has arisen from the cross-fertilization of advances in mathematics technology and shifts in social demands. MRE has followed a heterogeneous development trajectory and found applications in different disciplines, but it is still scarcely considered and applied in the food sector. Here, we take a novel angle by looking at food and life science applications of MRE, with discussion encompassing the specificities involved. After highlighting the pivotal steps that led to MRE (the "Pivotal Steps Toward Multi-Criteria Reverse Engineering" section), we illustrate ongoing advances with two contrasted case studies: MRE for food products (the "Multi-Criteria Reverse Engineering for Food: The Complex Case of Food Organoleptic Properties" section) and MRE for food packaging (the "Multi-Criteria Reverse Engineering for Food: the Case of Food Eco-Packaging Design" section). The "Discussion" section proposes a discussion of the bigger picture based on insight and feedback from various applications, before concluding on a set of guidelines for implementing an efficient MRE approach in the food sector.

Pivotal Steps Towards Multi-Criteria Reverse Engineering

From Empirical to Formal Approaches

The long-term competitiveness of food and bioproduct companies and the general health and wellness of citizens depend on the availability of safe, tasty, affordable, ready-to-use, and eco-friendly products [7]. To meet such expectations, there is a need to merge heterogeneous data in order to develop the necessary decision support systems [8].

The food industry has developed from traditional companies relying on a lot of experience and little innovation to a dynamic industry geared to follow consumer trends [9]. Until recently, food design had relied more on experience than on science, but recent efforts have substantially increased the number of research projects, improved knowledge of the phenomena involved, and drastically rationalized the food sector [10], prompting an explosion of scientific papers and at the same time a need to integrate them into a comprehensive corpus of knowledge. Therefore, there is a pressing need to channel effort into developing the necessary tools and decision support systems. The industry today requires knowledge from its own know-how as well as from integrative approaches and knowledge engineering disciplines. One challenge is to identify and exploit all the key information—and only the key information—from the mass of data available. Today, the value of information comes not from its scarcity but from how it can be contextualized, managed, and integrated into a system to make it available with the relevant features at the right time and the right place [11, 12].

From Mono- to Multi-Criteria Concerns

In food engineering, choices concerning the best characteristics of the end-product rely on various sources and cover different points of view. They include health–hygiene and environmental impact concerns, sensory and nutritional aspects, cost, and, possibly, practicality aspects too (Fig. 1). Moreover, factoring these aspects into a reverse engineering approach means that they have to be technically feasible and economically viable given the skills, knowledge, and profit expectations of the enterprise.
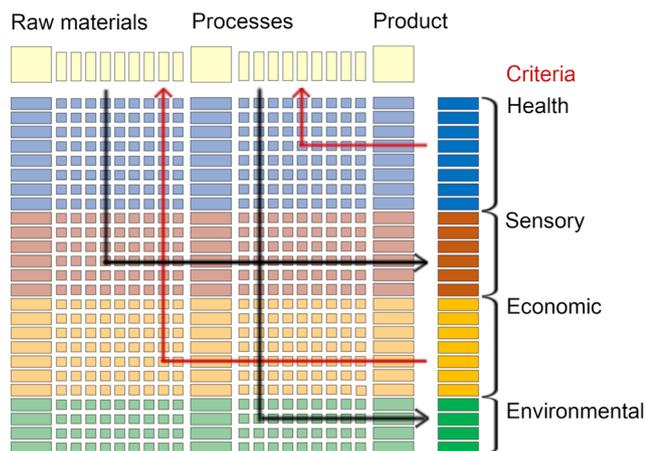
Fig. 1 Illustration of MRE applied to manufacture a product having many and varied qualities. Using various raw materials that undergo numerous processes led to the production of a given product having certain criteria (direct impact, black arrows). MRE is needed to define the processes and/or raw materials necessary to obtain a product having the defined criteria (reverse impact, red arrows)

Studies and syntheses in the economics and management fields, such as [13, 14], address the linkage with enterprise profit expectations. Information sources go from websites, project meetings, expert interviews, scientific articles, and manufacturing practices to consumer patterns, opinions, preferences, and choices, available through online forums, to sales statistics, new marketing trends, and the list goes on [15].

Within the framework of these general criteria (environment, nutrition, etc.), more specific goals are expressed concerning the outcomes expected for the end product. Examples of such goals are "25% increase of soluble fibers" for the nutritional criterion, "keeping pesticide contamination risk low" for the food safety criterion, "no packaging waste" for the environmental criterion, etc. Simultaneously achieving several goals is not always possible and depends, in particular, on whether or not the actions leading to each of these goals are compatible. If they are not compatible, we need to find a compromise, and, so, we look for the "best" compatible sets of actions, which should be deduced from the preferences expressed by the decision-makers on the outcomes.

As an illustrative example, the evolution in the field of operations research, in general, and decision support systems (DSS), in particular, shows a transition from mono-criterion optimization approaches to multiple-objective optimization and multi-criteria decision-making [16]. We distinguish between both in "The Emergence of Compromise Computation" and "The MRE Issue Shared by Sectors Other than Food" sections.

The Emergence of Compromise Computation

Several types of approaches can be referred to as methods for "compromise computation." Here, we look at five of them,

which may be combined to solve a problem. Historically, the first was probably the social choice approach. Its utility value in food-related applications has recently been explored [17]. It is premised on the principle that the food design process should internalize the opinions of all categories of food chain actors, and, so, actors' opinions are computed as votes. The second type of approach, called multi-criteria decision [18], can be broken down into the following two categories of issues: evaluation issues, in which a set of pre-defined alternatives is to be evaluated according to various criteria (environment, cost, etc.), and design issues, in which the alternatives are not defined a priori but have to be found through satisfying constraints (e.g., maximizing digestibility while minimizing energy consumption). In cases where the set of alternatives is large (possibly infinite), mathematical combinatory approaches for optimization are then used, which takes us into the scope of a third type of approach called multi-objective optimization [19]. A recent concern in both multi-criteria decision and multi-objective optimization scholarship is the need to explain and trace the conclusions obtained. Why was a given alternative chosen? Which criteria were best satisfied, and which were left aside? Do all actors benefit equally from the solution? What arguments served for or against each alternative? How did possible compromises emerge from them? This way of reasoning is central to the fourth type of approach, called argumentation theory [20], which has also been explored in food applications [2, 15, 21, 22]. The fifth type of approach for compromise computation becomes relevant in cases where data and/or knowledge describing each alternative is available in a data or knowledge base. It consists in formulating the compromise search problem as a query answering the problem submitted to the data or knowledge base [23]. Preferences are expressed as optional search criteria in the query, whereas constraints are expressed as mandatory search criteria in the query. If the system fails to find a response, meaning that there is no answer that perfectly matches the query, then some of the criteria have to be relaxed until an answer is found. This answer then serves as a candidate for a compromise solution.

