

# An online tool for semantic-driven WSIS

**Deliverable 2.1** 

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### **Executive Summary**

**Summary of Deliverable** 

D2.1 is mainly focused on the elaboration of the water smart industrial symbiosis ontology that will permit to establish informational links between industries and processes that permit to understand the possibilities and the impacts to share resources between industries. The work performed has derived on the publication of the WSIS Ontology as the initial asset to establish a common vocabulary to understand the information and share information across industries about this potential reusability of resources (water, material, etc). The main novelty of this ontology relies on the representation of process interlink in terms of different resources. Also, it is important to highlight the interlink on the potential benefits aligned with key performance indicators (KPIS) of the nexus (related to Task 2.4) to facilitate data understanding at different levels (from micro levels to meso levels). Considering these aspects, this ontology has been constructed following an agile semantic developing methodology called <u>SAMOD</u> to facilitate ontology construction, documentation, and publication. Based on this methodology, the ontology has been published under the following link for their reuse and extension:

#### https://aolite.github.io/WSISOntology/

For the construction of the ontology, we used process information about the "<u>CS#2-Nieuw Prinsenland</u>". Complementary to the ontology design, this information have served to the elaboration of the initial version of an online tool called "RIOTER" (Reactive Internet of Thinks). This online tool permit to explore semantic enriched datasets in regard to industrial symbiosis and help to establish strategies to determine industrial symbiosis in companies. All of these assets finally contribute to the main objective of the task in relation to link cross-domain information (water, energy, food, climate and environment) with socio-economic parameters and technology options to generate and assess the medium- and long-term performance of alternative symbiotic strategies and increase eco-efficiency and reliability.

Definitely, the design and implementation of the ontology and the semantic repository contributed to the following aspects:

- Support the data representation to enable circular economy and process symbiosis strategies.
- Provide metadata and context-based information to interlink water management information with industrial process, material and energy industrial fluxes.
- Generating open linked data related to industrial process and the process symbiosis information.
- Support the construction of data models that permit to harmonize the information exchange and the production of Open APIs to explore such information.
- Provide online tool to navigate and explore the information for their understanding and support to elaborate WISIS strategies.





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### **1.Introduction**

#### 1.1. Context

This document is mainly focused on the description of the semantic model (ontology) of WSIS. This ontology and the subsequent semantic repository (called RIOTER) is envisioning to support the rest of WP2 tools to share data and also, to support to understand collected data from the entire WP. Considering these aspects, the WSIS ontology is devoted to (i) elaborate a methodology to interlink processes and industries wastes and needs to enable WSIS; (ii) interlink data and information with representative cross-domain and nexus key performance indicators to support the understanding of actions at different temporal and spatial levels; (iii) align economic costs of the waste categories to complement the WSIS modelling. The elaborated ontology can be accessed through the following URL:

#### https://aolite.github.io/WSISOntology/

The WSIS ontology will be one of the main elements to represent the information and the subsequent context. This ontology will support the decision-making with the interlink between water management, industrial processes and, the use of other reusable resources in industry. Therefore, one of the main challenges of the ontology is to support the data understanding about circular economy and industrial symbiosis practices. Moreover, the ontology will be able to harmonize information exchange, understanding and exploration among different modules that compose the AQUASPICE architecture. Despite the availability of different ontologies like SIM4NEXUS ontology [1], WatERP ontology [2], OFIS [3] or e-Symbiosis [4] developed during the past years, there is the challenge to represent wider linked information to establish a more large-scale, representing more operational information about the process to enable the generation of monitoring and control tools. Also, there is need to disaggregate the information from site-specific information, making the ontology like a catalogue of potential process representation, material representation and also a model to detect waste resource events. Moreover, latest developments on the field for enabling the approaching of industrial symbiosis strategies have been deprecated an not further maintained. This impedes to share knowledge and data using common vocabularies and digital industrial tools. Therefore, this situation has derived to the highlight of industrial siloes and the limitation of the circular economy solutions implementation, scalability and also, transferability.

