# PO2/TransformON: A New Domain Ontology for Integrating Food, Feed, Bio-products and Waste in a Circular and Sustainable Approach

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**Abstract**

We are experiencing an acceleration in the global drive to converge consumption and production patterns towards a circular and more sustainable approach to the agri-food system. To meet the challenge of reconnecting agriculture, environment, food and health, data from heterogeneous sources and formats need to be integrated and exploited. In this context, ontologies may play a relevant role as they provide a formal representation of knowledge and structure for integrating data. We present a new domain ontology on food and bio-products engineering for data integration in a circular agri-food system. This ontology is based on a core model for a generic process, the Process and Observation Ontology (PO2), which has been specialized to provide the required vocabulary to describe any biomass transformation process and to characterize the food, bio-products and wastes involved as inputs and/or inputs of these processes. Much of the vocabulary comes from authoritative references such as the European food classification system (FoodEx2), European Waste Catalog (EWC) and other international nomenclatures. The ontology is built using Semantic Web standards, aiming to be compliant with the Findable Accessible Interoperable Reusable (FAIR) principles and willing to provide system interoperability and software-driven intelligence. This ontology may provide the link between the different drivers (environmental, socioeconomic, nutrition and health) involved into the food system.

**Keywords**

agri-food system, material transformation process, knowledge base, data integration, ontology, semantic web, food classification system



## 1. Introduction

Food systems are complex and multidimensional systems defined by the Organisation for Economic Co-operation and Development (OECD) as the elements and activities related to the production and consumption of food and their effects, including economic, health, and environmental outcomes. We are witnessing an acceleration of the global drive to converge consumption and production patterns toward a circular and more sustainable approach to the

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food system [1, 2]. In addition, the need to develop more integrative approaches to reconnect agriculture, environment, food, and health has been reaffirmed recently [3]. This nexus approach combines the issue of the sustainability of diets with that of the sustainability of agricultural and food production systems, leading to sustainable agri-food systems. To address this challenge, collections of large data sets must be exploited, which are by nature heterogeneous and multidimensional as they cover nutritional, sensory, physicochemical, rheological, microbiological, environmental, and socio-economic aspects. In this context, the FAIR (Findable, Accessible, Interoperable, Reusable) principles [4], and the Semantic Web standards and technologies promoted by the World Wide Web Consortium (W3C), are promising solutions for structuring, linking, querying and reusing data. Ontologies play a relevant role in some of the FAIR principles, especially with regard to data interoperability and re-usability [5]. As a formal representation of knowledge, ontologies provide logical meaning to the data and the possibility to develop a machine-readable data format [6]. Some of them are promoted either by the W3C (https://www.w3.org/standards/semanticweb/) or the Open Biological and Biomedical Ontology (OBO) Foundry (https://obofoundry.org/) which focus on life science research.

Among the OBO Foundry ontologies, FoodOn, the “farm to fork” Food ontology aims to cover food products and broad food processing steps [7] and provides a lingua franca for representing knowledge about food. This ontology addresses animal and plant food sources, food categories and products, and other descriptive facets coming from LanguaL, a mature and popular food indexing thesaurus (http://langual.org). LanguaL has been used to index numerous food composition databases, including the United States Department of Agriculture (USDA) Nutrient Database for Standard Reference (SR) and the European Food Information Resource (EuroFIR) Network of Excellence [8]. However, in 2015, the European Food Safety Agency (EFSA) developed a standardized food classification and description system called FoodEx2 revision 2 (https://www.efsa.europa.eu/en/data/data-standardisation). This system is built to be compliant with European legislation for pesticide residues, chemical contaminants, food additives, biological monitoring data of zoonoses and zoonotic agents, and microbiological criteria for foodstuffs. FoodEx2 consists of descriptions of a large number of individual food items aggregated into food groups and broader food categories in a hierarchical parent-child relationship called the “master hierarchy”.

