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Relating transformation process, eco-design, composition and sensory quality in cheeses using PO^2 ontology

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ABSTRACT

To provide answers to sustainability challenges, a database called BaGaTel, guided by the PO^2 ontology, has been built to integrate data to reformulate dairy products taking into account nutritional and sensory properties together with environmental concerns. In this paper, BaGaTel was queried to address questions dealing with the eco-design of hard cheese processing, in relation to composition, sensory quality and rheological properties. For the formulation of hard cheese, BaGaTel made it possible to estimate missing data in a dataset supposing that samples have common characteristics. For environmental concerns, BaGaTel gave hints about relevant data that need to be acquired and made possible the estimation of missing data. The common vocabulary and structure provided by the PO^2 ontology allowed combining and integrating into BaGaTel data from different projects, giving relevant answers to different questions, and therefore proving its suitability as a support tool for multi-criteria assessment of food systems.

1. Introduction

The food processing sector is facing sustainability challenges of growing complexity, such as global warming, the increase in overweight, obesity or population ageing. These problems, while having a tremendous impact on populations, urge the food industry to develop new strategies to formulate well-balanced products in terms of nutritional requirements (e.g., less fat, sugar and salt), animal/vegetable protein supply and sensory acceptability by consumers, while using eco-friendly transformation processes. In this paper, we will focus on dairy products, which have been reported to have a high environmental impact (Weidema et al., 2008) and more specifically cheeses. Cheeses have a variety of compositions (e.g., different fat and protein types and content), structures (i.e., from liquid to solid) and micro-structures (e.g., fat droplets, protein networks), which open up many reformulation opportunities for their production. However, even if a lot of studies have been conducted on dairy products, considering on one hand the environmental impact of food processing and on the other the nutritional and sensory quality of foods, there is no integrated study combining all these data.

To tackle this challenge, data and knowledge from different domains in science (e.g., nutrition, sensory perception, eco-design, microbiology, biochemistry, process engineering) need to be combined with data and knowledge from environmental analysis.

The environmental impact of food and food processing is seriously questioned. Food products have been reported to contribute to 20–30% of European environmental impact (Tukker et al., 2006). Life Cycle Assessment (LCA) is a standard method (ISO 14040:2006; ISO, 2006) that allows quantification of the environmental impacts of a product, process or service during its whole life cycle, and it is widely applied to food systems (Roy et al., 2009) and more specifically on semi-hard cheeses (Berlin, 2002). However, environmental impacts are more frequently related to the mass of food produced than to its quality, which can lead to ineffective and even counterproductive eco-design process options (Igos et al., 2013; Pénicaud, Monclus, Perret, Passot, & Fonseca, 2018). As an

example, Berlin (2002) suggested that the environmental impact of semi-hard cheese should be reduced by decreasing the wastage of the milk, but this could affect quality of the cheese.

There is thus a crucial need to take into account relevant parameters of food quality in any environmental impact assessment. Product quality can be assessed by taking into account its sensory quality, for instance. Sensory quality is the result of all the sensory modalities (i.e., aroma, taste and texture) perceived during the physiological process necessary for in-mouth food breakdown and varies with product formulation and technology. Relationships among food composition, structure, sensory properties and food breakdown in the mouth have already been investigated by in vivo and/or in vitro studies conducted on dairy products (Doyennette et al., 2011; Guichard, Repoux, Qannari, Laboure, & Feron, 2017; Lauverjat, Deleris, Trelea, Salles, & Souchon, 2009; Lawrence et al., 2012). However, these studies were conducted on different dairy food products, did not measure the same parameters and did not take into account environmental parameters. It is thus difficult from these data to link quality assessment to environmental impact. The obtained data are also difficult to compare because of (i) their heterogeneity (e.g., qualitative data such as flavour perception versus quantitative or semi-quantitative data such as energy consumption), (ii) their measurement scales (e.g., micro-structure of product vs impact of the whole system on global warming) and (iii) their evolution over time: some measured properties may change over time through the different unit operations for production (e.g., content in unsaturated lipids), whilst others do not (e.g., process working conditions).

In addition, data are generally acquired during a specific research project, for a given food product and are focused on specific parameters. Because of natural variability of food products, it is hard to directly compare two products coming from different projects. Moreover, one project may not produce a great number of measurements: a standard experimental procedure is usually based on triplicates, which is relatively low from a statistical point of view. Besides, data coming from a specific project are generally stored in laboratory books and/or on personal computers of the persons involved in the project, and not widely shared with the scientific community.

The great challenge is thus to combine, aggregate and integrate all data and knowledge that have been collected in different projects covering specific domains. Data heterogeneity, their multi-scales dimension, sparseness and their evolution over time through different unit operations of the production process represent important bottlenecks. Moreover, expert knowledge is often implicit and difficult to acquire. Nevertheless, data and knowledge storage and integration enriched with the bibliographic data is of utmost importance for sustainable process development.

To address data and knowledge integration, a relevant solution is the use of an ontology (Doan, Halevy, & Ives, 2012). Ontology is defined as a formal common vocabulary of a given domain, shared by the domain experts. Ontology is designed to represent the knowledge from one domain in terms of concepts, relationships among these concepts and instances of these concepts (Guarino, Oberle, & Staab, 2009). Moreover, publishing ontologies on the Linked Open Data (LOD) cloud (http://linkeddata.org) and building networks of interconnected ontologies (Suárez-Figueroa, Gómez-Pérez, & Fernández-López, 2012) facilitate data integration and data sharing, such as giving access to data from specific disciplines or data produced within specific geographic regions (Bizer, 2013).

In the food and human nutrition domain, eleven ontologies are listed on the portal providing the map of agri-food data standards (http://vest.agrisemantics.org), a recent initiative within a GODAN (Global Open Data for Agriculture and Nutrition) Action project (http://www.godan.info). For instance, Food Track & Trace Ontology has been developed for traceability purposes, with the aim of being connected with a global track and trace information system (Pizzuti, Mirabelli, Sanz-Bobi, & Gomez-Gonzalez, 2014). This ontology has been extended into MESCO (Meat Supply Chain Ontology) for supporting the management of meat traceability along the whole supply chain, from farmer to final consumer (Pizzuti, Mirabelli, Grasso, & Paldino, 2017). Another example is the OFPE (Ontology for Food Processing Experiment; Muljarto, Salmon, Neveu, Charnomordic, & Buche, 2014) dedicated to food processing experiments and reused in AFEO (Agri-Food Experiment Ontology; Muljarto et al., 2017) to guide data integration in viticulture and winemaking. Moreover, close to environmental concern, a decision support system has been created to allow the use of data found in the literature

116 to assess environmental sustainability of biorefinery systems (Lousteau-Cazalet et al., 2016). This
117 couples ontologies, soft computing techniques and environmental factor computation. However,
118 none of these ontologies was suited to represent a food transformation process described by a set of
119 experimental observations available at different scales and changing over time through the different
120 unit operations of the production process. Only such an ontology would permit handling of multi-
121 criteria indicators associating the quality of the food product, the transformation process constraints
122 and the environmental impact of the whole system.

