[MS]^{2}O: A Multi-scale and Multi-step Ontology for Transformation Processes: Application to Micro-Organisms

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Abstract. This paper focuses on the knowledge representation for an interdisciplinary project concerning transformation processes in food science. The use case concerns the production of stabilized micro-organisms performed at INRA (French National Institute for Agricultural Research). Experimental observations are available for some inputs of the production processes, at different steps and at a certain scale. Available data sets are described using different vocabularies and are stored in different formats. Therefore there is a need to define an ontology, called $[MS]^2O$, as a common and standardized vocabulary. Users' requirements were defined through competency questions and the ontology was validated against these competency questions. $[MS]^2O$ ontology aims to play a key role as the representation layer of the querying and simulation systems of the project. This leads to the possibility of comparing different production scenarios and suggesting improvements.

Keywords: domain ontology building, multi-step and multi-scale ontology, transformation processes

1 Introduction

There is a challenging need for food companies to design and to control the transformation of raw materials into final products, ensuring their quality while applying appropriate technologies for minimal economic, environmental and social costs. For that, they have to better understand the food production system in order to adopt an eco design approach by considering concomitantly product quality, production process parameters, and its environmental impacts. Such an eco design approach supposes to take advantage of all available data and experts' knowledge for performing the analysis of the production system. However, data have been collected for different purposes, in different sub-domains, at different scales. Data have also been encoded in various formats using heterogeneous vocabularies and are processed in different information systems. Moreover, expert's knowledge is often implicit and difficult to acquire. There is therefore a need to uniformly model and store available data and experts' knowledge in order to compare different production scenarios and to perform a cause and effect analysis.

Ontologies are nowadays used as a common and standardized vocabulary for representing concepts and relations from a particular field (e.g. life-science, geography). An ontology is designed to represent the knowledge from a domain in terms of concepts, relations between these concepts and instances of these concepts [8]. Building networks of interconnected ontologies [5] and publishing ontologies on the Linked Open Data (LOD) cloud[3] should facilitate data integration and data sharing, such as giving access to data from specific disciplines or data produced within specific geographic regions [2]. However, domain ontologies are built for a specific task and it is not easy to reuse them for a different one. Data available at different scales and the challenge to take into account the environmental impact of the food production process cause the knowledge management in food production more complex.

This paper focuses on building an ontology, called $[MS]^2O$, for transformation processes and more particularly the production of stabilized micro-organisms, performed at INRA (French National Institute for Agricultural Research) in an inter disciplinary project called LIONES.

A process may be represented as an industrial process [7], a bussiness process [12] or a food transformation process [10]. However, none of these representations was suited to represent a food transformation process described by a set of experimental observations available at different scales. Different Ontology Design Patterns (ODP)[4] exist as for example the ODP for material transformation [13] or the ODP for life cycle assessment data [9]. As disscused in [3], ODPs bring a promise of compositional modeling and true ontology reuse, but many barriers to their adoption still remain.

Building the ontology from scratch, one of the scenarios of the NeON methodology [5] was used for the construction of $[MS]^2O$. Users' requirements were defined through competency questions and the ontology was validated against these competency questions.

$[MS]^2O$ core component is implemented in OWL[5] and all the available data were structured in files using the $[MS]^2O$ vocabulary. The domain component of $[MS]^2O$ is under development.

The paper is organized according to the NeOn methodology. In Section 2 the ontology specification is presented, then the ontology conceptualization is detailed in Section 3. In Section 4, we present the ontology implementation and user evaluation. Finally, we conclude in Section 5 and present our further work.

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[3] http://linkeddata.org
[4] http://ontologydesignpatterns.org
[5] https://www.w3.org/2001/sw/wiki/OWL

2 Ontology Specification

This section briefly presents the LIONES Project, then the competency questions expressing users' requirements and finally our ontology specification.