In this paper, we present PO2/TransformON, a new domain ontology on food and bioproducts engineering for data integration in circular agri-food systems, based on the PO2 core model [9, 10, 11]. New ontology requirements were identified leading both to an evolution of the PO2 core model and to a definition of terms and concepts covering the scope and purpose of the studied domain. We considered that FoodEx2 is an authoritative reference complementary to the Standard Sample Description (SSD2) at the European level used by national agencies in European countries for database annotation and data exchange. We decided to reuse the vocabulary of FoodEx2 for the food and feed hierarchies to build PO2/TransformON concepts and hierarchies. In addition, we built a hierarchy for non-food products to cover the newly defined domain. To this end, the legacy vocabulary of FoodEx2 and other valuable non semantic resources were transformed into linkable data thanks to the fairification process (https://www.go-fair.org/fair-principles/fairification-process/) and transformed to be compliant with the PO2 core model. The PO2/TransformON ontology is built using Semantic Web standards, aiming to be compliant with the FAIR principles, and to be aligned with relevant existing

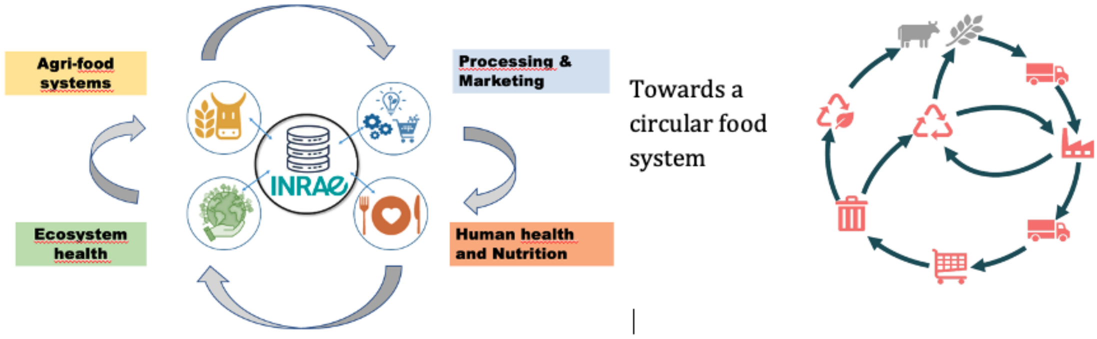


**Figure 1:** Scope and purposes of the domain ontology PO2/TransformON at INRAE.

resource, as e.g. the FoodOn food ontology, which has become an interconnected resource for various academic and government projects that span agricultural and public health domains.

## 2. Why a New Domain Ontology on Food and Bio-products Engineering?

The objective of our domain ontology is to describe food and bio-products engineering, from raw materials (e.g. animal, plant) to end-products (e.g. food), including waste recycling. It covers the characterization of food, feed-stuff, by-products and wastes trough the whole cycle, starting with animal and plant production in agri-food systems, followed by transportation, processing and marketing, then by human consumption and recycling as shown in Figure 1. The scope of our ontology concerns the activities from French National Research Institute for Agriculture, Food and the Environment (INRAE).

The purposes of the domain ontology PO2/TransformON is to model and structure data in order to address/tackle the following general research questions:

1. Life cycle assessment of agri-food systems.
2. Reduction of food loss and valorization of agri-food waste.
3. Process engineering and food eco-design in relations with consumer's perception and preference.
4. Assess and improve nutritional and health aspects of food.

We wanted to reuse and harmonize existing vocabularies from other sub-domain ontologies and reengineer them into a new overarching ontology in order to integrate various data in a unified view. As our main driver was data stewardship, a very strong constraint was to ensure backward compatibility with our existing data-sets [12, 13, 14, 15, 16, 17], structured by the PO2 core model during our former projects. During the specification phase of building the PO2/TransformON ontology, the following needs were identified to cover the targeted domain: 1) process engineering and life cycle assessment, 2) bio-based composite making and characterization of bio products, 3) food eco-design and relations with consumer's perception and preference, and 4) nutritional and healthy aspect of food.