123 With this objective, our collaborative network gathering scientists in food process, oral
124 physiology and sensory perception, eco-design and computer science, built a first ontology for the
125 eco-design of transformation processes (Dibie, Dervaux, Doriot, Ibanescu, & Pénicaud, 2016). This
126 ontology has been extended to PO², a process and observation ontology in food science (available at
127 http://agroportal.lirmm.fr/ontologies/PO2/), to integrate data for the formulation of dairy products,
128 taking into account nutritional and sensory properties (Ibanescu, Dibie, Dervaux, Guichard, & Raad,
129 2016). A database, called BaGaTel, structured by the PO² ontology has been built, hosted by the
130 PLASTIC platform of INRA (http://www.pfl-cepia.inra.fr). Data from different sources (e.g.,
131 experiments, papers, databases) are manually annotated with concepts and relations from PO²
132 ontology and are thus stored into specific EXCEL files that were previously designed according to the
133 structure of PO². Data from EXCEL files are uploaded into the BaGaTel database. Once the ontology
134 has been built, the specific vocabulary has been fixed, and the data and knowledge collected have
135 been integrated in a common database, the question of their querying and analysis for decision
136 support issues can be addressed.

137 The database and the vocabulary of the ontology have been designed for two
138 complementary applications. The first one is to allow researchers in food science to answer research
139 questions. The second is to help food producers formulate food products that answer different
140 constraints (nutritional, sensory, and environmental). The structure of the database and the
141 vocabulary had to be suitable to facilitate the querying of data by both researchers and food

142 producers. The objective of this paper is to demonstrate the ability and the suitability of the
143 developed tools to provide relevant data in response to questions which involve multi-criteria
144 indicators. Several questions in the context of formulation and environmental concerns are
145 addressed.

146 In Section 2, this paper presents the different data available on dairy products in BaGaTel
147 database, and more specifically on hard cheeses, with a focus on the parameters used to formulate
148 the requests. Section 2 also describes briefly PO^2 ontology. Section 3 reports on how the use of
149 BaGaTel database structured according to PO^2 allows answering to specific questions relating
150 process, product quality and eco-design parameters.

151

152 **2. Materials and methods**

153

154 *2.1. Hard cheeses*

155

156 Among dairy products, cheese is widely consumed, especially in Europe and North America,
157 and is the main growth product within the dairy sector (Fox, 2011). Cheese is a fermented food
158 derived from milk. Although cheese making is a linear process, it involves many manufacturing steps
159 and at each step, different parameters can be measured for production control. This makes cheese a
160 very interesting model food product to study to understand and qualify the links among
161 manufacturing parameters, product quality and environmental impact. Considering the fact that a
162 great number of different types of cheese exists, due to the diversity of composition, processes and
163 ripening steps, the present paper will focus on hard cheeses and related model systems.

164

165 *2.1.1. Available data and addressed questions*

166 There are a significant number of research projects conducted on hard cheeses, from which
167 data were successfully imported into the BaGaTel database following the PO^2 structure. Available

168 data on hard cheeses including technical process descriptions and parameters, composition and
169 structure of the studied cheese during different process steps and sensory perception parameters,
170 were collected during the following projects: TRUEFOOD (EU-FP6-FOOD-16264: 2006-2010;
171 https://cordis.europa.eu/result/rcn/46734_en.html); SmartRipe (EU-FP7-KBBE-613827: 2013-2015;
172 https://cordis.europa.eu/project/rcn/111141_fr.html); and PRASEL (Programme de recherche en
173 alimentation sur le sel. French national project 2005-2008). Summaries of TRUEFOOD, SmartRipe and
174 PRASEL projects are provided as Supplementary material files SF1, SF2 and SF3, respectively.
175 Complementary data were imported into the field of in-mouth food breakdown, aroma and taste
176 compounds release and sensory acceptability from projects done on model cheeses similar to hard
177 cheeses (Bigaski Ribeiro et al., 2016; Boisard et al., 2013, 2014; Feron et al., 2014; Gierczynski,
178 Labouré, Sémon, & Guichard, 2007; Guichard et al., 2017; Lawrence et al., 2011; Mosca, Andriot,
179 Guichard, & Salles, 2015; Phan et al., 2008; Tarrega, Yven, Sémon, & Salles, 2008, 2011).
180 These projects covered a wide range of cheese composition (e.g., lipid, protein, salt,
181 microorganisms), technical processes from very simple model systems to real cheese production,
182 cheese structure at different scales, sensory perception (i.e., aroma, taste and texture), in-mouth
183 breakdown (e.g., masticatory parameters, food bolus structure), as well as in vitro and in vivo aroma
184 and taste compounds release.
185 Other data from a process eco-design project (CellExtraDry; Eco-design preservation
186 processes of functional yeast enriched with anti-oxidants. Funded by ANR-IC-Qualiment) were also
187 imported into BaGaTel, covering inputs and outputs used for the transformation processes (e.g.,
188 consumptions and wastes of energy, water, steam) of stabilised micro-organisms, together with
189 quality data for yeasts (e.g., enumeration, antioxidant capacity), the processing conditions (e.g.,
190 temperature, pressure) and resulting environmental impacts computed by LCA. The summary of
191 CellExtraDry project is provided as Supplementary material file SF4. Energy consumption for
192 processes and processing conditions in the case of hard cheeses are also available from TRUEFOOD
193 (EU-FP6-FOOD-16264: 2006-2010) and SmartRipe (EU-FP7-KBBE-613827: 2013-2015) projects.

As not all parameters were measured at the same time on the same cheese sample, the aim of this study is to investigate how and to what extent it is possible to benefit from data integrated from different projects to answer to specific questions. Questions focus on relationships among composition, sensory quality and rheological properties of hard cheeses, and also on their environmental impact.

The first three questions addressed the problem of formulation by combining data about cheese composition during production, sensory quality and rheological parameters. In fact, sensory description and rheological parameters are commonly used in the literature to assess the quality of cheese samples differing in composition and process (Foegeding, Brown, Drake, & Daubert, 2003; Hailu et al., 2018). The last two questions address the environmental impact issue of the production process. The questions were:

Q1. Which hard cheese sample has the highest value for “taste intensity”?

Q2. What is the composition (participant part) of this sample at different steps in the process?

Q3. What are the characteristics (observation part) measured on this sample?

Q4. Which parameters need to be measured throughout the process to perform a LCA of the sample?

Q5. What are the values of the relevant parameters (observation part) needed to conduct the LCA?