2.1 LIONES Project

LIONES Project involves domain experts and computer scientists researchers from INRA, the French National Institute for Agricultural Research. It addresses the issue of modeling semantic **LI**nks between **ON**tological multi-scal**ES** objects involved in transformation process. LIONES Project is applied to the production of stabilized micro-organisms. Micro-organisms are biological agents which present a large scale of applications in food (e.g. yoghurts, cheese, wine, beer) and non-food (e.g. probiotics, microbial production of chemical molecules, biofuels) domains. The need for concentrated micro-organisms (called starters) to be stabilized and in ready-to-use form is increasing. Their production process [1] is composed of a set of steps or unit operations (e.g. fermentation, cooling, concentration, formulation) that transforms inputs into outputs. The inputs of the system are the raw materials (e.g. micro-organisms, sugar), energy and water. The outputs of the system are the final product, some co-products, energy and effluents. Figure 1 presents the production system for stabilized micro-organism from the domain experts point of view. Two distinct axes were identified: the multi-step axis composed of the different steps of the production process and the multi-scale axis which represents the different scales of the studied product. Moreover, the multi-criteria analysis of the production system should help the experts to guarantee the product quality during the transformation process while reducing economical costs and environmental impact.

The modeling of semantic links in LIONES Project first requires to qualify and represent the multi-scales objects involved in the transformation process. This paper focus on the knowledge representation task of the LIONES Project: the building of $[MS]^2O$, a Multi-Scale and Multi-Step Ontology for modeling the production of stabilized micro-organisms.

The available data sets in LIONES Project concerns different steps of the production process at different scales, from the microbial cell components to the target functionality at the population level. Data sets are heterogeneous and sparse and come from many different sources such as databases, EXCEL files, text files, sensor outputs, scientific publications [11, 6, 14], Master reports, laboratory technical reports. They are gathered for many different purposes by different experts with their own experimental itineraries, vocabularies and technical materiel and methods. Since the experts work on the same domain, reaching a consensus about a common vocabulary was quite easy. Nevertheless (i) extracting and expressing implicit experts' knowledge, (ii) understanding and structuring the whole transformation process with all the involved entities, their properties and interactions using the available data and documents and the implicit experts' knowledge and (iii) identifying the users requirements for data retrieval

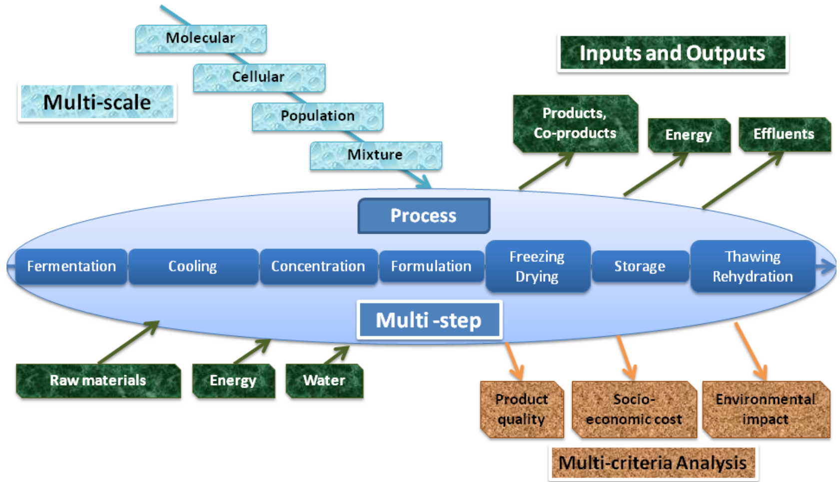

Fig. 1. The production system for stabilized micro-organism

and reasoning were less easier and required extensive conversations with domain experts to model the ontology.

In the next sub-section, we present the users' requirements through competency questions (CQ), which are natural language sentences that express a pattern for a type of questions domain experts expect the ontology to answer.

2.2 Competency questions

Domain experts involved in LIONES Project have the following criteria for the product process analysis: the product quality, the environmental impact, and the economical cost. We helped the domain experts to express their users' requirements through a set of competency questions, as for example:

- Competency questions about product quality analysis

CQ_1 Find all the production conditions of stabilized *Lactobacillus delbrueckii* subspecies *bulgaricus* CFL1 that allowed obtaining a specific acidifying activity lower than 20 min/log (CFU/mL).

CQ_2 Find all the datasets about cultivability losses and membrane integrity of *Yarrowia lipolytica* during drying.

CQ_3 Find the Yeast having the most cultivability losses during drying.

CQ_4 Find which process step was the most damaging for the micro-organisms viability.

CQ_5 Find all the datasets about drying resistance of *Yarrowia lipolytica* during the fermentation step.

- Competency questions about environmental impact analysis

CQ_6 Find all the process steps that are involved in global warming.

CQ_7 Find the energy consumptions of freeze-drying measured in France during the year 2014.

– Competency questions about economical cost analysis

CQ_8 Find all the freeze-drying conditions that allowed producing more than 10t/month of stabilized bacteria.