From Forward to Reverse Engineering

In agrifood chains, products traditionally go through the intermediate stages of processing, storage, transport and packaging, and reach the consumer (demand) from the producer (supply). As quality constraints have become increasingly critical, several parties are now involved in production process, from consumers to industry players and back to health and hygiene authorities, etc., each defending their own positions and expressing their own potentially conflicting requirements on the final product [24]. This is where reverse engineering, in which it is the demand (and not the supply) that sets the specifications of

desired products and it is up to the supply to adapt and find its ways to respond, can be considered as a way forward [2, 11].

This paper focuses on decision support in the reverse engineering mode and highlights the need for many valued information. Several aspects are considered. Reverse engineering implies a preliminary assumption: having defined the desired outcome of the process. Defining goals for possible outcomes is a complex, multi-actor process based on ubiquitous information. Once identified at best, several alternative scenarios may lead to the desired outcome. Evaluating these alternative scenarios is an early issue. While taking into consideration the positive consequences that the different alternatives will generate, decisions also have to account for possible negative impacts, which are not explicitly expressed in the defined goals. Several examples of such goals, alternatives, and positive/negative consequences are provided on the best technological choices in breadmaking [11, 15]. For instance, the choice of whole wheat products is beneficial from a nutritional standpoint due to the micronutrients and the fibers they provide, but it also implies an increased risk of contamination by pesticides and other contaminants. Another example of methodology for dealing with this type of issue is the CoGUI-Capex approach [25], in which an unexpected food quality defect (e.g., bitterness) is corrected through process solutions and then sorted according to the possible negative impacts on other food qualities (e.g., texture). Thus, the reverse engineering process has to be "bipolar," in the sense that it also factors in undesirable effects.

The previous paragraphs have sketched a picture of advances in MRE applications in the food sector. To facilitate a mental grasp of the array of approaches and tools involved, Fig. 2 gives a global view. The food example presented, i.e., cheese, illustrates the complementary of the different approaches that could be used to obtain a cheese having desired qualities.

Multi-Criteria Reverse Engineering for Food: The Complex Case of Food Organoleptic Properties

Beyond being fit for consumption, food primarily has to cover physiological needs in terms of both energy and macro/micronutrient intake. Nevertheless, environmental constraints are increasingly part of the food product development framework as a factor for ensuring food security and sustainability [26]. The big food sector trend today is towards the concept of personalized food. This paradigm shift implies that once we know the properties desired by the consumer, we want to know how modifying the raw product will affect it and how to restore the original properties via the process.
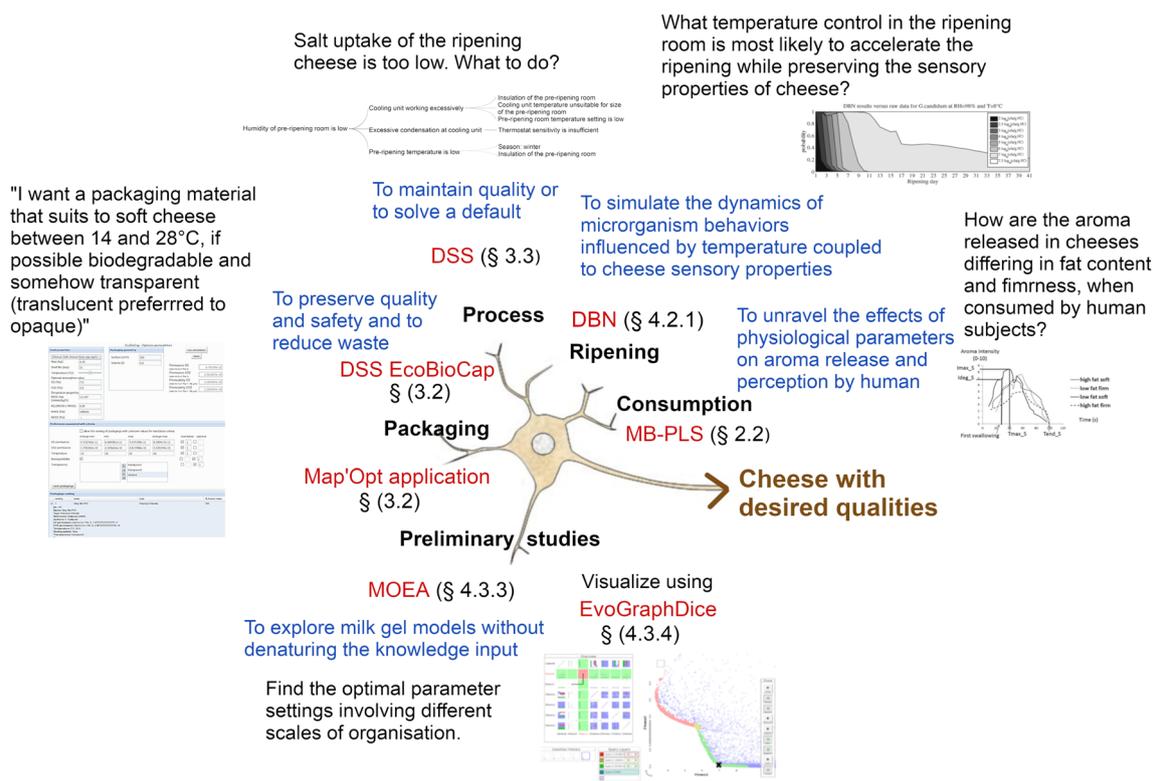

Fig. 2 Overview of the network of approaches usable to obtain a cheese having desired qualities; it is as complex as a neural network. Each tool (in red) has a purpose (in blue) and answers a specific question (in black). All together they contribute to the qualities of the final product. § refers to the corresponding paragraph in the text

The Main Criteria of Food Expectations: Problem Statement

From an evolutionary point of view, the optimization of food intake has been linked to a source of satisfaction. Indeed, pleasure from eating is assumed to be a strong driver of consumption both in terms of food choices and in terms of amount of food consumed [27]. The most important drivers of food pleasantness are the sensory sensations that food procures. For a food product to be consumed, it has to fulfill relevant hedonic values, namely to produce pleasant sensations like, for a cake, sweet taste, smooth texture, and vanilla flavor. As we eat a food, it gets broken down in the mouth, but differently according to the individual's physiology (e.g., mastication abilities, salivary properties), which contributes to the release of the flavor stimuli responsible for sensory perception. The development of food that targets the needs of specific populations therefore has to take these physiological parameters into account [28]. Sensory characteristics need to be critically optimized to ensure actual effective food consumption, which is a prerequisite to the fulfillment of any other criteria—including nutritional or environmental criteria. Nevertheless, the pleasantness of a food product is not driven exclusively by sensory features—the social context of food consumption also plays a role, as does the psychosocial dimension, especially the cognitive representation of food which is gaining importance [29]. The cognitive representation of food is largely modulated by labels or other types of information that cannot be properly assessed during consumption, such as freshness, naturalness, geographic origin, and ethics, among others. Such features, which consumers are now increasingly informed and aware of, may orient the choice of raw materials or food transformation processes and, therefore, become further criteria to be considered within the product development process.