2.1.2. Hard cheese production process

Data imported into BaGaTel describe the production of French hard cheeses made from raw cows’ milk in the Franche-Comté region of eastern France. The general outline of French hard cheese production steps can be described as follows (data from TRUEFOOD, 2008). The composition of the milk is analysed (i.e., lipid, protein, lactose and water content) during the *Milk reception* step. Then, a cream separator is used to separate the cream from the skim milk by turning the milk at high speed

220 at the *Skimming* step. During the *Milk standardisation* step, cream and skimmed milk are combined
221 to ensure a standard fat / protein ratio. The *Cooling* step consists of cooling the standardised milk in
222 refrigerated tanks. After pumping into the manufacturing vat, the milk is inoculated with lactic
223 starters during the *Inoculation of the milk* step. During the *Renneting* step, rennet is added to the
224 milk causing milk gelation. Different treatments are then applied to the milk in the vat at the *Step in*
225 *the vat*. To remove part of the whey trapped in the coagulated matrix, the curd is cut, then stirred
226 and heated. Withdrawal of whey is favoured by increasing outlet surfaces and by retracting the
227 matrix. In the *Draining* step, the mass of curd grains is separated from the whey, and put into moulds
228 during the *Moulding* step. During the *Pressing* step, the remaining intergranular whey is evacuated
229 and the cheese is given its final form. The *Demoulding* step consists in removing the cheese from the
230 mould in which it has been set to take its specific shape. During the *Pickling* step, the cheese is
231 immerged in an aqueous solution saturated with sodium chloride. Finally, the cheese is placed in
232 three successive ripening cellars with different controlled temperatures and relative humidities
233 where it is regularly rubbed with salt solution. During this *Cheese ripening* step, fermentations
234 continue and transform the cheese.
235
236 *2.1.3. Sensory description of cheese samples*
237 Sensory taste and texture profiles of cheeses were carried out by different trained panels
238 using conventional sensory profiling (AFNOR, 2009). The main attributes used in this paper to
239 describe the texture are springiness, firmness, granularity, hardness and moisture, while the
240 attributes used to describe the taste are taste intensity, salty, sour and sweet. Their definitions are
241 given in Table 1.
242
243 *2.1.4. Rheological measurements*
244 Rheological properties of the cheeses were determined by a uniaxial compression test at
245 constant displacement rate. Rheological measurements were made with a Texture Analyser TA XT2

246 (Stable Microsystems Ltd). During the test, the sample was compressed at a constant crosshead
247 speed according to its main axis between two parallel plates. Samples were compressed to 80 %
248 maximum deformation at 0.8 mm s^{-1} between parallel plates. Using recorded force and displacement
249 data, engineering stress and Cauchy strain were calculated. From these data, the Young modulus MD
250 (kPa), fracture stress σf (kPa), fracture strain εf (-), and work to fracture Wf (kJ m^{-3}) were determined
251 as described by (Noël, Zannoni, & Hunter, 1996).
252 The Young modulus is an estimation of the apparent elastic modulus and characterises the
253 elastic properties of the cheese. The work to fracture describes the total deformation work up to the
254 fracture. Fracture stress and the work to fracture describe the mechanical resistance of the cheese.
255 Fracture strain characterises the deformability of the cheese.
256
257 *2.1.5. Life Cycle Assessment methodology*
258 LCA can be divided in four steps: goal and scope definition, data inventory, impact
259 assessment and interpretation (ISO 14040:2006).
260 *Step 1: Goal and scope definition.* This phase consists in defining the objectives of the study,
261 system boundaries, functional unit, data needed, assumptions and limits. The goal of the LCA
262 presented in this paper was to show to what extent the BaGaTel database can help LCA practitioners
263 perform the data inventory step. A simplified LCA was thus performed on a specific sample to
264 illustrate the contribution of BaGaTel in a LCA approach. The system boundaries exactly fitted the
265 system described in section 2.1.2. The functional unit was the production of one cheese of 10.5 kg
266 ripened for 120 days, corresponding to the use of 115 L of raw milk. The data needed mainly came
267 from data included in databases, no complementary measurement was performed. Because of the
268 production process of the sample under study, no allocation had to be assumed. Obviously, such
269 assumptions on data and allocation can limit the reliability of the obtained results. Nevertheless, this
270 paper aims to show how the BaGaTel database can be helpful in LCA studies, but does not claim to
271 provide thorough LCA results. Such a simplified approach was sufficient to achieve our goal.

Step 2: Data inventory. This stage concerns quantification of the mass and energy flows used and emitted by the system under study. Modelling of the system requires data collection for the entire life cycle and this is often the most time-consuming stage of an LCA. Primary data are measured data, secondary data are obtained from calculations or databases (e.g., Ecoinvent). The data inventory is detailed in the results section to show how the BaGaTel database can be useful to perform this step. Briefly, data used to perform the simplified LCA came from BaGaTel database, supplemented by Ecoinvent database.

Step 3: Impact assessment. Environmental impacts are evaluated by using identified inputs and outputs through specific indicators usually fixed in internationally recognised methods (e.g., ILCD). In this paper, environmental impacts were calculated by using ILCD 2011 Midpoint+ method (European Commission, 2011). This method provides environmental impacts with regards to sixteen indicators (climate change, ozone depletion, human toxicity - non-cancer effects, human toxicity - cancer effects, particulate matter, ionising radiation HH, ionising radiation E (interim), photochemical ozone formation, acidification, terrestrial eutrophication, freshwater eutrophication, marine eutrophication, freshwater ecotoxicity, land use, water resource depletion, mineral, fossil and renewable resource depletion). However, for clarity reasons, only results on climate change, ozone depletion and acidification indicators are presented in the results section. System modelling and impact assessment were performed by using Simapro software (V8.4.0.0 PRé consultant).

Step 4: Interpretation. An LCA is an iterative process and the aim is to analyse results and hypotheses and discuss them at each step 1, 2 and 3. This will help decision makers to make an improved choice. This paper aims at showing how the BaGaTel database can be helpful in LCA studies, but does not claim to provide thorough LCA results. As a consequence, LCA assumptions and results are not deeply discussed in this paper.

2.2. PO² ontology description

PO² ontology (Ibanescu et al., 2016) allows representation of a food transformation process described by a set of experimental observations available at different scales and changing over time through the different unit operations of the production process. Ontology is designed in two layers: a core layer and a domain layer. The core layer is composed of three main parts, presented in Fig. 1 (adapted from Ibanescu et al., 2016).

The domain layer allows one to represent a specific domain, here the hard cheese production process. PO² ontology description:

1. Part concerning the production *process* that contains the concepts: process, itinerary and step. An *itinerary* is an execution of a production *process*, i.e., a set of interrelated steps. It allows for description of different possible technological processes. A *step* is characterised by its participants and its temporal duration.
2. Part concerning the *participant* that contains the concepts: product, mixture, material and method. A participant may be a *mixture*, a *material* or a *method*. Each participant is characterised by its experimental conditions. A *mixture* is characterised by its composition (i.e. the *products* it contains). For instance, the *mixture* “cheese” is composed of several *products* such as “proteins” and “lipids”. Fig. 2 gives an excerpt of the milk products hierarchy in the PO² domain ontology. Notice that the concept “hard cheese” belongs to the concept “cheese”, which belongs to the concept “milk products” which belongs and to the core concept “product”.
3. Part concerning the *observation* that contains the concepts: observation, scale and attribute, which can be symbolic or quantitative. An *observation* observes a *participant* (e.g., a mixture, a material) at a given *scale* during a given *step*. An observation stored in BaGaTel allows one to have both raw and computed data about several different *attributes* such as pH, taste intensity or energy consumption of the equipment.

PO² ontology is implemented in OWL 2 (https://www.w3.org/2001/sw/wiki/OWL) and its core layer is available on the AgroPortal repository (http://agroportal.lirmm.fr/ontologies/PO2)

under the license Creative Commons Attribution International 4.0 International (CC BY 4.0) (https://creativecommons.org/licenses/by/4.0/).

