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Caroline Pénicaud, Liliana Ibanescu, Thomas Allard, Fernanda Fonseca, Stephane S. Dervaux, Bruno Perret, Herve Guillemin, S Buchin, Christian Salles, Juliette Dibia-Barthelemy, et al.

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1 **Relating transformation process, eco-design, composition and sensory quality in cheeses using PO<sup>2</sup>**  
2 **ontology**

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24 ABSTRACT

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

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38 **1. Introduction**

39

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

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

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

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

66         There is thus a crucial need to take into account relevant parameters of food quality in any  
67 environmental impact assessment. Product quality can be assessed by taking into account its sensory  
68 quality, for instance. Sensory quality is the result of all the sensory modalities (i.e., aroma, taste and  
69 texture) perceived during the physiological process necessary for in-mouth food breakdown and  
70 varies with product formulation and technology. Relationships among food composition, structure,  
71 sensory properties and food breakdown in the mouth have already been investigated by in vivo  
72 and/or in vitro studies conducted on dairy products (Doyennette et al., 2011; Guichard, Repoux,  
73 Qannari, Laboure, & Feron, 2017; Lauerjat, Deleris, Trelea, Salles, & Souchon, 2009; Lawrence et al.,  
74 2012). However, these studies were conducted on different dairy food products, did not measure the  
75 same parameters and did not take into account environmental parameters. It is thus difficult from  
76 these data to link quality assessment to environmental impact. The obtained data are also difficult to  
77 compare because of (i) their heterogeneity (e.g., qualitative data such as flavour perception versus  
78 quantitative or semi-quantitative data such as energy consumption), (ii) their measurement scales  
79 (e.g., micro-structure of product vs impact of the whole system on global warming) and (iii) their  
80 evolution over time: some measured properties may change over time through the different unit  
81 operations for production (e.g., content in unsaturated lipids), whilst others do not (e.g., process  
82 working conditions).

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

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

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

104           In the food and human nutrition domain, eleven ontologies are listed on the portal providing  
105 the map of agri-food data standards (<http://vest.agrisemantics.org>), a recent initiative within a  
106 GODAN (Global Open Data for Agriculture and Nutrition) Action project (<http://www.godan.info>). For  
107 instance, Food Track & Trace Ontology has been developed for traceability purposes, with the aim of  
108 being connected with a global track and trace information system (Pizzuti, Mirabelli, Sanz-Bobi, &  
109 Gomez-Gonzalez, 2014). This ontology has been extended into MESCO (Meat Supply Chain Ontology)  
110 for supporting the management of meat traceability along the whole supply chain, from farmer to  
111 final consumer (Pizzuti, Mirabelli, Grasso, & Paldino, 2017). Another example is the OFPE (Ontology  
112 for Food Processing Experiment; Muljarto, Salmon, Neveu, Charnomordic, & Buche, 2014) dedicated  
113 to food processing experiments and reused in AFEO (Agri-Food Experiment Ontology; Muljarto et al.,  
114 2017) to guide data integration in viticulture and winemaking. Moreover, close to environmental  
115 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 PO<sup>2</sup>, 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 PO<sup>2</sup> 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 PO<sup>2</sup>  
132 ontology and are thus stored into specific EXCEL files that were previously designed according to the  
133 structure of PO<sup>2</sup>. 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<sup>2</sup> ontology. Section 3 reports on how the use of  
149 BaGaTel database structured according to PO<sup>2</sup> 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<sup>2</sup> 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](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](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.

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

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

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

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

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

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

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

213

#### 214 2.1.2. *Hard cheese production process*

215 Data imported into BaGaTel describe the production of French hard cheeses made from raw  
216 cows’ milk in the Franche-Comté region of eastern France. The general outline of French hard cheese  
217 production steps can be described as follows (data from TRUEFOOD, 2008). The composition of the  
218 milk is analysed (i.e., lipid, protein, lactose and water content) during the *Milk reception* step. Then, a  
219 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 immersed 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  $0.8 \text{ mm s}^{-1}$  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  $\sigma_f$  (kPa), fracture strain  $\epsilon_f$  (-), and work to fracture  $W_f$  ( $\text{kJ m}^{-3}$ ) 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.