As a consequence, the formulation or reformulation of food products, under nutritional and/or environmental constraints, needs to reversely consider raw materials and/or physiological and cognitive processes that affect the hedonic dimension of the food product, which in turn needs to be optimized to ensure sustainable consumption for a given segment of the population. The application of reverse engineering to food formulation with the objective of tackling nutritional–environmental–organoleptic qualities is, therefore, clearly multi-criteria.

State of the Art

Achieving health objectives, while maintaining food pleasantness, is not an easy target. Different strategies have already been used to reduce fat, salt, and sugar content in food, known to be associated with pleasant sensory sensations. Public health authorities, such as the US Food and Drug Administration (FDA), have taken a stance on the issue [30]. For instance, sugar can be replaced using both sweeteners and bulking agents, with good acceptability from consumers [31].

However, as adding non-nutritive sweeteners often causes off-flavor, an alternative strategy could be to add congruent aroma, using multi-sensory integration principles, or to modify the food microstructure [32]. Several projects have attempted to assess, by a direct engineering approach, the extent to which food composition, especially a decrease in fat, sugar, and salt content to target nutritional guidelines, can affect flavor compound release and perception as well as overall food liking, and then empirically apply reverse engineering to restore the liking by modifying food composition and process.

For example, one study carried out with model cheeses varying in fat, salt, and aroma content clearly showed that the time-course release of aroma compounds was affected by the lipids-to-proteins ratio and salt content as a function of aroma compound hydrophobicity [33]. As aroma perception increased by increasing both fat and salt content, a compromise had to be found between nutritional value and sensory acceptability. As an example, in the TeRiFiQ EU project [34], perceptual interactions between fat and salt perception have been used in a reverse engineering process to restore the food liking of healthier products. It was shown that salt congruent aromas (e.g., Comté cheese aroma), but not carrot aroma, could enhance salty taste perception in low-salt solid-food matrices and low-salt low-fat model cheese [35] and thus compensate for up to a 20% decrease in salt content in this type of food. Nevertheless, the observed compensation effects were dependent on the composition and texture characteristics of the cheeses. The effect of product composition and structure on the aroma-induced salt and fat perception enhancement appeared to be complex and mostly unpredictable, suggesting a combined influence of stimuli release kinetics and perceptual interactions, which would need a lot of data on the direct effect of food composition and process on sensory perception. In these studies, two criteria were simultaneously considered for the development of low-fat low-salt food that keeps sufficient overall flavor to preclude consumer rejection: one was level of salt and fat reduction and the other was the taste and texture properties that dictate the acceptability of a given food product. The data obtained can now be used to formulate this kind of dairy product with a good nutritional value and good acceptability for consumers. However, the relationships between fat and salt that shape food composition are so intricate and different from one product to another that it has not yet been possible to generalize food sensory perception and pleasantness to several types of products.

Moreover, food acceptability is a consumer-dependent variable. In order to better understand the variability in sensory perception and liking between consumers, several projects have set out to unravel the effect of human physiological parameters on aroma release and perception [36]. For example, a statistical multi-block partial least squares (MB-PLS) approach was successfully applied on four model cheeses differing in fat content and firmness, consumed by 48 well-characterized human subjects. The results indicated that all

aroma compounds were released faster from the firmer cheeses when food bolus was more consistent, among which only hydrophobic aroma compounds were more persistent in the breath for high-fat soft cheeses and subjects having a higher amount of product remaining in the mouth after swallowing. Another MB-PLS was conducted to explain sensory perception by in vivo aroma release and physiological parameters on the same cheeses, and 14 subjects [37] showed that in vivo aroma release could not fully explain aroma perception. The fruity aroma was mainly explained by the release of ethyl propanoate before swallowing, whatever the cheese composition. However, the cheese aroma was only partly explained by the release of 2-nonanone after swallowing but was highly impacted by saliva composition and by amount of product remaining in the mouth. It was thus concluded that other sensory perceptions, such as saltiness and fattiness, are expected to influence aroma perception by cross-modal interaction. These results on the effect of human physiology on sensory perception can be used in reverse engineering to formulate foods for specific populations, such as elderly people with low salivary flow [38].

Overall, these results highlighted that sensory perception of food is not a linear combination of ingredients but results from a complex process shaped not only by food composition but also by the consumer's physiological parameters, neurobiological sensory integration mechanisms, and a host of cognitive factors (Fig. 3). All these factors should be considered in the context of MRE designed to optimize food nutritional, hedonic, and sustainability qualities. In fact, MRE can be a powerful way to help food producers engineer personalized food. In food perception, simultaneously mobilizing ME and MRE appears a good way to conceive and design target food.

Integrating Data and Knowledge Ready for Multi-Criteria Reverse Engineering

In the context of food design or redesign under multiple intricate constraints, the MRE problem can be expressed as being the reformulation of the raw materials and processes used to produce a food product, meeting nutritional and hedonic criteria defined for a given segment of the population, possibly completed by safety, price, and environmental considerations if the process change is liable to affect them. To do this, data and knowledge collected in various projects covering complementary issues, such as those mentioned in the previous paragraphs, need to be combined, aggregated, and integrated. A relevant solution to address data and knowledge integration is to use an ontology, which can be defined as a formal common vocabulary of a given domain, shared by the domain experts. This ontology allows multi-criteria querying associating the nutritional and sensory quality of the food product, the transformation process constraints, and the environmental impact of the whole system. As a pioneering example, the BaGaTel database already aggregates data imported from collaborative projects conducted on dairy foods, covering technological processes with their environmental impact (hard cheese, yogurt), food composition and structure, sensory properties, and food bolus properties, all connecting with human oral physiology and nutritional properties (http://plasticnet.grignon.inra.fr/PortailNutriSensAl/). It was built using the PO² ontology [39]. PO² is a food science process and observation ontology dedicated to the eco-design of transformation processes and nutritional and sensory properties in the field of dairy products [33, 35–37, 40–43]. The experimental observations are obtained on a participant (e.g., food matrix or processing
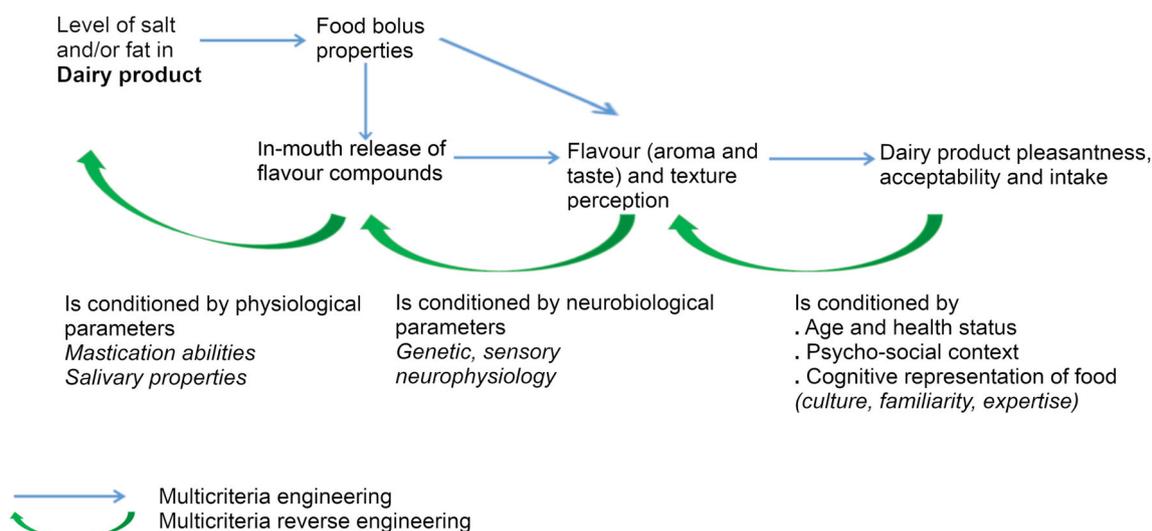