The next sub-section presents the ontology specification aiming to answer to the domain experts' competency questions.

2.3 Ontology Specification

Using the Figure 1, the available data sets and the related documents, we established, in close collaboration with domain experts, a new representation of the production system as given in Figure 2.

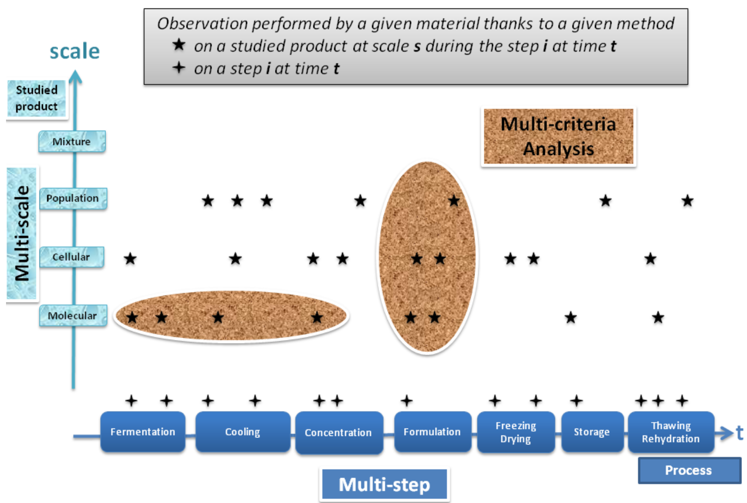

Fig. 2. Global schema of the production system

In this new schema, the two axes of Figure 1 remain: the multi-step axis where the process is described by its different steps and the multi-scale axis where the studied products can be considered at different scales (i.e. as a whole inside a mixture, at the population scale, the cellular or molecular ones). Moreover, we give the following definitions:

D1 **a transformation process is composed of steps, non necessarily in sequence** (e.g. two steps can occur simultaneously), **which transforms inputs into several different outputs**;

D2 **the representation of a transformation process relies on experimental observations**;

D3 **experimental observations are performed with a given material according to a given method either on a mixture (i.e. a set of**

combined products) at a certain scale during a certain step (e.g. observations about the membrane integrity of *Yarrowia lipolytica* performed at its cellular scale during the drying step in CQ_2) **or on a step** (e.g. observations about energy consumption by the freeze-drying step in CQ_7).

D4 **the inputs and outputs of the system** (e.g. raw materials, water, co-products and effluents) of Figure 1 **are components of the mixture and can be evaluated through observations on it at different steps and different scales**.

D5 **The product quality, the economic cost and the environmental impact** of Figure 1 **can be deduced from attributes associated with the studied products, the steps of the process and the materials**.

These five definitions correspond to our understanding of the studied domain and guide our $[MS]^2O$ conceptualization.

3 Ontology Conceptualization

In this section, we present our Multi Scale and Multi Step Ontology for transformation Processes, $[MS]^2O$. Our ontology is designed from scratch by an iterative process in a modular way in order to be able to import and reuse existing ontologies, which will be the next step of our work, as recommended by the NeOn methodology. $[MS]^2O$ is composed of two components: a core component to represent the transformation processes as defined in `D1` to `D5` and a domain component to represent the production of stabilized micro-organisms. The core component of $[MS]^2O$ is composed of the five following modules (see Figure 3):

- a Process module
- a Studied object module
- an Attribute module
- an Observation module
- a Material and Method module

In the next sub sections, we detail its main entities presented in Figure 4, with examples on the production of stabilized micro-organisms. The Material and Method module is not presented in this paper since a complementary expertise is necessary to develop it. Even if its existence seems obvious for the domain experts, this module was not in the initial user requirements. The definition of the competency questions for this module is in progress.