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

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

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

295

296   2.2.   *PO<sup>2</sup> ontology description*

297

298 PO<sup>2</sup> ontology (Ibanescu et al., 2016) allows representation of a food transformation process  
299 described by a set of experimental observations available at different scales and changing over time  
300 through the different unit operations of the production process. Ontology is designed in two layers: a  
301 core layer and a domain layer. The core layer is composed of three main parts, presented in Fig. 1  
302 (adapted from Ibanescu et al., 2016).

303 The domain layer allows one to represent a specific domain, here the hard cheese production  
304 process. PO<sup>2</sup> ontology description:

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

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

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

326 PO<sup>2</sup> ontology guided the structure of the BaGaTel database, as detailed in Supplementary  
327 material file SF5, integrating and storing all the available data presented in Section 2.1.1. These data  
328 are represented with the standard format Resource Description Framework (RDF). RDF integrated  
329 data can be queried by using semantic queries expressed in SPARQL.

330

### 331 2.3. *Implementation of data*

332

333 In a first step, experts in food science, especially in food process, oral physiology, sensory  
334 perception and eco-design worked to develop a consensual vocabulary gathered in PO<sup>2</sup> ontology,  
335 which has been used for the structuring of BaGaTel.

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

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

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

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

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

357

### 358 **3. Results and discussion**

359

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

364

#### 365 *3.1. Combining data about hard cheese composition, process, sensory quality and rheological* 366 *parameters*

367

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

372 By using the RDF integrated data, BaGaTel was queried with Q1 (Which hard cheese sample  
373 has the highest value for “taste intensity”?) by a SPARQL query shown in Supplementary material Fig.  
374 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)]:

$$404 \text{ Firmness} = 0.0086 \times \text{Young modulus} + 1.95 \quad (R^2 = 0.74) \quad \text{Equation (1)}$$

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  $\text{mg kg}^{-1}$  of cheese) at  
411 the “ripening” step of the same order of magnitude as the sample Fd24 ( $\pm 20\%$ ).

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)):

$$418 \text{ Firmness} = 0.0074 \times \text{Young Modulus} + 3.1899 \quad (R^2 = 0.83) \quad \text{Equation (2)}$$

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<sup>2</sup> 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<sup>2</sup> 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)