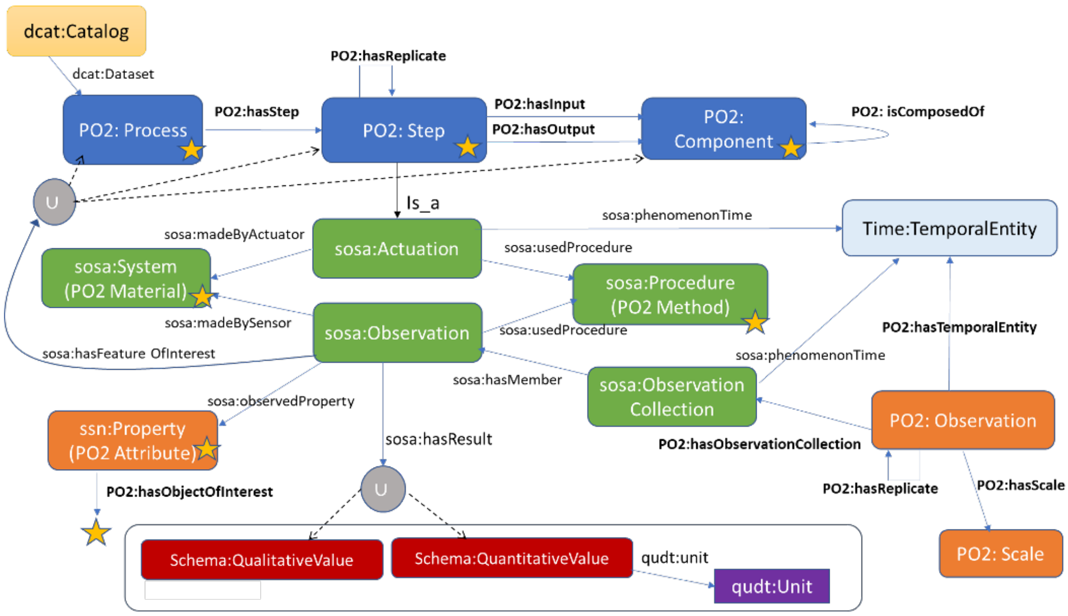


**Figure 2:** PO² core model. Concepts in dark blue constitute the Process part. Concepts in green are SOSA concepts. Concepts in orange constitute the Observation part. Concepts in red and purple constitute the Result part. Objects of interest are materialized by a yellow star.

Those needs where, for the most part, already identified in the previously existing PO2 domain ontologies, but we needed to re-analyze them in the scope of the PO2/TransformON ontology.

## 3. Evolution of the PO² Core Model

This new domain ontology is based on a core model, the PO2, which has been designed to represent a generic process described by a set of steps and experimental observations available for the input and output components of each step of a process. The PO² core model reuses various existing ontologies such as Semantic Sensor Network Ontology (SOSA/SSN) (https://www.w3.org/TR/vocab-ssn/), Time Ontology (https://www.w3.org/TR/owl-time/) and Quantity, Unit, Dimension and Type (QUDT) (https://qudt.org/) and is aligned with the Basic Formal Ontology (BFO) hierarchy (https://basic-formal-ontology.org/).

Figure 2 shows an excerpt of the current version of the PO² core model (V2.3), organized into three parts:

- The "Process part" describes the sequence of steps and the input and output components of a step (concepts in dark blue in Figure 2). A step is a `sosa:Actuation` and has a temporal duration thanks to `Time:Temporal` entity (in light blue).
- The "Observation part" reuses the `sosa:System` and `sosa:Procedure` concepts to the conditions under which the measurements were obtained and describe `PO2:Material` and `PO2:Method` (concepts in green).

- The “Results part” deals with the qualitative or quantitative values obtained from the observations, and units of measure (concepts in red and purple).