3.1 The Process module

According to definition `D1`, a transformation `process` is composed of steps, non necessarily in sequence (e.g. two steps can occur simultaneously) which transforms inputs into several different outputs. A `process`, which corresponds to one experimentation for the domain experts, is composed of several itineraries (see `hasForItinerary` property in Figure 4). An `itinerary` is composed of a set of

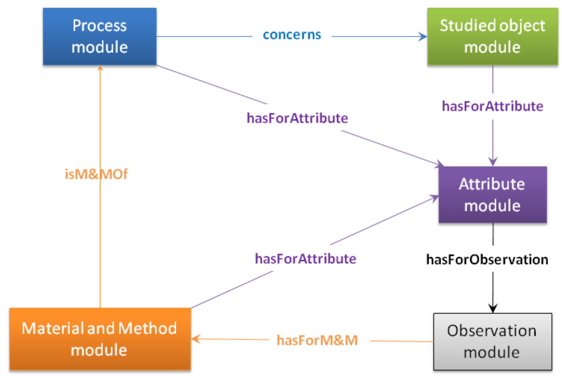

Fig. 3. The five modules of the $[MS]^2O$ core component

steps (see `hasForStep` property in Figure 4) characterized by some experimental conditions linked by time relations (see `TimeRelation` property on `step` concept in Figure 4).

Example 1. Let us consider a process on the production and stabilization of the yeast Yarrowia lipolytica *performed with two distinct itineraries. The first itinerary is composed of the steps: fermentation, concentration, drying into stove during 75 minutes and storage. The second one is composed of: fermentation, concentration, drying into fluidized bed during 90 minutes and storage.*

A `step` may be composed of substeps (see `hasForSubstep` property in Figure 4), which are considered as steps. A `step` is characterized by its material and method (see `hasForM&M` property in Figure 4). Figure 5 gives an example of the possible substeps of the fermentation step in different cases.

Each `itinerary` and `step` is characterized by the time when it starts (see `hasForTimeProperty` property in Figure 4).

A step can be compared with the perdurant object *Phenomenon* in DOLCE[6] and with the concept *Process* in SUMO[7].

3.2 The Studied object module

A studied object may be a `product` or a `mixture`. The studied product is the one on which is applied the transformation process (see `hasForStudiedObject` property between `process` and `product` in Figure 4).

Example 2. The studied product of the process presented in Example 1 is the yeast: Yarrowia lipolytica.