479 Results are presented in Table 3.

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

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

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

502

#### 503 **4. Conclusions**

504

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

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

527

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529

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532

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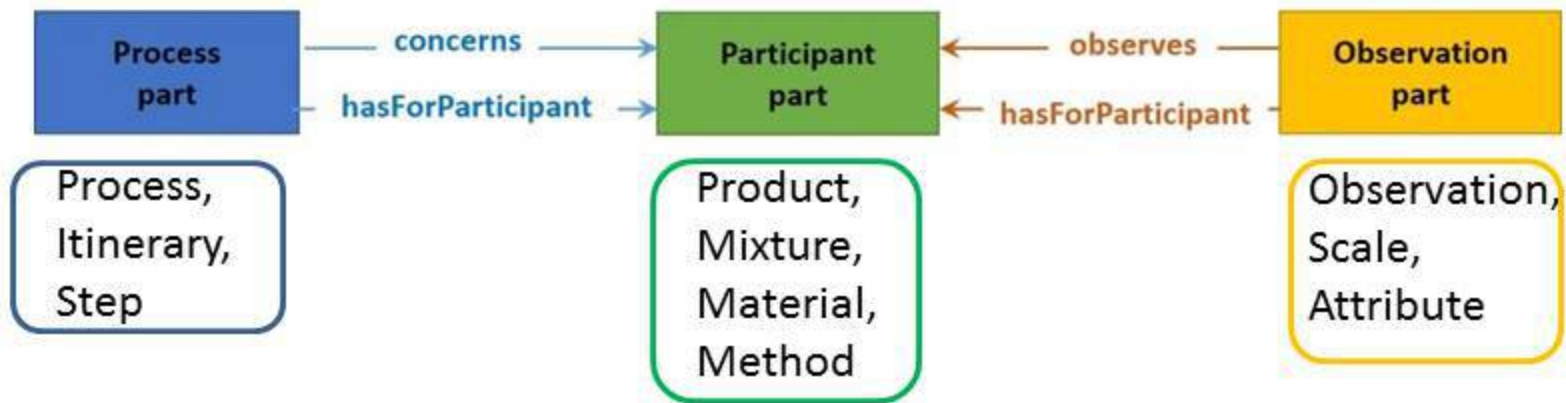
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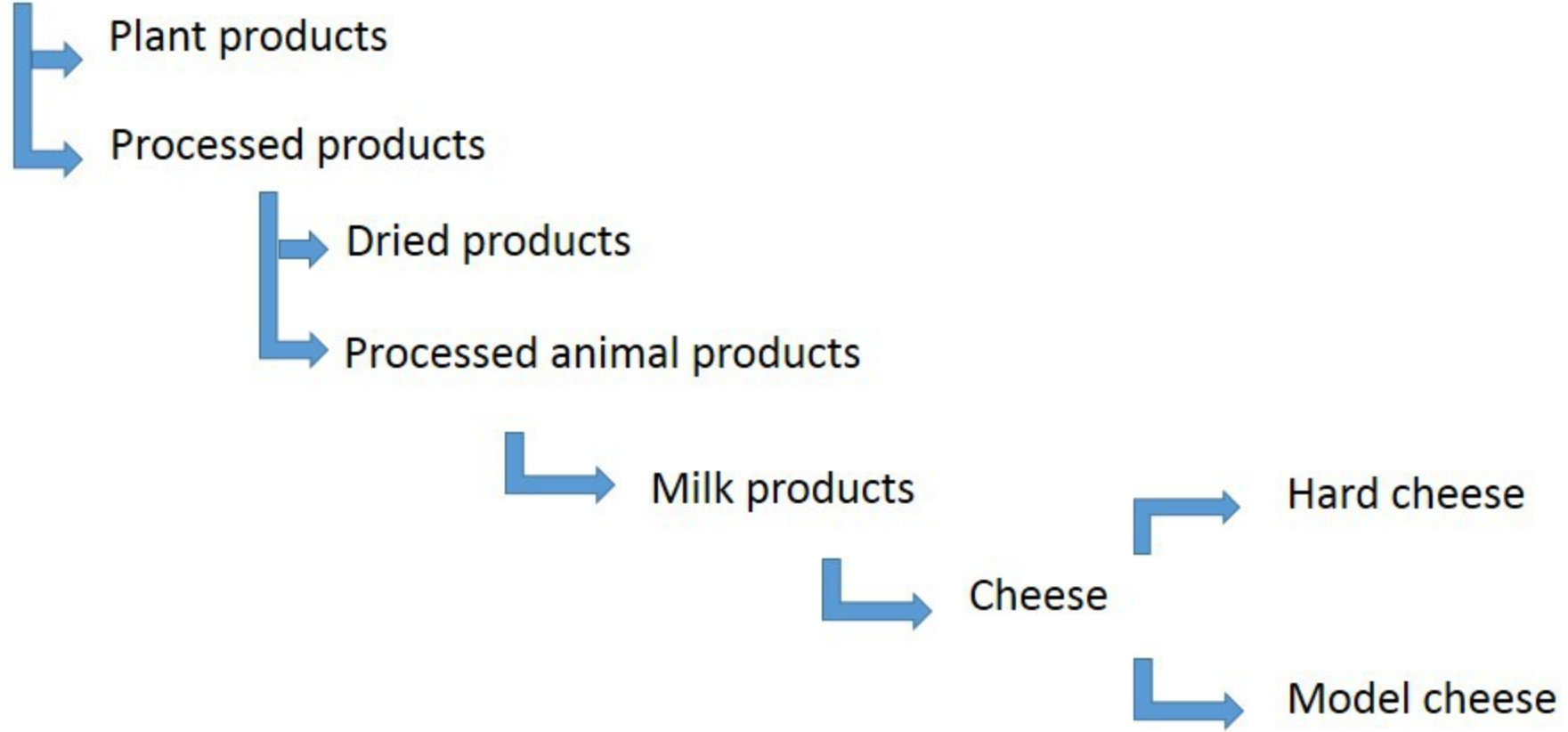
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657