Fig. 3 Food acceptability and sustainable intake are driven by food sensory features and the individual and social context of consumption. Food composition conditions food pleasantness, acceptability, and intake through flavor and texture perception (multi-criteria engineering, blue arrows), which are in turn governed by psychosocial, cognitive, neurobiological, and physiological parameters (multi-criteria reverse engineering, green arrows)

equipment) at different steps of a process (e.g., product manufacturing or the "in-mouth" process) and described by their outputs (data) and the methods used to compute them. The common vocabulary and the structure provided by the PO^2 ontology make it possible to answer different questions related to food formulation in the field of dairy products using data from different projects, in a reverse engineering approach (Pénicaud et al. in revision). This kind of knowledge integration approach, which to our knowledge is the first example of concrete application in the food composition framework, offers a promising pathway for multi-criteria optimization following a reverse engineering approach.

Multi-Criteria Reverse Engineering for Food: The Case of Food Eco-Packaging Design

The Decision-Making Process in the Field of Food Packaging

Packaging is part and parcel of the food product itself: almost all our food products are stored and sold packed in a packaging material which is much more than a simple container or support for marketing and communication. Indeed, packaging is a key element of food preservation, as it serves to prevent and limit the degradation reactions inherent to the biological status of our foodstuffs and which occur throughout the processing, storage, distribution, and in-home preparation steps of the product. The major challenge for food packaging is to preserve food quality and safety, reduce food waste and foodborne diseases, and reduce the wastefully negative burden that producing and distributing uneaten or inedible food has on our environment and economy. Making packaging sustainable also means saving resources by using renewable instead of oil-based resources and mitigating the negative burden of accumulating packaging waste. Multi-criteria decision-making is thus particularly relevant in the field of food packaging to help the user choose a material that complies with numerous requirements and find the necessary compromise between sometimes antagonistic expectations.

Note that in most cases, food is a living product—its cells, the microorganisms it sometimes contains, are continuously metabolizing. The role of food packaging in increasing food shelf-life is principally related to its gas and vapor barrier properties (or permeability) that help shroud the product in an atmosphere suitable for its preservation (e.g., starved of oxygen to slow down metabolism and oxidation reactions) [44]. In the specific case of modified atmosphere packaging (MAP) for respiring products, such as fresh fruit and vegetables, the gas (O_2/CO_2) permeability of the packaging material needs to match the respiration properties of the product [45, 46]. Respiration is an intrinsic food property that differs in rate from one product to another, making it impossible to generalize the use of one

packaging film formulation to every single variety of fruit and vegetables. To avoid having to repeat numerous experimental tests to fit each packaging to a given product, a virtual MAP modeling tool called "Tailorpack" has been developed that computes the evolution of gas composition inside the packaging headspace using Fick's law for permeation and the Michaëlis–Menten equation for gas consumption/production and using packaging and food characteristics as input parameters [47].

When packaging characteristics are unknown, the same model can be used in a reverse manner to identify the window of gas permeability suitable for obtaining and maintaining, at equilibrium, the optimal internal atmosphere for the preservation. This type of modeling tool empowers all food chain stakeholders with a more rational approach to packaging design instead of the prevailing empirical "pack-and-pray" approach. This modeling approach represents a successful advance of reverse engineering in the field of food packaging.

However, the choice of a packaging material for a given application often revolves around more than just its permeability characteristics, encompassing a combination of several criteria including, in addition to permeability, the cost of the raw material, its machinability, its sealability, its environmental impact, type of resource, end-of-life management issues, consumer acceptability, and more. This combination of criteria represents the desired outcomes of the food packaging material selection process. To handle this growing complexity, MRE is indispensable, enabling the development of a tailored answer to a multi-criteria query and finding compromises between antagonistic aspects when necessary. MRE emerges as a promising tool for multi-criteria decision-making in the food packaging field, as illustrated in the following section.

Multi-Criteria Reverse Engineering for Decision-Making in the Field of Food Packaging

MRE could be used to mimic the decision-making process of the human brain and develop decision support systems (DSS) like EcoBioCAP software that help users take the right decision in the field of food packaging [23]. In the subsequent texts, we borrow the EcoBioCAP tool as our main example to show how such tools have been developed at the junction between different fields of expertise, such as food engineering, computer science, knowledge engineering, argumentation, and numerical simulation.

EcoBioCAP is a powerful MRE tool able to answer a complex multi-criteria query such as: "*I want a packaging material that will maintain the quality of strawberries (i.e. with the permeability properties that match the respiration of strawberries), at a cost of less than €3 per kg, and if possible transparent and derived from renewable resources.*" Flexible querying methodologies employed in knowledge engineering were used to develop this tool [48]. EcoBioCAP retrieves respiration characteristics from the product database and uses this data plus other

user-entered characteristics, such as pack geometry, to compute the optimal permeabilities for the product. These permeabilities are automatically considered as mandatory preferences associated to selection criteria for the query, to which are added other mandatory or optional preferences that are determined by the user. The flexible querying module polls the packaging database to retrieve the material that best satisfies the query preferences and proposes as output a ranking of these materials. The DSS can manage both imprecise and missing data [48]. An answer is guaranteed even if no material satisfies the mandatory criteria. This type of tool marks a significant breakthrough, as it had never before been attempted in the field of food packaging.

The first step in the process of building a DSS in the field of food packaging is to develop the numerical program that will serve to compute the evolution of food quality in relation to mass transfers in the food/packaging system. Several mathematical models have been developed that combine mass transfer models (based on Fick's laws) with food degradation models, such as the Mickaëlis–Menten equation for respiration or first-order reactions for oxidation [49]. In addition to the aforementioned Tailorpack application developed for fruit and vegetables, we developed the Map'Opt application for non-respiring products. Map'Opt can predict microbial growth as a function of packaging permeabilities and initial gas concentrations initially flushed in the packaging headspace [50, 51]. The Map'Opt application is used to adjust the packaging material to "the strict minimum", i.e., just those mass transfer properties necessary to maintain the protective atmosphere within a given range of values. This approach is an alternative to that currently used in industry for MAP of non-respiring products, which is based on the by-default use of high-barrier films to be sure of maintaining the protective atmosphere throughout the product's shelf life.