Recent trends in ontology modelling are confluence to the use of standard data models and ontologies represented by <u>NGSI-LD specification</u> and <u>SAREF</u> ontological ecosystem. At more industrial level, there are proliferating ontologies related to raw materials and materials modelling. In this regards, there are published standard ontologies like <u>MODA</u>, <u>CHADA</u>, <u>OSMO</u> or <u>EMMO</u>. All of this semantic model representation are maintained by relevant institutions like the European Commission, EMMC, or ETSI standardization body. Using these practices, the long-term maintenance of the ontologies are ensured.



Apart from the ontologies, there is also a lack of tools to explore, visualize and navigate through semantic-enhanced data (see Figure 1). This field of semantic enhanced data exploration using facets were initially established in <u>Rizhomer online tool</u> [5]. Under this tool, there is the main key aspect of exploring and filtering information using facets (or interlinks between the information). Another approach were exposed in RDFSurveyor [6] as a tool to explore SPARQL endpoints dynamically through a REST API and SPARQL queries. Complementing types of visualization of SPARQL information, GraFa [7], <u>STOP-IT</u> and eLinda [8] advances on the visualization of dashboarding information from numeric information coming from the queries. Despite the advances on data visualization and exploration, querying SPARQL information through the web is still time consuming and, in some cases, gathering certain information makes these systems to run slowly. As an innovation, ULTIMATE will index and store relevant knowledge graph information through and Open API to make this information available but also to make more dynamic information querying and exploration.

W3C	RDF OWL		SPARQI		Linked Data			OWL 2 ARQL 1.1	RDF :	1.1		RDF Schema 1	.1				* RDF Schem (1999)
Browsers & Exploratory		Flamenco		E		Disco	UI Expl	ed Explorer RIBurner orator Marbles VisiNav Sig.ma Faceted	Visor Sewel et LESS	VВ	X-ENS	Sparklis			nuzzy.link Farbie DFSurveyo		
Specialized Visualization							DBp	edia Mobile	Who's	Who Map4RDF CubeViz LinkedGeoD		Facete Payola LDCE OpenCube Spacetime		ESTA-LD	1		
Multi Visualization					Rhizomer		v	1zBoard	LODW SemL			loon Synopsi Vis Wizard SynopsViz LDVizWiz	is LinkDaViz ViCoMap		LPVA YDS	Elinda	
	2002		2004	+	2006		2008	20	10	2012		2014		2016		2018	2020
Graph-based Visualization		lsaViz Graph Visu RDF-Gravit		PGV			Fenfire	Trisolda RelFir Flext Zoom 3-S Cytosj	Viz RDF	Lodlive LODWheel	S		QueryVO	F4U F2Graph		VizLOD GIG H-BOLD WISP Graphless Tarsier	

Figure 1. Overview of Semantic enhanced visualization (source: "Linked Data Visualization" [9])

Considering these aspects, key innovation of the ULTIMATE ontology and semantic repository is the support and advance on the representation of WSIS data and their subsequent understanding. This innovation derives in the informational interlink between resource parameters, process parameters and process/industries that consumes or produces certain resources. This will definitely contribute to aid decision-making and establish a set of semantic rules and axioms that facilitate the detection of waste processes or circular strategies hotspots. Considering these aspects, the present deliverable will:

• Analysis of the existing semantic development methodologies to select the most appropriate for the development of ULTIMATE semantic model.





- Describe the requirements collected to build the ULTIMATE semantic model.
- Describes the current version of the ontology and their validation over the information collected from case studies.
- Describes the mechanism to test the ontology and the initial dataset loaded into an open shared repository.
- Describe the mechanism to publish the ontology.
- Describe the initial version of RIOTER, the semantic repository and visualization/exploration tool.