Product

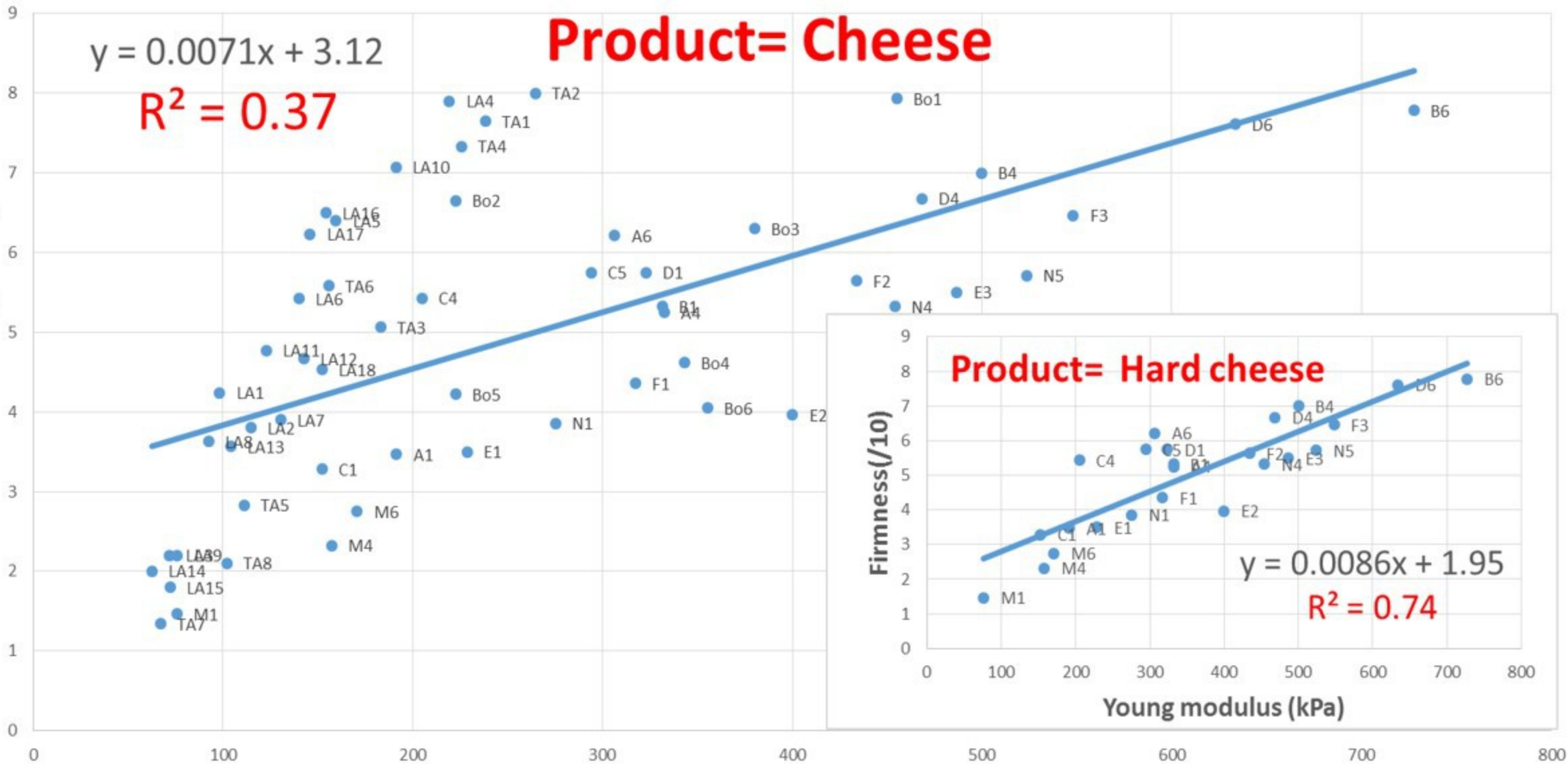


# Product= Cheese

$$y = 0.0071x + 3.12$$

$$R^2 = 0.37$$

Firmness (/10)



Young Modulus (kPa)