PO² ontology guided the structure of the BaGaTel database, as detailed in Supplementary material file SF5, integrating and storing all the available data presented in Section 2.1.1. These data are represented with the standard format Resource Description Framework (RDF). RDF integrated data can be queried by using semantic queries expressed in SPARQL.

2.3. Implementation of data

In a first step, experts in food science, especially in food process, oral physiology, sensory perception and eco-design worked to develop a consensual vocabulary gathered in PO² ontology, which has been used for the structuring of BaGaTel.

In a second step, data were utilised in BaGaTel from different collaborative national or international projects, theses and scientific publications from scientists involved in the NutriSensAl project (http://plasticnet.grignon.inra.fr/PortailNutriSensAl/). BaGaTel contains data for different types of parameters covering different steps of the process, raw materials (useful data to perform LCA), composition of the food product at the different steps, structure of the food product, evaluation of the environmental, sensory and nutritional qualities of the final product, taking into account food breakdown in the mouth and digestive track when relevant.

In a third step, data from different projects dealing with the same type of food product were compared. The challenge was then to identify data that were comparable. For example, concerning cheese products, measurements made using various devices and different calibrations of the device, sensory evaluations were made with various panels and on products from different sensory spaces, according to the specific project.

Thanks to our network of scientific and technical experts in the field, it was possible to identify types of cheeses and parameters that could be compared among them. After selection of the

most relevant parameters, with the aim of always having the same parameter and same unit of measurement, some transformations of data and adjustments were done. For example, all scores obtained in sensory analysis were standardised on a 10-point scale. Physico-chemical data of composition were all expressed as gram of the item concerned (lipid, protein, dry matter…) per kilogram of total product.

All these modifications and adjustments must absolutely be validated by experts in food science and by scientists in charge of the thesis, the publication or the project.

3. Results and discussion

Results presented in this section aim at demonstrating the added value of the PO^2 ontology for querying the BaGaTel database to answer questions that need data from different projects. The integrated use of data coming from different projects allows for estimation of missing data in one specific project from a combination of data from other projects.

3.1. Combining data about hard cheese composition, process, sensory quality and rheological parameters

We chose to focus on “hard cheeses”; these cheeses have common characteristics, such as composition, technological process and structure. In the BaGaTel database two projects, PRASEL and TRUEFOOD, on real hard cheeses had common steps in their processing: renneting, draining, pressing, moulding, demoulding, and ripening.

By using the RDF integrated data, BaGaTel was queried with Q1 (Which hard cheese sample has the highest value for “taste intensity”?) by a SPARQL query shown in Supplementary material Fig. S1. The answer, presented in Supplementary material Fig. S2, is sample “Fd24” that has a taste

375 intensity of 6.82/10. This sample also had the highest aroma intensity (6.45/10). This sample belongs
376 to TRUEFOOD project.

377 The answer to Q2 ("What is the composition of this sample at different steps in the
378 process?") is given in Table 2. The lipid and protein content are given at three steps "milk reception",
379 "in the vat" and "cheese ripening". Table 2 also shows the answer given by BaGaTel to Q3 ("What are
380 the characteristics measured on this sample?"). The pH value has been measured at different steps
381 ("moulding", "step in the vat", "demoulding") and the sensory properties have been measured at the
382 "chewing" step.

383 No rheological properties could be found in BaGaTel database to answer to Q3, while these
384 parameters are important to evaluate the quality of cheeses. Hence, it was necessary to estimate this
385 missing data using data from other projects imported into BaGaTel.

386 The rheological parameters such as Young modulus have been demonstrated to be relevant
387 to predict masticatory activity, especially with the aim of formulating food products for specific
388 populations such as elderly people (Engelen, Fontijn-Tekamp, & Bilt, 2005; Peyron, Maskawi, Woda,
389 Tanguay, & Lund, 1997). They can be used to select samples that are easily broken down in the
390 mouth. Samples for this population are known to present reduced masticatory facilities. The aim of
391 the following query is to estimate rheological parameters for the sample Fd24 using relationships
392 between rheological parameters and sensorial parameters in BaGaTel.

393 We focused on one specific rheological parameter, Young modulus. The literature shows a
394 good correlation between the Young modulus and the sensorial parameter "firmness" for cheese
395 products (Foegeding et al., 2003), and for other food products like banana (Finney, Ben-Gera, &
396 Massie, 1967) and apple (Mohsenin, Cooper, Hammerle, Fletcher, & Tukey, 1965).

397 By using this correlation, we wanted to estimate the Young modulus value for sample Fd24.
398 Fig. 3 contains for all cheese samples in BaGaTel the value for the sensory characteristic "firmness" as
399 a function of the Young modulus in kPa. However, a poor correlation is observed between "firmness"
400 and "Young modulus" if we consider all the cheese samples in BaGaTel ($R^2 = 0.37$).

401 However, if we focus only on cheese samples belonging to “hard cheese” category, the linear
402 relationship between “firmness” and “Young modulus” (Fig. 3, bottom right), is higher (R^2 = 0.74)
403 [Equation (1)]:
404 *Firmness* = 0.0086 x *Young modulus* + 1.95 (R^2 = 0.74) Equation (1)
405 To estimate Young modulus’ of the sample Fd24, a selection was made among all samples.
406 The database was queried to identify samples characterised by the following criteria (query denoted
407 Q3bis):
408 1. belongs to the category “hard cheese” in the ontology,
409 2. has been characterised for its “firmness” and for its “Young modulus”,
410 3. has a composition in terms of lipid content and protein content (in mg kg^{-1} of cheese) at
411 the “ripening” step of the same order of magnitude as the sample Fd24 (± 20 %).
412 The assumption in criterion 3 is that the protein network and the lipid content play an
413 important role in the firmness of a product (Fu et al., 2018). Therefore, the query Q3bis imposed that
414 the protein and lipid content values of a sample could not be lower or higher than 20 % of the
415 respective values for the sample Fd24.
416 Only six samples matched all the criteria of the query Q3bis. A linear relationship exists
417 between “firmness” and “Young modulus” (Equation (2)):
418 *Firmness*= 0.0074 x *Young Modulus* + 3.1899 (R^2 = 0.83) Equation (2)
419 The correlation between “firmness” and “Young modulus” is higher considering a selected
420 set of samples [Equation (2), R^2=0.83, Fig. 4] than for samples matching only the first two criteria of
421 Q3bis [Equation (1), R^2=0.74, Fig. 3].
422 Lipid and protein contents, firmness characteristic and Young modulus parameters of the six
423 samples found in the BaGaTel database to answer the criteria from Q3bis are presented in
424 Supplementary material Fig. S3. As given in Table 2, the “firmness” value for the sample Fd24 was
425 4.64. Among the six samples from Fig. 4, one has a “firmness” value lower than 4.64 while the other
426 five samples have “firmness” values higher than 4.64. We chose the sample with the lower value (i.e.,

427 sample C1) and the sample with the value just above (i.e., sample C4). Therefore, the value of the
428 Young modulus of the sample Fd24 was estimated between the values of the Young modulus of
429 sample C1, i.e., 152.37 kPa, as lower limit and the value of the Young modulus of sample C4, i.e.,
430 205.13 kPa, as upper limit (Fig. 4).