Mathematical models for food engineering do allow some technical outputs to be computed but are not sufficient for decision making in an industrial world where choice of a packaging material is a multi-criteria decision. To take into account this aspect, the EcoBioCAP tool was developed to choose the most suitable packaging material for respiring produce from a dedicated database by answering bipolar multi-criteria querying (currently four criteria considered in the first prototype). Bipolarity refers to the human reasoning that combines information on pros with information on cons to make decisions, choices, or judgments. Some preferences are modeled as constraints for which satisfaction is mandatory, while others are "nice-to-haves" for which satisfaction is optional. Any packaging material that fails to satisfy the constraints is definitively discarded, while preference for a packaging increases the more it satisfies the optional nice-to-haves. It is, thus, natural, in this context, for the querying process to make use of a bipolar approach, since as it can enable to handle compound preferences made of mandatory conditions and optional conditions.

Practical Implementation and Description of the Tool

The DSS was implemented as a web application accessible at http://pfl.grignon.inra.fr/EcoBioCapQuerying/. Short demo videos are available for download at http://umr-iate.cirad.fr/axes-de-recherche/ingenierie-des-connaissances/themes-de-recherche/ecobiocap-dss.

The application interface is made of three parts as presented on Fig. 4:

– The upper part is dedicated to the permeability simulation and can be used to set the fresh food and packaging parameters. It plugs into the product database to retrieve the characteristics associated with the selected fresh food. Figure 4 (upper part) displays the optimal permeability properties for a soft cheese from raw ewe's milk, computed by the DSS, for a shelf life of 21 days in ambient temperature (20 °C), a food mass of 0.25 kg, a volume of 0.5 l, and a surface area of 350 cm^2.

– The middle part allows the user to express his/her preferences. In this version, the user can specify his/her preferences on O_2/CO_2 permeabilities, storage temperature, biodegradability, and transparency of the packaging material. The text of the multi-criteria querying shown in Fig. 4 would be: "*I want a suitable packaging material for my product, a soft cheese from raw ewe's milk (e.g. its O_2 and CO_2 permeabilities match the soft cheese requirement) for a 14 °C–26 °C temperature range and is ideally biodegradable and translucent or transparent.*" Note that the optimal permeabilities computed by the DSS are automatically replicated in the middle part with a predefined deviation for the min–max and enlarged min–max intervals. These values correspond to the fuzzy preferences associated with permeabilities as presented on Fig. 5 and can be modified by the user before launching the querying of the packaging database. The use of fuzzy preferences allows to deliver a set of discriminated answers, which are ranked from most to least preferred.

– The lower part is dedicated to the result of the query, as shown in Fig. 4, again in the case of soft cheese. Note that, in this example, the process can rank the packaging with unknown values for mandatory criteria (the highest percentage of known values in the ranking is 60%).

Discussion

The Brief on Both Cases Studied

In the first case, which includes sensorial and nutritional aspects of food, expressing the properties expected from the end

Fig. 4 Permeability values obtained in the case of a soft cheese and associated packaging solution fitting all the mandatory criteria and one of the two optional criteria. The upper part is dedicated to the permeability simulation and can be used to set parameters for the fresh food and packaging. It plugs into the fresh food database to retrieve the characteristics associated with the selected fresh food. The middle part allows users to express their preferences on the O_2/CO_2 permeances, storage temperature, biodegradability, and transparency of the packaging material. The lower part is dedicated to the results of the query—for a soft cheese in this example

food product is no trivial task. The need to take into account considerations as complex as cultural impact, inter-individual variations in preferences and needs, and the "dilution" effect of each food product in the whole diet with the huge number of possible and existing combinations involved [52], expressing the expected properties is an ill-defined problem. In this situation, a main input criterion (e.g., nutrition) is generally considered as a priority, after which other criteria are consecutively explored. The multi-criteria integration is thus at an earlier stage of completion, but still addressed through the building of a shared ontology. In contrast, in the second case concerning food eco-packaging, the expected properties of the packaging are well-defined through criteria describing physical properties of the materials, which are themselves dependent on the gas exchange characteristics of the food product considered. In this case, the MRE can be re-expressed as a
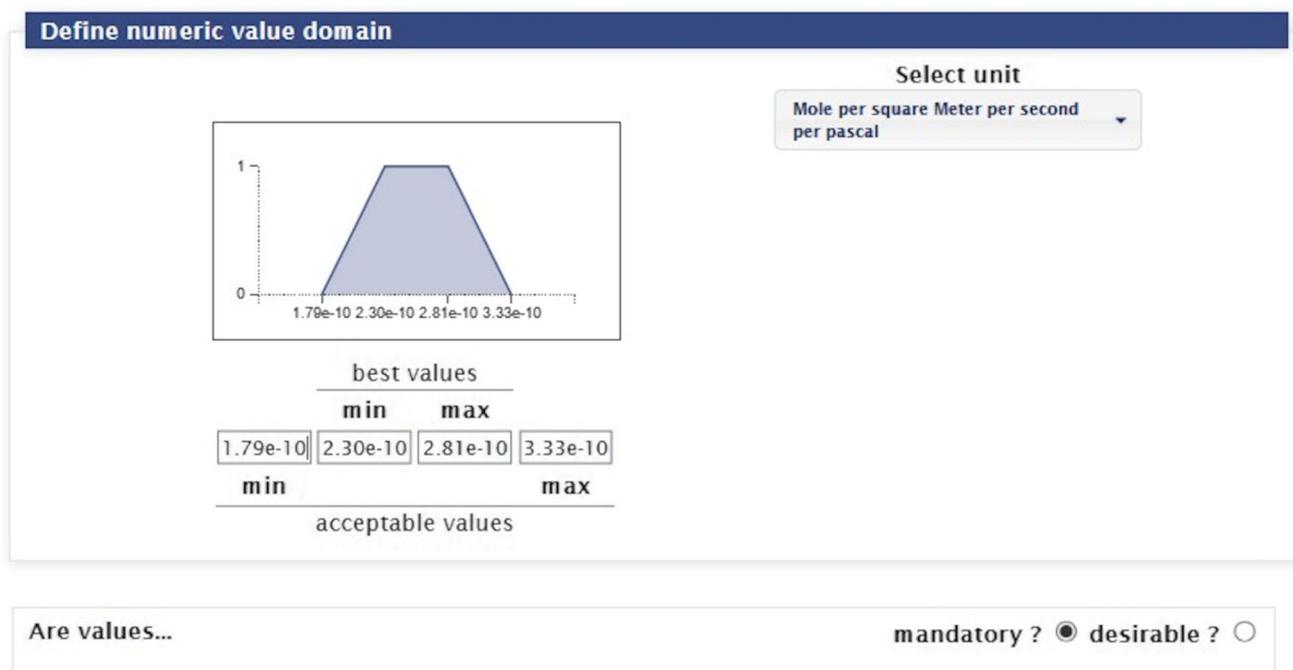
Fig. 5 Fuzzy preferences can be associated with diverse parameters. Here, the fuzzy preferences associated with CO_2 permeability, the fuzzy set "CO_2perm" corresponding to the optimal permeances computed by the DSS and presented on Fig. 4, are presented

query-answering problem and handled through an advanced search engine that distinguishes between constraint- and preference-expressing search criteria.