[6] http://www.loa.istc.cnr.it/old/DOLCE.html
[7] http://www.adampease.org/OP/

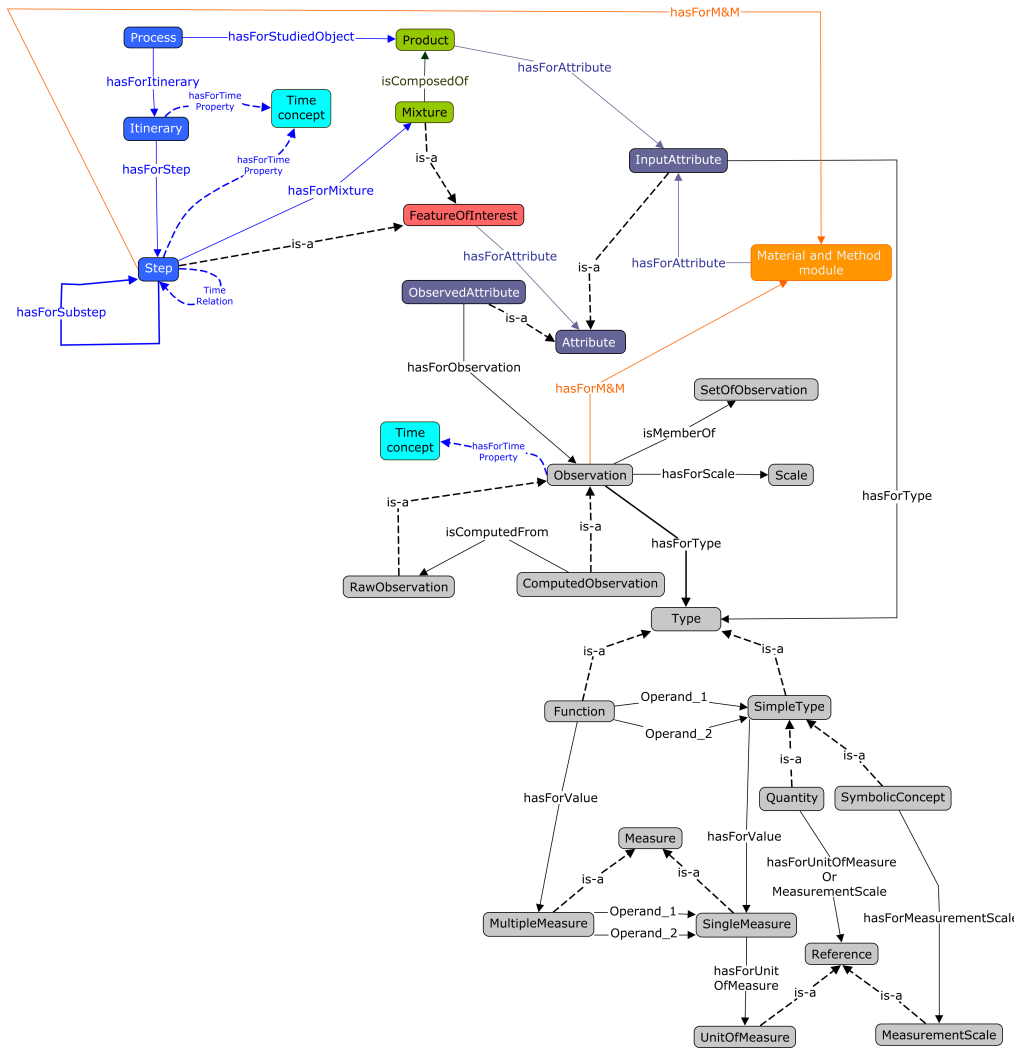

Fig. 4. Detail of the modules Process, Studied object, Attribute and Observation of the $[MS]^2O$ core component

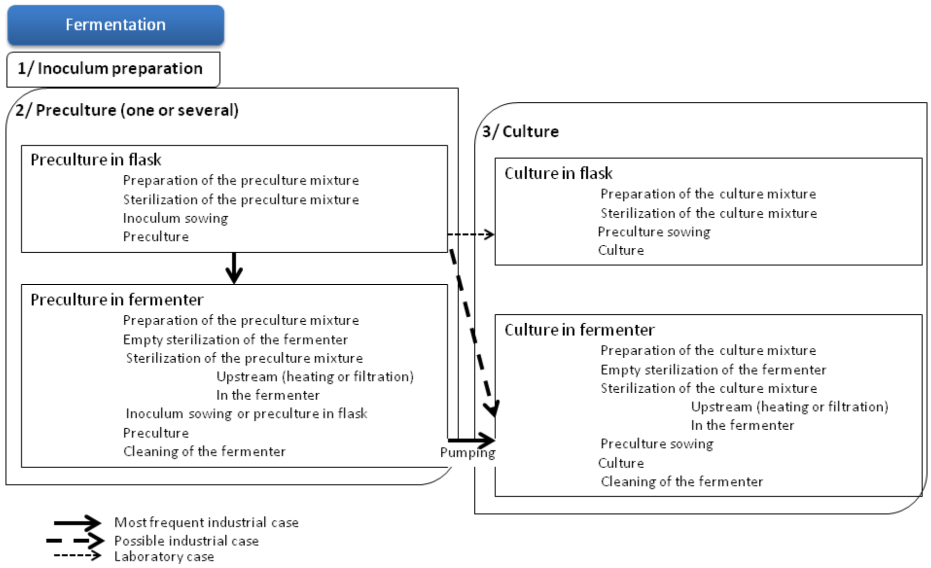

Fig. 5. The possible substeps of the fermentation step

A `mixture` is a composition of several products (see `isComposedOf` property in Figure 4), but may be composed of only one product. A `mixture` is characterized by its composition (e.g. raw materials, water). It contains in particular the studied product. The different `steps` and sub-steps of an itinerary are applied on `mixtures` (see `hasForMixture` property in Figure 4). Let us notice that a `step` may be applied on several `mixtures`.

A mixture can be compared with the DOLCE concept *Non-Agentive-Physical-Object*.

3.3 The Attribute module

The features of interest of our domain are the steps and the studied mixtures. They are characterized by `attributes` which may have input values or may be observed (see `hasForAttribute` property between `FeatureOfInterest` and `Attribute` in Figure 4). An attribute can therefore be either an `input attribute`, it is then associated with input values (see Section 3.4), or an `observed attribute`, it is then associated with observations (see `hasForObservation` property between `ObservedAttribute` and `Observation` in Figure 4). Let us notice that the material and method are also characterized by input attributes (see `hasForAttribute` property between `Material and Method module` and `Attribute` in Figure 4).