431 To have another estimation of the Young modulus value of sample Fd24, it was also possible
432 to use the linear relationships between firmness and Young modulus for hard cheeses. As sample
433 Fd24 has a firmness rating of 4.64, the calculated estimation of the value for the Young modulus
434 using Equation (2) was 196 kPa. This value is in the first estimated interval [152.37 kPa; 205.13 kPa].
435 An estimation with Equation (1) that only takes into account criteria 1 and 2 of query Q3bis gave an
436 estimation of 312.5 kPa for Young modulus value for sample Fd24. This value is out of the previous
437 estimated interval. This validates the usefulness of criterion 3 in Q3bis for this estimation, assuming
438 that the relationship between firmness and Young modulus depends on the protein and lipid content
439 of the cheese.

440 Therefore, this approach can estimate the missing rheological parameters for hard cheese
441 samples by combining and reusing data from different projects. This estimation was only obtained by
442 mathematical thinking and has to be confirmed by a computation of numerous data sets or by
443 performing real experiments.

444

445 *3.2. Combining data about hard cheese composition, processing and environmental impact*

446

447 The other questions, Q4 and Q5, address environmental concerns to BaGaTel database. No
448 environmental data have been collected for the Fd24 sample. Therefore, this section will show how
449 BaGaTel database could be used to estimate environmental impact of sample Fd24.

450 Environmental impact has been quantified by using LCA in the CellExtraDry project (2014-
451 2016), in the case of production of stabilised micro-organisms. BaGaTel database can be very useful
452 to support life cycle inventory of data [step (ii) in LCA methodology] since it already contains data

453 coming from LCA inventories and results from the CellExtraDry project. The answer to the question
454 Q4 ("Which parameters need to be measured throughout the process to perform a Life Cycle
455 Assessment of the sample?"), is summarised in Supplementary material Table S1.

456 Measured parameters (e.g., electricity consumption, mass of water, volume of compressed
457 air) are obtained as well as the step when data related to these parameters have been collected.
458 That provides detailed items that have been previously measured to perform LCAs. LCA practitioner
459 then has to consider if these are relevant for their system, and if other similar items have to be
460 included. For instance, the mass of saccharose used for the fermentation step in CellExtraDry project
461 might not be relevant to a cheese production system. However, by analogy, a LCA practitioner can
462 easily extrapolate this result to conclude that it would be important to measure the initial mass of
463 raw milk. Combination of BaGaTel querying and expertise of a LCA practitioner is crucial to state all
464 relevant data that have to be gathered. This approach may help LCA practitioners to transfer
465 knowledge from one domain to another domain by suggesting relevant parameters to be measured.
466 This is possible thanks to the high-level description of the available data using the PO^2 ontology.

467 The BaGaTel database can therefore be also queried to obtain relevant quantified data on
468 specified items. For instance, from Supplementary material Table S1, it can be deduced that energy
469 consumption is an important parameter, since it was measured at different steps (fermentation,
470 centrifugation, drying). The query Q5, ("What are the values of the relevant parameters needed to
471 conduct the Life Cycle Assessment?"), could be reformulated as "What is the energy consumption of
472 a French hard cheese production process?". Unfortunately, no data were directly available in the
473 BaGaTel database to answer this question. Nevertheless, because PO^2 ontology also integrates
474 material and methods related to the experiments, the BaGaTel database could be queried on this to
475 evaluate the energy consumption during the different steps of hard cheese production presented in
476 Section 2.1.2. For each step, the material used could be identified, duration of its use and power of
477 the equipment. Then energy consumption was calculated by using Equation (3):

478 Energy consumption = Power of equipment × Use duration of equipment Equation (3)

Results are presented in Table 3.

Mass flow data concerning sample Fd24 could also be obtained by querying BaGaTel database, these are presented in Table 4.

Finally, using data described in Tables 3 and 4, supplemented by data and emission factors of Ecoinvent database, a simplified LCA could be performed. This simplified LCA referred to the production of one cheese of 10.5 kg ripened over 120 days, corresponding to the use of 115 L of raw milk. A simplified LCA was performed, but not detailed, because this paper aims at showing how the BaGaTel database can be helpful in LCA studies, but does not claim to provide thorough LCA results. For this reason, LCA results will not be deeply discussed. Results for climate change, ozone depletion and acidification indicators are presented in Fig. 5. For clarity reasons, other indicators are not shown. Milk reception was the main contributor to climate change and acidification, as well as for ten other indicators (not shown), due to raw milk production. On the other side, cheese ripening was the main contributor to Ozone depletion, as well as for three other indicators (not shown), due to energy demand by the ripening rooms. These results are consistent with other LCA studies which showed that raw milk production and energy use during ripening were the main causes of environmental impacts of ripened cheese (Berlin, 2002; Finnegan, Yan, Holden, & Goggins, 2017).

Finally, when a LCA practitioner has finished: LCA inventory data and LCA results can be stored in the BaGaTel database, together with all the corresponding metadata (e.g. system boundaries, functional unit, impact assessment method) necessary to eventually re-use them. From these inventory and results, LCA data could enrich existing databases (e.g., LCA Food database, World Food LCA database, EcoInvent database) that are currently poorly documented with regards to impacts due to processes as a function of (i) the food product submitted to the process and (ii) the process operating conditions.

4. Conclusions

This study demonstrates that the common vocabulary and structure provided by PO^2 ontology allow for combining and integrating data from different projects in a common database, BaGaTel, and therefore giving relevant answers to several questions. BaGaTel can add value to evaluate the relevance of a data set to be used for the estimation of missing data for a specific sample, taking into account the data available. The question addressing the formulation of hard cheese, BaGaTel database could be useful in estimate missing data on cheese rheology, by restricting the query to a set of samples with similar measured characteristics. On the question about eco-design of a food product, it gave hints about relevant data that have to be acquired and could also be useful in estimate missing data. Thanks to the fact that data on cheese quality, process and eco-design are in the same database, it will now be possible to estimate missing data on the environmental impact of projects only focused on food quality and also estimate relevant parameters for food quality in samples from project only focused on eco-design. Such an approach is very useful for knowledge and data capitalisation, as well as to produce new knowledge and data by combining and integrating existing resources. As a consequence, the number of available observations in the database is a key-parameter for making BaGaTel structured by PO^2 valuable. At the same time, such a tool makes it possible to identify the lack of data, which have to be estimated or experimentally measured, to be able to answer challenging questions.

Further work should be done to investigate to what extent open data available on the LOD (Linked Open Data) could be reused in connection with PO^2. In addition, by combining the presented tools with artificial intelligence techniques, a decision support tool could be developed to formulate future foods answering specific quality properties and produced with a controlled environmental impact. This would be a big step towards more sustainable food systems.