As shown in Figure 2, the definition of the range of the property `sosa:hasFeatureOfInterest` implies that observations are about process, steps, or input/output compositions (`PO2:Process`, `PO2:Step`, `PO2:Component`). Both quantitative and qualitative variables are described as results of the observation part (`sosa:hasResult`). `PO2:Observation` is a core concept defined as a `sosa:ObservationCollection` allowing to represent data tables. `PO2:scale` allows to specify the scale of the observation. Each `sosa:Observation` is associated with a value thanks to the relation `sosa:hasResult`. Finally, each value is typed according to the Schema.org vocabulary (Schema.org, https://schema.org/) and quantitative values are associated with a QUDT unit. Besides, Data Catalog Vocabulary (DCAT) metadata (https://www.w3.org/TR/vocab-dcat/) were added to document the data-set annotated with the ontology.

This generic model of PO2 is already well adapted to transformation or characterization processes as illustrated in [10, 11, 18, 14, 19, 20, 21, 22], but Ontology Requirement (OR)s needed to be revised and refined:

- to model a global process of biomass transformation by being able to distinguish between food and non-food products (OR1),
- to be able to distinguish between what comes from primary production, secondary processing and waste (OR2),
- to represent the experimental observations throughout the process by being able to distinguish the object of interest in the observation (OR3),
- to represent the list of types of equipment of a given platform (OR4),
- to be able to retrieve the replications of a process with respect to an experimental design (OR5),
- to identify metadata allowing traceability and harvesting of the ontology and corresponding data-sets once published on the Web (OR6).

These requirements implied considering some evolution of the $PO^2$ core model:

- the control parameters or characteristics (`ssn:Property`) are associated with an object of interest: `PO2:hasObjectOfInterest` property has as range all the concepts with a yellow star in Figure 2.
- the addition of two SOSA/SSN concepts (`sosa:Platform` and `sosa:System`) to be able to register the equipment of a facility or experimental platform.

Let us notice that with the introduction of the new relation `PO2:hasObjectOfInterest`, $PO^2$ core model is compliant with InteroperAble Descriptions of Observable Property Terminology (I-ADOPT) (https://www.rd-alliance.org/groups/interoperable-descriptions-observable-property-terminology-wg-i-adopt-wg), a general framework for representing the variables derived from observations.

When building a domain ontology, seven classes of the $PO^2$ core model should be specialized: `PO2:Process`, `PO2:Step`, `PO2:Component`, `PO2:Material`, `PO2:Method`, `PO2:Attribute` and `PO2:Scale`.

## 4. Collection of Terms and Concepts for the Domain Ontology

To collect the terms and concepts required for knowledge representation in PO2/TransformON, we combined two complementary approaches: first, we followed a bottom-up approach with the existing use cases and data-sets (data-driven approach) [12, 13, 14, 15, 16, 17] and second, we followed a top-down approach for selecting knowledge resources. We used specific services for ontology retrieval such as the Ontology Lookup Service (OLS) (https://www.ebi.ac.uk/ols/index), a repository for biomedical ontologies, and AgroPortal (https://agroportal.lirmm.fr/), an ontology repository for agronomy and related domains. We selected FoodON (https://foodon.org/) as a main resource with respect to food, as well as other OBO Foundry ontologies (https://obofoundry.org/), namely Chemical Entities of Biological Interest (ChEBI) (https://www.ebi.ac.uk/chebi/), Compositional Dietary Nutrition Ontology (CDNO) (https://obofoundry.org/ontology/cdno.html), Ontology for Biomedical Investigations (OBI) (https://obi-ontology.org/), Chemical Methods Ontology (CHMO) (https://www.ebi.ac.uk/ols/ontologies/chmo), Phenotype And Trait Ontology (PATO) (https://obofoundry.org/ontology/pato.html) or The Environment Ontology (ENVO) (http://www.environmentontology.org/), among others.