This highlights the linkage between MRE and data management issues. One way to implement MRE in the food sector is to take data management into account. Indeed, a DSS is nothing without its data, which are input parameters for the system to provide answers to the question asked. In order to design MRE systems, data management is required to parameterize numerical models. If numerical models are not available, we have to reason based on what data there is, by using database as well as descriptive data (e.g., text) querying techniques for example. Data sources in the food domain are heterogeneously structured and notoriously scattered. To break this deadlock, a recent initiative aims to gather shared vocabularies and data structures into a common open repository [53]. Other initiatives aim to adopt shared vocabularies and data structures for specific agriculture subdomains (see for example [54] for the wheat community). This effort has prompted proposals for new open data platforms implementing FAIR—a set of guiding principles to make data Findable, Accessible, Interoperable, and Re-usable—to re-use and manage these shared vocabularies and data structures [55, 56]. Before re-using data, it should first be assessed for data quality. Note that models have already been proposed to assess data-source reliability [57] and have already been implemented in data management platforms [55, 56]. Note too that re-using the huge amount of text-format data in the scientific literature relevant to populating MRE systems remains a

challenging task, although there are proposals to semi-automatically extract relevant data using text-mining tools guided by ontologies [58]. Although the aim of this research is to also apply to complex situations, in real-world case studies, if the problem is too complex and computation time becomes prohibitively long, it is not unusual for practitioners to resort to problem-dependent heuristics, i.e., calculation methods that quickly provide feasible, although not necessarily optimal, solutions [59, 60] or to explore the space of possible combinations with expert knowledge. This point is addressed further in the "MRE Through Multi-Objective Optimization" section.

The MRE Problem in Different Food Sectors

Example of the Cheese Sector

To our knowledge, no real MRE application has been developed before in the cheese sector either. Nevertheless, there has been an effort [25] to rise in collective competence at the supply chains level. A DSS was recently created to link quality and default descriptors with guidelines for maintaining quality or actions to be undertaken to solve the default, all within a decision tree. Moreover, explanatory mechanisms are included in the decision tree in order to make the explicit link between descriptors and guidelines. For example, in the Comté food chain, the default "salt uptake of the ripening cheese is low" may be explained by "low salt uptake after fifteen days" which can be solved by "cheese moistening with

brine." A complete methodology has been proposed in three steps to apply mono-criterion RE to "salt uptake of the ripening cheese is low":

1) Knowledge structuring in decision trees using mind map tools (like the Freeplane open source software for example, www.freeplane.org) based on interviews with domain experts (scientists, technical center engineers, cheesemakers, etc.);

2) Knowledge translation into a knowledge representation formalism that enables automatic reasoning: the conceptual graph model has been chosen, as its graphical representation is easily understandable by non-specialists;

3) Reasoning on the decision trees encoded in conceptual graphs to find the actions associated with a given descriptor and, inversely, to find the descriptors impacted by a given action.

This current application is only a mono-criterion RE app, but the current tools will be almost certainly extended to MRE applications in the near future, as each cheese food chain has to manage a huge number of decision trees (more than 60 just for Comté cheese alone; see Fig. 6 for an excerpt of a decision tree).

Within machine learning models, dynamic Bayesian networks (DBNs) [61] have been used to develop a simulation of the dynamics of microorganism behavior influenced by temperature coupled to the sensory changes of cheese during ripening [62]. DBNs provide a practical unifying mathematical formalism that makes it possible to describe complex dynamical systems tainted with uncertainty. They rely on probabilistic graphical models where the network structure provides both an intuitively appealing interface, enabling humans to model highly-interacting sets of variables, and a qualitative representation of knowledge. Uncertainty tied to the system is taken into account by quantifying dependencies between variables in the form of conditional probabilities. This use of probabilistic networks, known as inference, consists in a query expressed as conditional probabilities. The most common task we wish to solve is to estimate the marginal probabilities $P(X_Q|X_E = x_E)$, where X_Q is a set of query variables to be predicted and X_E is a set of evidence variables which are observed. In the MRE framework, the model established is

able to compute the most likely explanation given observed evidence [63] and to answer questions such as what temperature control inside the ripening room is likely to accelerate the process while preserving the organoleptic properties of the cheeses [62]. More generally, the probabilistic graphical models framework can help guide stakeholders towards strategic decisions and actions.

Example of the Meat Sector

Studies on meat and meat products have clearly recently switched from one-criterion optimization, often on only one product quality during processing, to full multi-criteria decision analysis that combines sensory, health–hygiene, and nutritional product qualities [64]. Indeed, the past ten years have seen a number of very interesting studies based on modeling and on emerging analytical approaches (analytical chemistry, toxicogenomics, etc.), particularly in the field of chemical safety for meat products [64–70]. These studies focused on the whole meat chain, from livestock exposure to micropollutants during farming [67] to meat digestion in the human gut [68, 71]. In terms of processes applied to meat, several papers have demonstrated the relevance of combining analytical techniques, such as multi-dimensional gas chromatography, olfactometry, and mass spectrometry, to investigate both the heat-induced toxicants and odor-active compounds formed when cooking meat [69, 70].

The most successful MRE-type application on meat and meat products was recently developed in the field of dry-cured meat products by Harkouss et al. [72] and Mirade [73] who used Comsol® Multiphysics software to create a 3D multi-physical finite element-based model that predicts proteolysis (i.e., the degradation of meat proteins that determines the final texture of the product), water activity, salt and water content distributions, and total weight loss during the different stages of dry-cured ham manufacture. This "numerical ham" model can also be used to calculate mean values of all the predicted parameters in different groups of muscles previously identified in the ham geometry during its construction, and in the whole ham volume. This numerical model constitutes a multi-criteria numerical tool that can help industrial operators define ambitious technological scenarios, used in MRE to fit expected end-product properties, for the manufacture of low-

Cooling unit working excessively
— Insulation of the pre-ripening room
— Cooling unit temperature unsuitable for size of the pre-ripening room
— Pre-ripening room temperature setting is low

Humidity of pre-ripening room is low — Excessive condensation at cooling unit — Thermostat sensitivity is insufficient