Example 3. In order to answer to CQ_5, we have to consider all the observations associated with the `Drying_resistance` attribute which characterizes mixtures composed of the yeast Yarrowia lipolytica*, during the fermentation step. Let us*

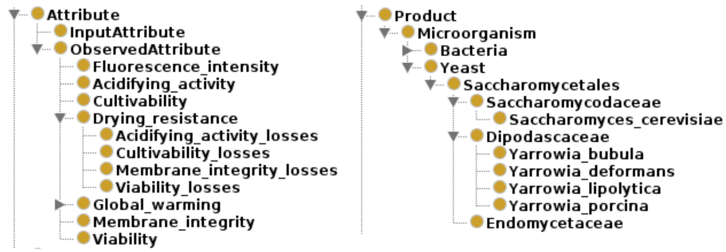

Fig. 6. An excerpt of the attribute hierarchy and the yeast hierarchy in the $[MS]^2O$ domain component applied to the production of stabilized micro-organisms

notice that the hierarchical links between the `Drying_resistance` attribute and the attributes `Acidifying_activity_losses`, `Cultivability_losses`, `Membrane_integrity_losses` and `Viability_losses` in Figure 6 eases the querying of all observations associated with the `Drying_resistance` attribute.

3.4 The Observation module

According to definitions D2 and D3, observations are very important for the transformation process representation. They correspond to the experimental results. Each observation is performed by a material (i.e. a sensor) using a given method (see `hasForM&M` property in Figure 4), on a step or on a mixture (see `hasForAttribute` property between `FeatureOfInterest` and `ObservedAttribute`, then `hasForObservation` property between `ObservedAttribute` and `Observation` in Figure 4) at a given scale (e.g. molecular, cellular, population) (see `hasForScale` property in Figure 4). It is important to stress on, as states in definition D3, that the multi scale property of $[MS]^2O$ is represented at the observation level. As a matter of fact, in our domain, what is important is to know at which scale a given experimental measure (i.e. an observation) is made, not to register the part-of links between different parts/scales of a product. Currently, the observations are made independently at different steps and different scales of the studied mixtures.

Example 4. The observations associated with the `Cultivability_losses` attribute are performed on mixtures at their population scale. In order to answer to CQ_3, we have to consider all the observations, associated with the `Cultivability_losses` attribute, which are performed on mixtures composed of a yeast during the drying step (see the excerpt of the yeast hierarchy in Figure 6).

An observation can be a `raw observation` or a `computed observation`. A `computed observation` is computed from `raw observations` (see `isComputedFrom` property in Figure 4). The observations are regrouped in a `set of observations`, which allows one to register that they were made together and represent the same set of experimental measures (see `isMemberOf` property in Figure 4).

An observation is characterized by the time when it is performed (see `hasForTimeProperty` property in Figure 4).

An observation and an input attribute are defined by their `type` (see `hasForType` property in Figure 4). This type can be either (i) a `SimpleType`, i.e. a quantity (e.g. temperature) or a symbolic concept (e.g texture), or (ii) a `function` composed of two operands (see `Operand_1` and `Operand_2` properties in Figure 4). The observation or the input attribute has then for value in the first case a `single measure` associated with a `unit of measure`, and, in the second case a `multiple measure`.

Example 5. The observations on the `Membrane_integrity` attribute, involved in CQ_2, are computed from the raw observations associated with the `Fluorescence_intensity` attribute. Each raw observation on the `Fluorescence_intensity` attribute has for type a function between the quantity `Fluorescence_intensity_quantity` and the quantity `NumberOfCells`. Each computed observation on the `Membrane_integrity` attribute has a simple type, the boolean symbolic concept. It has for value a boolean value, with the unit of measure 'no_unit '.

4 The ontology implementation and validation

The current version of $[MS]^2O$ core component implemented in OWL is available at http://lovinra.inra.fr/2015/12/16/multi-scale-multi-step-ontology/. Time ontology[8] recommended by the W3C[9] is used to represent the temporal concepts. For the measure part we reuse the modeling of the measures with their units from the @Web platform[10] [4] which was inspired from OM[11].

Available data concerning two production processes with two itineraries each were structured using the $[MS]^2O$ vocabulary and are stored into 162 EXCEL files. For each production process,

– 1 file describes the process,
– 66 files contain experimental observations, where the biggest experimental observation contains 297 results' raws,
– 4 files contain the mixture composition,
– 9 files describe the steps, and
– 1 file contains the environmental impact information.

Example 6. Figure 7 gives a screen-shot of an excerpt of the EXCEL file which describes a process.