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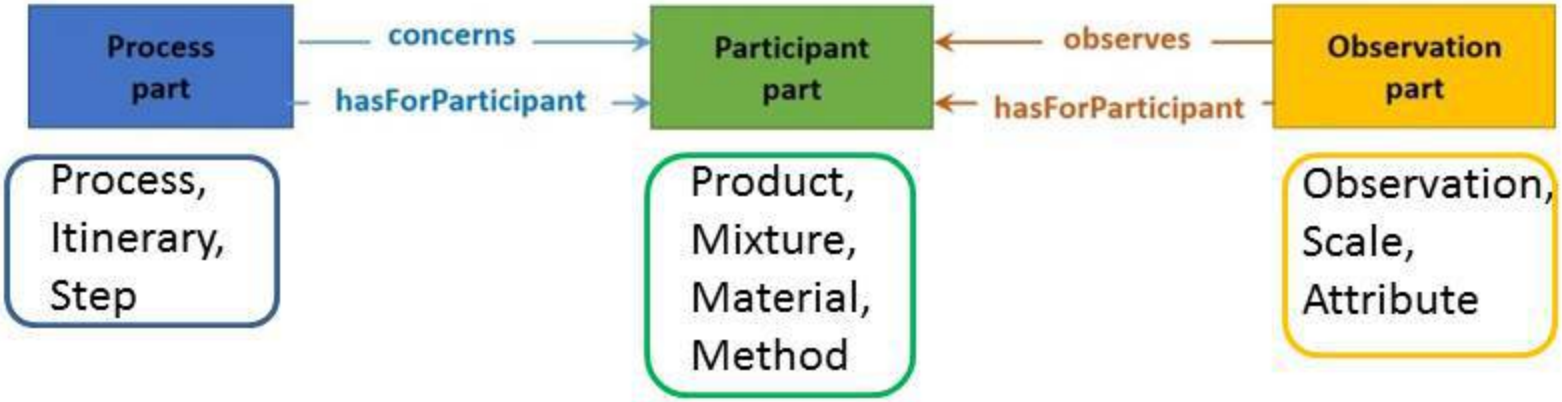
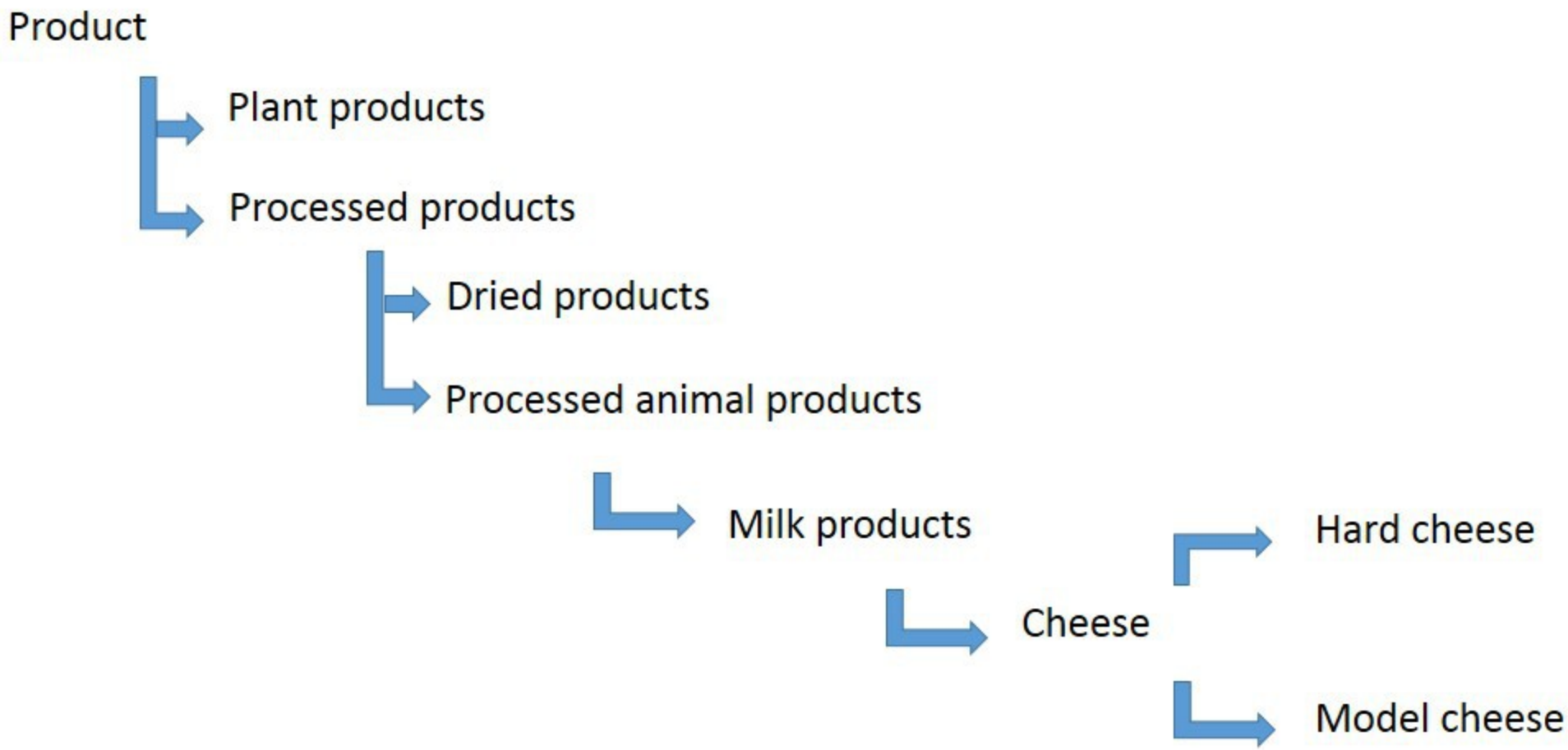