Pre-ripening temperatue is low
— Season: winter
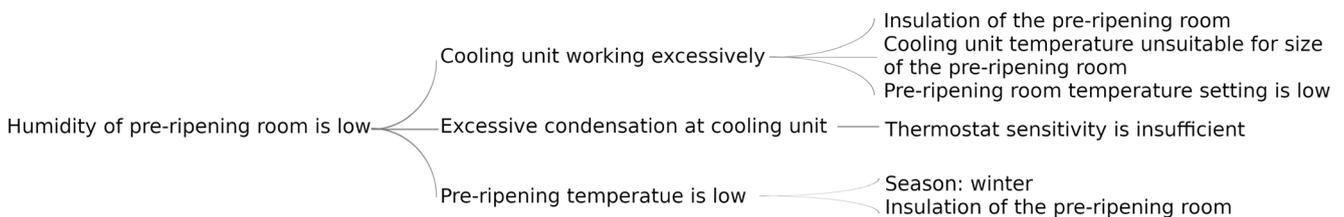— Insulation of the pre-ripening room

Fig. 6 Short excerpt of a decision tree created to link quality and default descriptors with guidelines for maintaining quality or actions to undertaken to solve the default. Here, the guideline to correct the default of humidity of pre-ripening room in the case of Comté cheese is presented

sodium dry-cured hams without impairing final microbial and product sensory qualities. Set with the objective of reducing salt content in dry-cured hams [74] by a 25% cut in duration of the salting stage, this model recently estimated three weeks as the extra time needed to be added to the duration of the low-temperature post-salting stage to arrive; first, at the end of post-salting with the same water activity as for normally salted dry-cured hams and, second, at the end of dry-cured ham manufacture with similar proteolysis and texture values.

Example of the Cereal Sector

In cereal processing, the early "Virtual Grain" system [75] used a database to gather heterogeneous information concerning the properties of cereal grains and the technical and agronomical routes to their production. The aim was to identify influential factors and potential relationships between morphological, biochemical, histological, mechanical, and technological properties that are usually studied separately. The database is connected to statistical and numerical computing tools, notably a wheat grain mapping tool developed using Matlab. Based on wheat grain properties and information on the distribution of wheat grain components, it proposes a local representation of the properties in each tissue. The Virtual Grain project was devised to explain grain behavior during fractionation and, in the longer term, in a MRE approach, to optimize the fractionation process so as to best meet structural and textural criteria in future food products.

In the overlapping domain of breadmaking technology, "Bread Advisor" was a pioneering knowledge software tool for the baking industry [76, 77]. "Bread Advisor," a tool exclusively based on expert knowledge stored in a database, does not propose experimental data or dynamic prediction, but it does provide three kinds of information: text information on processing methods, a list of possible defects and their causes, and generic messages on the effects of process changes.

The cereal sector has built up from these first attempts to develop a mature MRE approach, and is now probably one of the most MRE-advanced food sectors. To illustrate, Thomopoulos et al. [2] proposed a reverse engineering decision support method guided by the objectives defined for the end-products of the food chain. The "reverse" approach is materialized by "backward chaining" logic-based computation and uses argumentation. The maturity of this approach in the cereal sector is demonstrated by the fact that all of the three following aspects, mentioned separately in the "Pivotal Steps Towards Multi-Criteria Reverse Engineering" section, are considered simultaneously:

- Reverse engineering implies having defined a desired outcome of the decision process. This multi-actor process aims to identify several alternative scenarios (e.g., mass consumption vs nutrition-informed consumer) to be considered;

- Besides the positive consequences that the alternatives will generate (e.g., enhanced nutritional value), the decision process also has to anticipate unexpected negative impacts (e.g., safety impacts), even if not explicitly expressed in the defined goals;

- The feasibility of simultaneously achieving several goals depends on their inter-compatibility (e.g., the action "increasing flour extraction rate" improves nutrition but undermines safety). We, thus, search for "best" sets of actions rather than exact answers to the problem [11].

The MRE Issue Shared by Sectors Other than Food

Feedback from Other Application Domains

The term *reverse engineering* often carries a different connotation in sectors other than food, chiefly mechanical engineering, electronics, and computer science. Whereas both food case studies presented start out from the assumption of having information on the process under study, in other contexts, reverse engineering treats a target phenomenon as a black box where only inputs and outputs are considered as observable. Starting from available data defined as combinations of inputs and outputs, these approaches attempt to recreate a predictive model of the target phenomenon with no prior information. For example, most machine learning approaches can be classified as reverse engineering, as they use generic families of models (artificial neural networks, Bayesian networks, decision trees, support vector machines, etc.) whose parameters are automatically tuned to reproduce the phenomenon represented by a given training dataset.

The civil engineering and urban planning sector offers a particularly interesting case, since (a) it also deals with basic needs (housing); (b) it shares common issues regarding multi-criteria, multi-constraints, multi-stakeholders, and uncertainties; (c) some criteria are common (like pollution, energy consumption, cost, and security) while others share a common goal with the food sector, but translated in a different form (sensory/comfort, nutritive quality/quality of use, etc.); and (d) participatory approaches and consultation are well-developed. Moreover, reverse engineering is also required. Indeed, building design traditionally relies on a forward-path process in which a first design is made by an architect based on expert rules, then progressively refined by engineers, and the final building design is assessed against various different criteria using physical model simulations (mechanics, thermal, acoustics, and so on). However, this process makes it difficult to ensure optimality or even relevance, because each decision is taken locally without

considering the final global performance. To address this problem, researchers have proposed various methods and approaches, often in combination, from multi-objective optimization [78, 79] and multi-criteria decision support [80, 81] to network visualization [82], model reduction [83], and Bayesian networks [84]. A more complex variant of this problem is maintenance/refurbishment in a real property context, which adds uncertainty on the initial state and combinatorial issues, since different unitary actions can be proposed for each building, leading to an exponential set of solutions. The scholarship has proposed solutions based on multi-objective multi-dimensional knapsack optimization [85], typological analysis [86], and multi-criteria interactive approaches [87] which exploit interactivity in order to keep the goals to be reached by the decision-makers constantly in focus throughout the process and thus succeed in meeting the MRE objective. This domain also provides different approaches for participatory decision-making (notably in urban planning), i.e., dialog-based [88, 89], multi-criteria [90], and argumentation [91]. Although these approaches were developed in the area of civil engineering and urban planning, most of them can be transposed to the food sector and thus add to the researcher's arsenal for addressing the MRE issue (Fig. 7).