With respect to the scope and purposes defined in the specification phase, we also considered other non-semantic resources, such as FoodEx2 and the EWC, a hierarchical list of waste descriptions established by Commission decision 2000/532/EC2 for the non-food hierarchy. The International Union of Pure and Applied Chemistry (IUPAC) nomenclature (https://iupac.org/) was also considered as it is the universally-recognized authority on chemical nomenclature and terminology. Other terms and synonyms were also collected directly from the selected use cases with the help of domain experts and literature surveys. The ontology development process relied on human feedback and decisions using a human-centered method [23]. Finally, we integrate these concepts into Simple Knowledge Organization System (SKOS) hierarchies by specializing the PO2 core concepts taken as a SKOS concept scheme (https://www.w3.org/TR/skos-reference/#schemes). Each SKOS concept represents a class of the ontology. Figure 3 shows the top levels of the PO2/TransformON domain ontology together with the Unified Code for Units of Measure (UCUM) module (https://ucum.org/) allowing the standardization of units of measure. The UCUM codes are used to standardized the units of measure. An `owl:dataTypeProperty` associates a QUDT unit with its UCUM code (https://qudt.org/schema/qudt/ucumCode).

### 4.1. The Component Hierarchy

When building the “Component” branch (see Figure 4), we have considered the need to distinguish living organisms from inert substances (i.e., matter, energy, chemical compounds, ...). Living organisms are the sources of raw commodities entering the transformation processes. The “Living organism” sub-hierarchy gathers the categories of living organisms according to the common names of these organisms. Subsequently, alignments to taxonomic resources can be made to link these common names to scientific taxa (for example, the National Center for Biotechnology Information (NCBI) taxonomy, https://www.ncbi.nlm.nih.gov/taxonomy).

The “Substance” sub-hierarchy allows us to classify the substances into five subsequent categories: food, feed, non-food substances, biochemical constituents, and water (generic). The “Food” branch is based on the master hierarchy proposed in FoodEx2. It includes 4234 classes

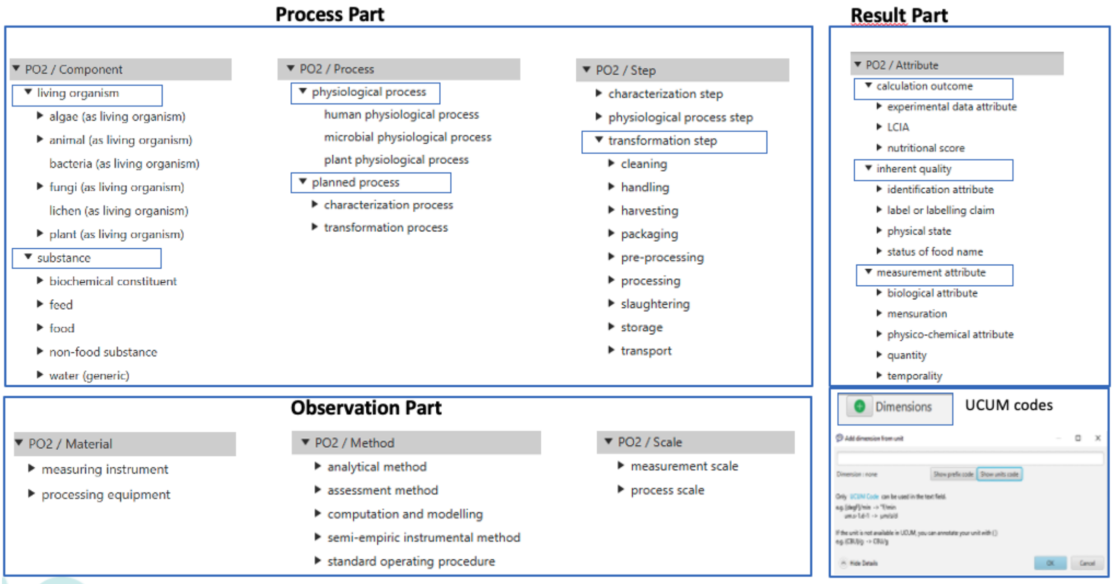


**Figure 3:** Overview of the three parts of the PO2/TransformON domain ontology 1) Process part: PO2/ Component, PO2/Process, PO2/Step; 2) Observation part: PO2/Material, PO2/Method, PO2/Scale; 3)Result part: PO2/Attribute and UCUM codes. Only the top levels are shown.