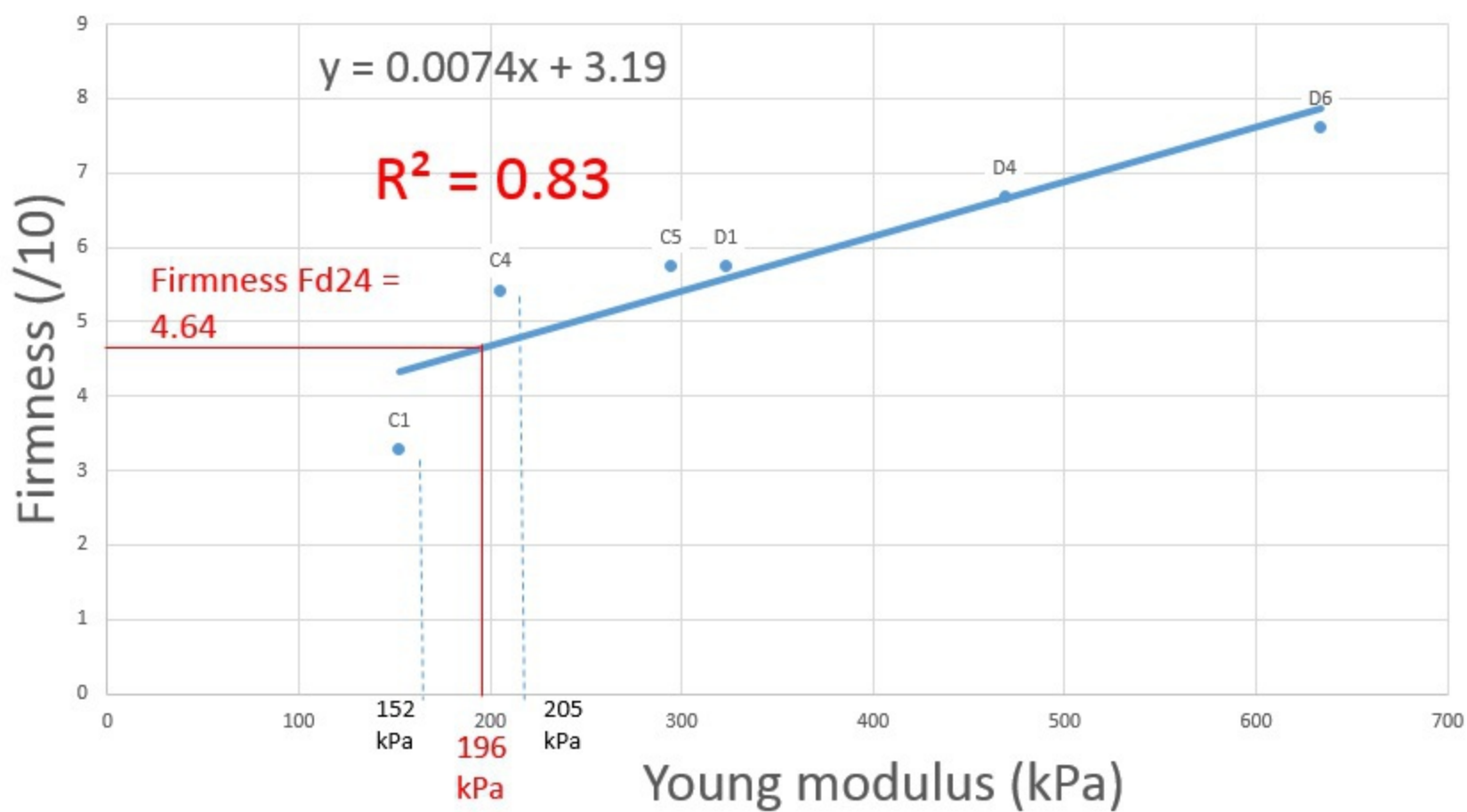
## Product= Hard cheese

$$y = 0.0086x + 1.95$$

$$R^2 = 0.74$$

Firmness (/10)

Young modulus (kPa)





**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 <sup>-1</sup>
Milk reception	Lipid	44.4	g L <sup>-1</sup>
Step in the vat	Protein	35.1	g L <sup>-1</sup>
Step in the vat	Lipid	38.5	g L <sup>-1</sup>
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 <sup>-1</sup>
Cheese ripening	Lipid	344.74	g kg <sup>-1</sup>

**Table 3**Energy consumption at different steps for French hard cheese production. <sup>a</sup>

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

<sup>a</sup> Results come from TRUEFOOD (2006-2010) project.

**Table 4**

Mass flow data involved in the production of sample Fd24. <sup>a</sup>

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

<sup>a</sup> Results come from TRUEFOOD (2006-2010) project.