These EXCEL files allow us to build the $[MS]^2O$ domain component and to validate that all available data in the use case can be represented as instances of $[MS]^2O$. To validate our conceptualization, we have checked that the SPARQL

[8] http://www.w3.org/TR/owl-time/
[9] World Wide Web Consortium. http://www.w3.org/
[10] http://www6.inra.fr/cati-icat-atweb
[11] http://www.wurvoc.org/vocabularies/om-1.8/

Date	2015-06-28
Project name	LIONES
Microorganism (species, stem)	Saccharomyces cerevisiae - CBS 8066
Code échantillon	2015-06-28-LIONES-001

Step	SubStep	time harvest	Measure	Measure level	Scale	File number	Type of data
Fermentation	Preparation of the culture mixture	NA	Composition	Mixture		1	raw
Fermentation	Sterilisation of the culture mixture	NA	Conduite	Step		1	raw
Fermentation	Culture	24h	Conduite	Step		3	raw
Fermentation	Culture	24h	Cultivability	Mixture	Population	1	raw - computed
Fermentation	Cleaning	NA	Composition	Mixture	Mixture	1	raw
Concentration	NA	20 min	Conduite	Step		1	raw
Drying into stove	NA	75 min	Conduite	Step		2	raw
Drying into stove	NA	75 min	GSH intracellular	Mixture	Cellular	1	raw - computed
Drying into fluidized bed	60°60'	60 min	Conduite	Step		1	raw
Drying into fluidized bed	60°60'	60 min	GSH intracellular	Step	Cellular	1	raw - computed
Storage	NA	NA	Energy consumption	Step		1	computed

Fig. 7. An excerpt of the EXCEL file which describes a process

queries deduced from the competency questions presented in Section 2.2 have answers in a subset of OWL instances built from the EXCEL files. A knowledge base built from EXCEL files is currently in progress.

Example 7. The SPARQL queries to answer to CQ_3 *and* CQ_5 *presented in examples 3 and 4 are:*

CQ_3:
```
SELECT ?prod (MAX(?value) AS ?valueMax) Where {
 ?attr rdf:type ms2o:Cultivability_losses .
 ?attr ms2o:hasForObservation ?obs .
 ?obs ms2o:hasForType ?type .
 ?type ms2o:hasForValue ?value .
 ?foi ms2o:hasForAttibute ?attr .
 ?foi ms2o:isComposedOf ?prod .
 ?prod rdf:type ms2o:Yeast .
 ?step ms2o:hasForMixture ?foi .
 ?step rdf:type ms2o:Drying
 }
```

CQ_5:
```
Select ?obs Where {
 ?attr rdf:type ms2o:Drying_resistance .
 ?attr ms2o:hasForObservation ?obs .
 ?foi ms2o:hasForAttibute ?attr .
 ?foi ms2o:isComposedOf ?prod .
 ?prod rdf:type ms2o:Yarrowia_lipolytica .
 ?step ms2o:hasForMixture ?foi .
 ?step rdf:type ms2o:Fermentation
}
```

5 Conclusions and Further Work

In this paper, we presented the building of $[MS]^2O$, a Multi-Scale and Multi-Step Ontology for transformation processes, applied to the production of stabilized micro-organisms use case, performed at INRA (French National Institute for Agricultural Research). To build $[MS]^2O$, we have followed the NeOn methodology. We detailed the $[MS]^2O$ core component in which a transformation process is composed of steps, non necessarily in sequence, that allows inputs to be transformed in several different outputs. We stated that a transformation process relies on experimental observations that are performed either on a mixture (i.e. a set of combined products) at a certain scale during a certain step or on a step, the mixture being transformed during the steps of the process.

Future work is to define the module Material and Method and its connections with the other modules. We are currently investigating if the Semantic Sensor Network ontology[12] recommended by the W3C could be used. We are also evaluating how to enrich the product hierarchy with the FAO thesauri, AGROVOC[13] and the EFSA classification, FoodEx2[14].

In order to test the genericity of our $[MS]^2O$ core component modeling we are currently investigating how to use it in an other project concerning transformation processes on dairy gels.

$[MS]^2O$ ontology aims to play a key role as the representation layer of the querying and simulation systems of the LIONES project. This leads to the possibility of comparing different production scenarios and suggesting improvements while increasing efficiency (e.g. costs for the company). Moreover modeling the production processes of multi-scale objects may help domain experts to discover new semantic links between concepts and perform a cause effect analysis.

Acknowledgments We are very grateful for the valuable inputs from all the domain experts partners involved in CellExtraDry French national project.

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[14] http://www.efsa.europa.eu/fr/datex/datexfoodclass

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