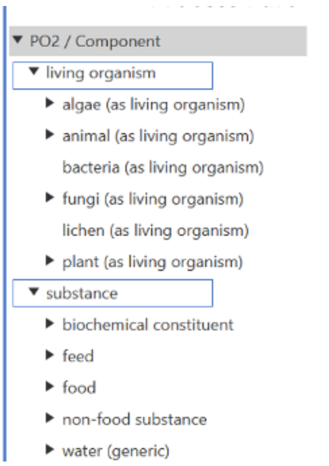


**Figure 4:** The Component Hierarchy.

directly imported from FoodEx2. The "Feed" branch includes 759 classes imported from FoodEx2. To be compliant with this approach, two main subclasses were created in the Feed hierarchy one for grouping all the primary sources of feed and the other one for grouping the compound feed. The ”Non-food substance” branch was created in PO2/TransformON to group all the chemical substances used or produced during transformation processes, considering the role or nature of the substances, namely whether they are organic or inorganic: chemical reagents, cleaning products, energy resources, matter, packaging gas, refrigerant fluids, polluting emissions, and recyclable wastes. The construction of the ”recyclable waste” branch was based on existing reference systems such as the EWC, a hierarchical list of waste descriptions established by the European Commission decision 2000/532/EC2 to harmonize the different nomenclatures existing in the Member States. following the same logic as for the ”Food” and ”Feed” branches of FoodEx2, namely the degree of transformation, we created classes of “primary organic wastes or residues” (animal or plant tissue waste or residues from agricultural production), “secondary organic wastes or residues” (residues or by-products from transformation processes), and “final biowastes” (liquid or solid organic wastes, including sludges and liquid wastes from waste treatment). The “Non-food substances” hierarchy includes 270 classes which can be further specialized into additional sub-classes for other types of by-products and waste encountered in future use cases.

Finally, the “Substance” sub-hierarchy includes two other branches for biochemical constituents and different forms of water. The “biochemical constituents” branch groups all the components that are part of food or feed products (i.e. nutritional compounds or dietary compounds). The “water (generic)” branch allows us to group the different types of water that can be encountered in different physical states or forms such as drinking water, process water, purified water, or water found as a food constituent. The biochemical constituents and water (generic) branches currently include 61 and 29 main classes respectively, but further work of mappings to OBO Foundry ontologies such as CDNO and ChEBI will provide other specific concepts dealing with dietary or chemical constituents [24].

### 4.2. The Process and Step Hierarchies

Two process types have been defined in the PO2/TransformON ontology. Planned processes are processes that follow procedures, whereas biological or physiological processes are unplanned processes. The hierarchy also covers unplanned processes such as spontaneous fermentations or human digestion which will be extended in an upcoming work with the FoodON curation group and the OBO Foundry community. A recent paper already proposed a comparison between W3C OWL ontologies (including PO2) and OBO Foundry’s FoodON ontology for modeling processes [25]. Further work is under progress for organizing material transformation processes into a new upper-level hierarchy within the OBO Foundry’s community. Mappings to OBI (https://obi-ontology.org/) or Core Ontology for Biology and Biomedicine (COB) (https://obofoundry.org/ontology/cob.html) will also provide a connection to analytical protocols and biological processes.

In the PO2 core model, steps are the elementary entities that compose a process itinerary. Each step is a `sosa:actuation` and is also situated under the `bfo:process hierarchy`. The step sub-hierarchy includes 396 classes which were grouped according to the kind of process they belong to (i.e. physiological steps, characterization, or transformation steps). These main subclasses were further divided into subsequent subclasses specializing steps according to the type of event or action they represent. It is worth mentioning that the transformation steps were further divided into several levels of subclasses according to the different nature of the operation (biological, chemical, and physical) involved. The list of steps was taken from the FoodEx2 process hierarchy and other internal resources such as research studies, courses, or books dedicated to food processing.