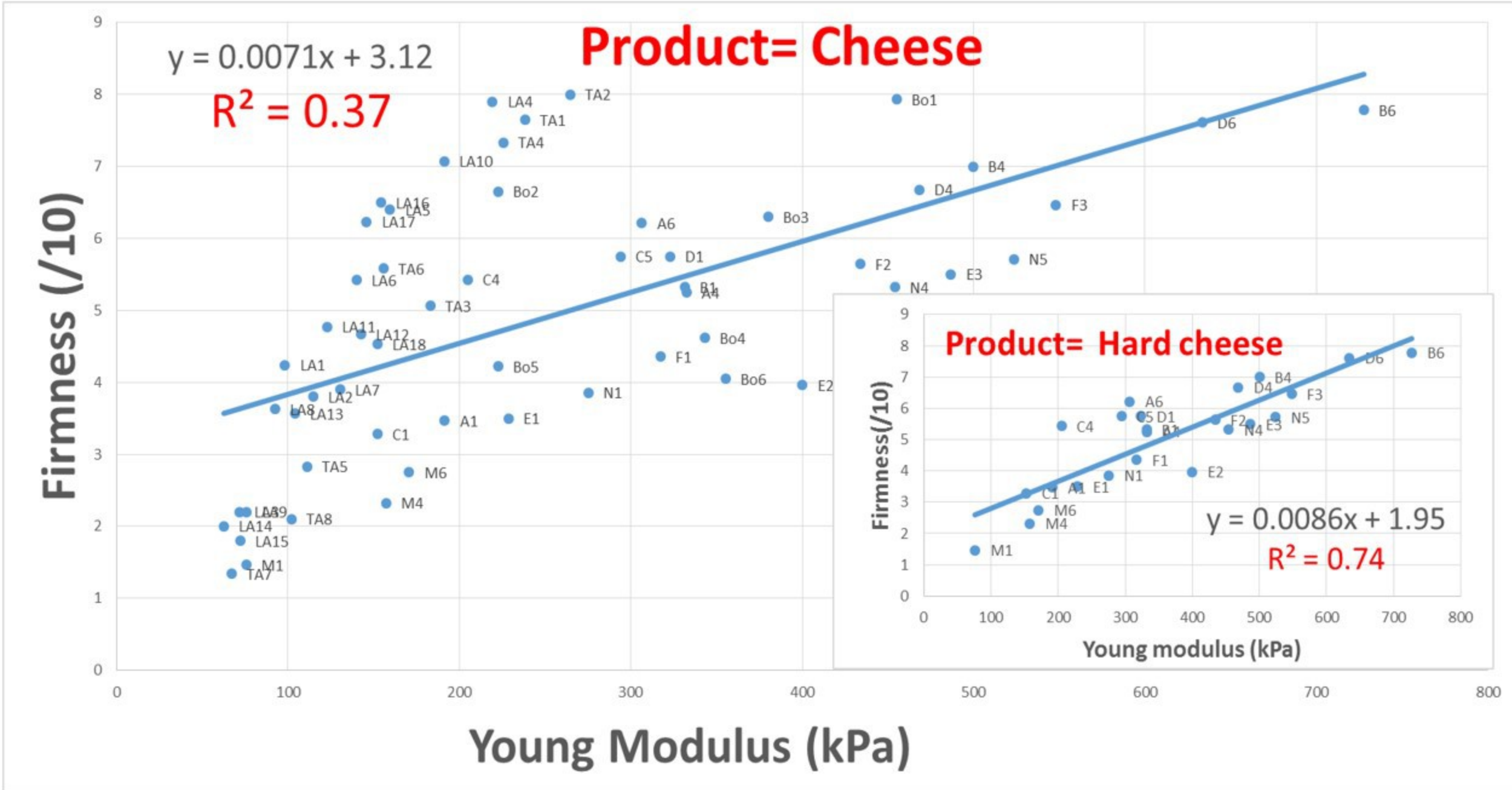
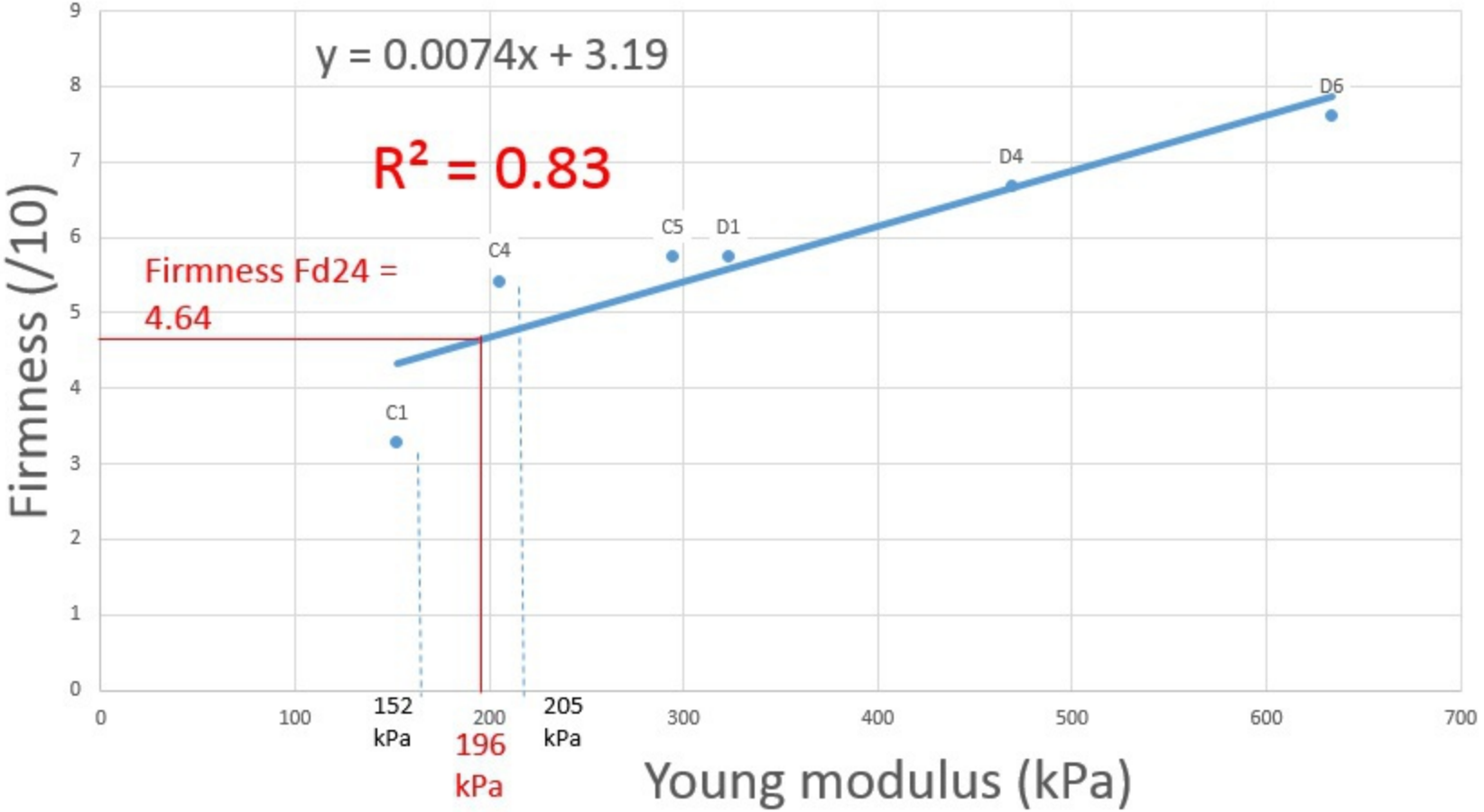
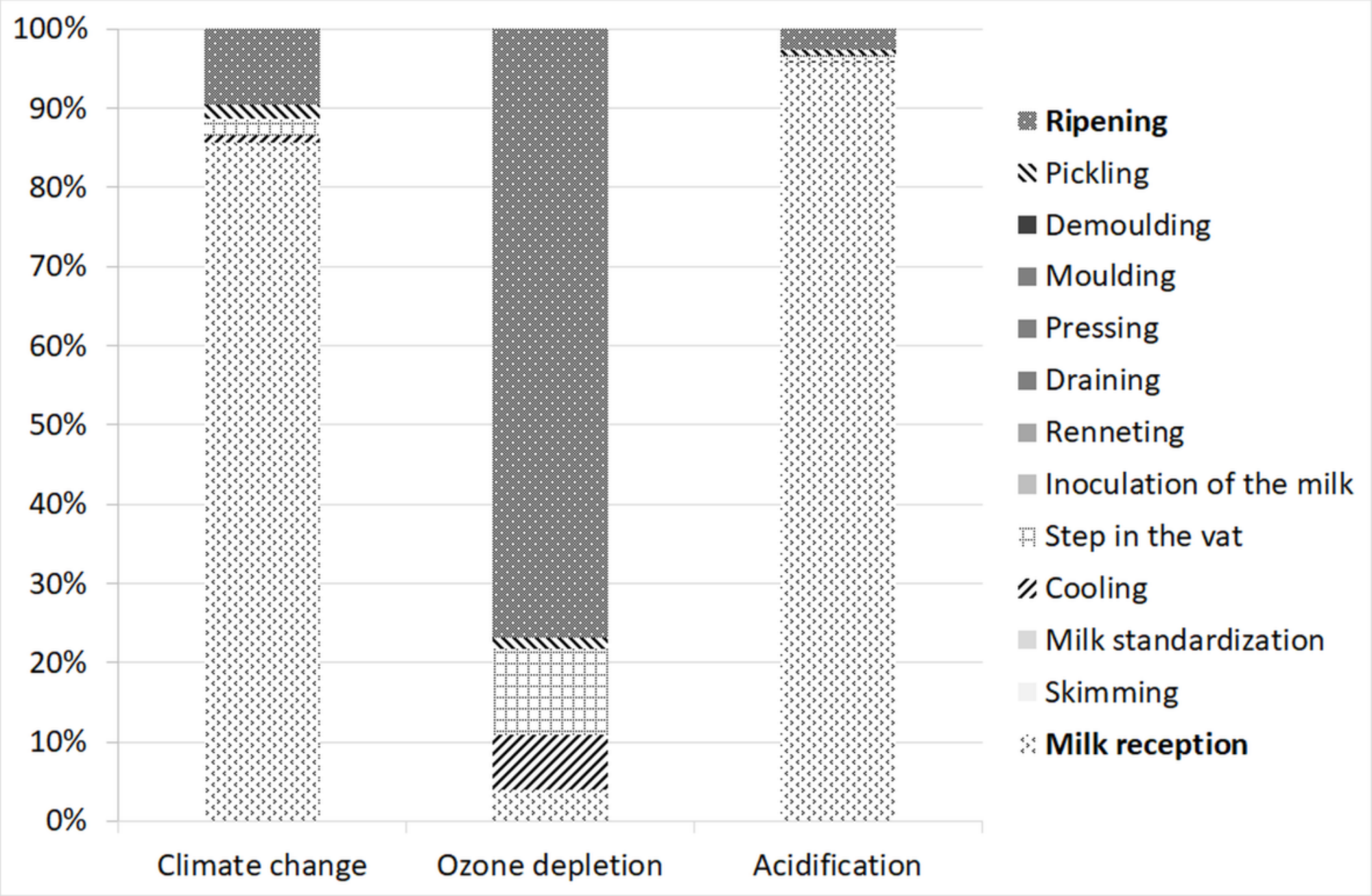