MRE Through Multi-Objective Optimization

In the field of computer science, but differently from black box approaches, multi-objective optimization can be an effective approach when dealing with multiple contrasting objectives to be simultaneously satisfied. As they usually stochastically explore the search space of all solutions, multi-objective optimization algorithms require support from explicit mathematical models (empirical or principle-driven) relating inputs and outputs, to evaluate every candidate solution with regard to all the considered objectives. While traditional optimization methodologies focus on finding the best values to maximize (or minimize) a single objective, multi-objective optimization focuses on obtaining a set of non-comparable compromises comprising a Pareto front ("non-dominated" solutions) and leaving the final choice to the user. However, finding the Pareto front for a given problem is no trivial task, and the best attainable result often remains an approximation. Multi-objective evolutionary algorithms (MOEAs) [92] currently represent the state of the art in multi-objective optimization, with NSGA-II [93] the most prominent, being implemented for several programming languages, from MatLab to C++ to Python (see, for example, http://pythonhosted.org/inspyred/ for a Python implementation). MOEAs thus count as a promising family of algorithms for computing MRE. Starting from a set of randomly generated solutions, a MOEA will create new candidate solutions for the problem, randomly changing and merging the existing ones. Ideally, the MOEA will push the solutions far apart in the objective space, in order to explore the compromises as far as possible and eventually approximate the Pareto front. MOEAs have successfully been used in multiple real-world problems, ranging from the optimization of thermal sterilization in food processing [94] to the selection of materials for sustainable products [95] and on to the exploration of milk gel models [96]. In this milk gel application, the learning task was to find the optimal parameter setting for a complex model involving different scales of organization of a milk gel: from the nanoscale of a whey protein to the macroscale of a network of colonized fat droplets. Combining multi-objective optimization with a visual exploration of the model offers an
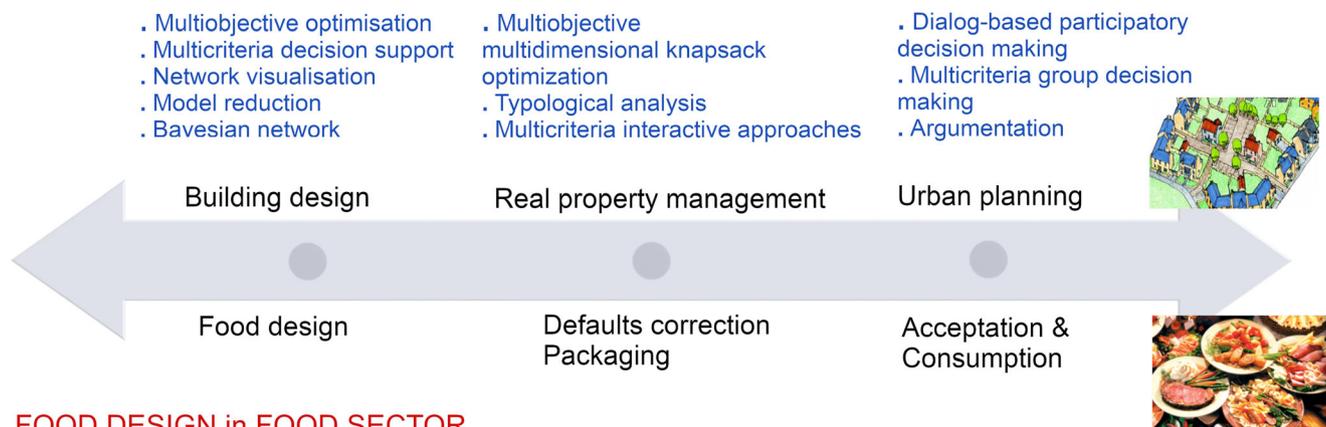
Fig. 7 Presentation of the methods and approaches (in blue) developed to ensure relevance for decision-making in civil engineering and which can be transposed to the food sector, as well in direct as reverse engineering

interesting exploration of this complex food model, and a way to simplify it without denaturing the knowledge input.

Interactive Visualization for MRE

As mentioned previously for several families of models, visual exploration offers the advantage of facilitating human intervention in MRE, which is often necessary as even today, decision-making remains an essentially human task: for example, while Pareto fronts are generated automatically, the final decision on what makes the best solution is left to the human authority. Due to the complexity of the search space in the presence of multiple objectives, interactive visualization can help humans navigate this trade-off space and act as a DSS.

To this end, the EvoGraphDice [97] visualization tool was used to explore the Pareto front of a wine fermentation model [98]. In this case, domain experts were interested in finding fermentation control strategies to obtain a target aromatic composition, while minimizing the amount of energy required to regulate the optimum temperature. The methodology consisted of bringing together experts from agronomy, modeling, optimization, and visualization domains in order to interactively explore the fitting of the model on a large tactile display. There are a number of visualization techniques available for multi-dimensional Pareto-optimal fronts [99], but the EvoGraphDice approach stands out as it enables domain experts to explore competing objectives and articulates new requirements with regard to the underlying model, the optimization constraints, and the visualization software. More generally, the dynamic confrontation of model simulations, multi-objective optimization, and visualization offers interesting perspectives for exploring, validating, and, ultimately, tuning MRE-implementing models.

Conclusion

This conclusion starts by sketching out a set of guidelines for setting up an efficient MRE approach in the food sector. The guidelines are structured in three key steps, and their associated questions, for practical implementation of a MRE approach.

    1st step   Problem statement: Setting the objectives and the scope of the study.

1) What is the food product, or part of it, to be optimized?
2) What is the target population of the MRE process?
3) Which criteria are considered? What are the variables describing them? Are they numerical or qualitative?

4) What data are available, and what data are missing, on the expectations of the target population for the considered criteria?
5) Are there any food formulation alternatives already envisioned?

2nd step   Identification of the method(s) to be used.

1) Are numerical models of the variables to be optimized available? If so, multi-objective optimization could be a candidate method.
2) Are descriptive data of the variables to be optimized available? If so, database querying could be a candidate method.
3) Can the variables be predicted from existing data? If so, machine learning approaches could be candidate methods.
4) Have opinions of the target population and/or other stakeholders been expressed on certain food alternatives and their associated variable values? If so, multi-criteria decision-making and social choice approaches could be candidate methods.
5) Have stakeholders provided explanations for their preferences? If so, argumentation theory could be a candidate method.

3rd step   Model analysis.

1) Provide a synthetic presentation of the different outcomes of the model.
2) Compare and discuss them: do some of the alternatives considered make innovative solutions?
3) Study how the model outcomes support/undercut stakeholders' expectations.
4) If possible, iteratively determine new cases to be modeled.
5) Identify how these assessments help improve food materials and process reformulation.

There are several cues and clues that MRE holds great promise for the future and is likely to develop further in the coming years and in various disciplines. On one hand, there is rising demand for multi-performance products, which designers have to respond to, creating a need for MRE tools. On the other hand, MRE seamlessly aligns with the booming open data initiatives as well as big data acquisitions that make the necessary data available.

Managing food quality issues hinges on simultaneously accounting for various criteria, whereas meeting target consumers' expectations hinges on defining the desired characteristics of the end product first. Since this is exactly the scope of MRE, the approaches proposed are expected to meet the needs of food industries and food chain

stakeholders, enabling both to move forward. With the forthcoming provision of standardized tools, it is, thus, more than likely that food sector enterprises will use MRE and will have the capacities to reap the benefits.

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