### 4.3. The "Observation" and "Result" parts

The observation part of PO2/TransformON includes the core concepts that enable the description of materials, methods, and scale of the observation. `PO2 Material` core concept are defined as systems in SOSA/SSN, which can be composed of either transformation equipment (sosa:actuator), or measuring instrument (sosa:sensor). Actuators and sensors can be devices or human agents (e.g., a tasting panel). `PO2 Method` core concept are defined as procedures in SOSA/SSN, which can be either techniques and analytical protocols, or operating instructions and recipes. `PO2:Scale` core concept allows specifying the size of the transformation process (process scale) and/or the size of the observed object (measurement scale). The observable properties are specialized in the `PO2 Attribute` hierarchy. An observable property is any characteristic that describes an object of interest, i.e. a component, a material, a method, an attribute, a step, or a process. `PO2 Attributes` are defined as properties in SOSA/SSN.

The Attribute hierarchy is divided into three main branches: 1) calculation outcomes (characteristics whose values are calculated from other values), 2) intrinsic qualities (characteristics inherent to the objects), and 3) measurement attributes (characteristics obtained from measurement). Much of the FoodEX2 descriptors (also known as "facets") have been imported into the Attribute hierarchy as intrinsic qualities. Measurement attributes were organized into sub-classes according to their nature: biological attributes or physico-chemical attributes, mensuration, quantity or temporality.

An extensive work has been achieved for capitalizing on existing data obtained from published studies involving different sensory evaluation methods. A data-centric typology of sensory evaluation measures [26] has been included in the Method's hierarchy of TransfomON. Work is also underway to ensure that the Attribute's hierarchy of TransformON incorporates sensory descriptors. Bondu et al. [27] proposed a lexicon and a generic wheel of texture descriptors and work is under progress to include the aroma/odor, flavor, and trigeminal descriptors into the Attribute's hierarchy.

## 5. Conclusion and Perspectives

The current version of PO2/TransformON domain ontology provides a vocabulary designed for specific needs to describe transformation processes and characterize food, bio-products, and biomass waste. Our main results consist in defining the ontology requirements, proposing an evolution of the PO2 core model fulfilling those requirements, semantizing FoodEx2, re-engineering existing domain ontologies, and creating a reference system providing unique resource identifiers (URIs) for food, biobased products, and biowaste engineering. In addition, the integration of sensory aspects in the vocabulary constitutes an added value compared to the purely "process" and "safety" points of view initially considered in FoodEx2. Further work is to align new PO2/TransformON concepts to other ontologies, namely FoodOn and interconnected OBO Foundry ontologies. This is the first step that will allow to conciliate production, transformation, and consumption in connection to safe, tasty, healthy, and sustainable food. This work of identifying and selecting useful resources, harmonizing vocabularies and defining and sharing a common reference system enables us to break out of the information silos that usually constitute individual projects.

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## Abbreviations

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|---|---|
| BFO | Basic Formal Ontology |
| CDNO | Compositional Dietary Nutrition Ontology |
| ChEBI | Chemical Entities of Biological Interest |
| CHMO | Chemical Methods Ontology |

| | |
|---|---|
| COB | Core Ontology for Biology and Biomedicine |
| DCAT | Data Catalog Vocabulary |
| EFSA | European Food Safety Agency |
| ENVO | The Environment Ontology |
| EWC | European Waste Catalog |
| FAIR | Findable Accessible Interoperable Reusable |
| I-ADOPT | InteroperAble Descriptions of Observable Property Terminology |
| INRAE | French National Research Institute for Agriculture, Food and the Environment |
| IUPAC | International Union of Pure and Applied Chemistry |
| NCBI | National Center for Biotechnology Information |
| OBI | Ontology for Biomedical Investigations |
| OBO | Open Biological and Biomedical Ontology |
| OECD | Organisation for Economic Co-operation and Development |
| OLS | Ontology Lookup Service |
| OR | Ontology Requirement |
| PATO | Phenotype And Trait Ontology |
| PO2 | Process and Observation Ontology |
| QUDT | Quantity, Unit, Dimension and Type |
| SKOS | Simple Knowledge Organization System |
| SOSA/SSN | Semantic Sensor Network Ontology |
| SSD2 | Standard Sample Description |
| UCUM | Unified Code for Units of Measure |
| USDA | United States Department of Agriculture |
| W3C | World Wide Web Consortium |