Process part
concerns
hasForParticipant
Participant part
observes
hasForParticipant
Observation part
Process, Itinerary, Step
Product, Mixture, Material, Method
Observation, Scale, Attribute


Product
Plant products
Processed products
Dried products
Processed animal products
Milk products
Cheese
Hard cheese
Model cheese


Product= Cheese
y = 0.0071x + 3.12
R² = 0.37
Firmness (/10)
Young Modulus (kPa)
Product= Hard cheese
y = 0.0086x + 1.95
R² = 0.74
Firmness(/10)
Young modulus (kPa)


y = 0.0074x + 3.19
R² = 0.83
Firmness Fd24 = 4.64
C1
C4
C5
D1
D4
D6
Firmness (/10)
Young modulus (kPa)
0
1
2
3
4
5
6
7
8
9
0
100
200
300
400
500
600
700
152 kPa
196 kPa
205 kPa


100%
90%
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30%
20%
10%
0%
Climate change
Ozone depletion
Acidification
Ripening
Pickling
Demoulding
Moulding
Pressing
Draining
Renneting
Inoculation of the milk
Step in the vat
Cooling
Milk standardization
Skimming
Milk reception

Table 1

The main attributes used during sensory profiling.

Sensory characteristic	Attribute	Definition or reference used
Texture	Springiness	Mechanical attribute related to the rapidity of shape recovery after the application of a deforming force (adapted from AFNOR, 2009)
Texture	Firmness	Mechanical textural attribute related to the force required to achieve a given deformation of the sample by teeth penetration (adapted from AFNOR, 2009)
Texture	Granularity	Geometrical textural attribute relating to the perception of the size, shape and amount of particles in a product (AFNOR, 2009)
Texture	Hardness	Mechanical textural attribute relating to the force required to achieve a given penetration, or breakage of a product (AFNOR, 2009)
Texture	Moisture	Surface textural attribute that describes the perception of water absorbed by or released from a product (AFNOR, 2009)
Taste	Overall taste intensity	Intensity of sensations perceived by the taste organ when stimulated by certain soluble substances (adapted from AFNOR, 2009)
Taste	Salty	Basic taste produced by dilute aqueous solutions of various substances such as sodium chloride (AFNOR, 2009)
Taste	Sour	Basic taste produced by dilute aqueous solutions of most acid substances (e.g., citric acid and tartaric acid) (AFNOR, 2009)
Taste	Sweet	Basic taste produced by dilute aqueous solutions of natural or artificial substances such as sucrose or aspartame (AFNOR, 2009)

Table 2

Characteristics measured on the sample Fd24 at different steps of the production process.

Step	Characteristic	Value	Unit
Milk reception	Protein	35.0	g L^{-1}
Milk reception	Lipid	44.4	g L^{-1}
Step in the vat	Protein	35.1	g L^{-1}
Step in the vat	Lipid	38.5	g L^{-1}
Step in the vat	pH	6.61	None
Moulding	pH	6.32	None
Demoulding	pH	5.07	None
Chewing	Salty	4 .55	/10
Chewing	Fat	8.27	/10
Chewing	Firmness	4.64	/10
Chewing	Aroma intensity	6.45	/10
Chewing	Taste intensity	6.82	/10
Cheese ripening	Protein	313.4	g kg^{-1}
Cheese ripening	Lipid	344.74	g kg^{-1}

Table 3

Energy consumption at different steps for French hard cheese production. [a]

Step	Material	Power (kW)	Usage duration (h)	Electricity consumption (kWh)
Skimming	Cream separator	0.065	1	0.065
Cooling	Refrigerated tank	14.52	2	29.04
Step in the vat	Heating equipment	9	0.75	6.75
Step in the vat	Heating equipment	9	1.15	9.45
Cheese ripening	Maturing cellar 1	1.25	720	900
Cheese ripening	Maturing cellar 2	1.25	1080	1350
Cheese ripening	Maturing cellar 3	1.25	1800	2250

[a] Results come from TRUEFOOD (2006-2010) project.

Table 4

Mass flow data involved in the production of sample Fd24. [a]

Step	Material	Amount
Milk reception	Milk	125 L
Vat cleaning	Sodium metasilicate	200 g
	Sodium carbonate	200 g
	Phosphoric acid	250 g
	Peracetic acid	250 g
	Hydrogen peroxide	250 g
	Ethanoic acid	250 g
Pickling	Pickle	25 L
Cheese Ripening 1	Pickle and Smear	20 g
Cheese Ripening 2	Pickle and Smear	20 g

[a] Results come from TRUEFOOD (2006-2010) project.