The work described under this document corresponds to the efforts performed under the WP2. Specifically, the work described under this document corresponds to Task 2.1 entitled as "Creating a common semantic representation for WSIS". T2.1 is mainly devoted to "elaborate an ontology to determine waste utilization potential of industries and subsequent processes and systems to support WSIS. This ontology will integrate cross-domain indicators (water, energy, environment, food, etc.) with socio-economic indicators to improve the understanding of waste utilization potential at process, industry or industrial cluster level. The innovation lies in integrating knowledge from existing "technical waste ontologies" with "economic cost ontologies", classifying the processing cost of the waste categories and compounds, and thus, extending the categorization of waste compounds and their physicochemical attributes. Then, industry information at process and system level will also consider economic costs to determine associated waste categories and the ability to make symbiotic links between them at local and region scales. This alignment between costs and processes will be complemented with the linkage of this information with the water-nexus ontology and social modelling (using FOAF or SNS ontologies among others). Through this combination we can determine WSIS decision-making implications at the short, medium- and long-term involving information from different domains and triple helix actors (based on semantic SPARQL queries and rules). The ontology will be delivered in the form of an online tool that will be compatible with the KPI tool (T2.4) and would allow interested industries to register their own water-related waste streams and identify promising opportunities for reuse at an industrial cluster and/or regional scale (to be further explored with tools identified in next tasks.".

All developments presented under this document applies an <u>Agile methodology</u>. That is, the work is continuously elaborated according to the project execution and casestudies engagement. For enabling the incremental elaboration of the digital tools, we also elaborated a fast-track methodology for evolving the tools based on the experience. Moreover, the ontology and the semantic repository will be also improved through the rest of the project, reporting the results in rest of WP2 deliverables.

#### **1.2. Document Structure**

The document is organised as follows:

- Section 2 presents the Fast track methodology to implement WP2 tools.
- Section 3 presents the different semantic development methodologies.





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- Section 4 describes the main ontology use-cases and requirements.
- Section 5 focuses on the ontology development and the corresponding parts.
- Section 6 describes the ontology validation and testing.
- Section 7 describes the ontology documentation and publication.
- **Section 8** described the semantic repository and data exploration from casestudy.
- Section 9 concludes the document and discusses the future work.





## 2. Fast Track Methodology

This part of the document is mainly focused on the description of the fast-track strategy for demonstrating the ULTIMATE solutions (see Section 2.1). This strategy will facilitate an early demonstration of the entire solutions to see their impacts and potential results. Moreover, the elaborated strategy will also serve to scale up the solution to the rest of the demo cases based on the best practices learnt.

Considering this fast-track demonstration strategy, Section 2.2 is mainly devoted to the description of The Netherlands (Nieuw Prinsenland) selected as initial demo case as for conducting the study. It has been selected based on the information available, the processes involved and the potential impact benefits to demonstrate the digital solutions.

#### 2.1. Fast-Track strategy

This initial phase of the ULTIMATE project has been devoted to understanding demo cases, their processes and the information available to mention a few. An important aspect of this understanding has been focused on the strategic planning of the physical and digital tools.

Thus, we decided to implement a fast-track for the development of the digital solutions of ULTIMATE with the main purpose of early demonstrate them under a controlled and real scenario. Based on our previous experience on EU projects, a fast-track implementation permit the project to: (i) early demonstrate the solutions; (ii) gather experience on the development and deployment of the solutions; (iii) gather early user feedback to enhance the solutions; and (iv) speed-up the demonstration of the rest of the case studies.



Figure 2. ULTIMATE demo cases (source: https://ultimatewater.eu/demonstration-cases/)

The elaboration of the fast-track strategy was initiated by the pre-selection of potential relevant cases for this first demonstration of the digital solutions. Hence, considering the ULTIMATE demo cases depicted in the following table:





CS#	Name
1	Tarragona (ES)
2	Nieuw Prinsenland (NL)
3	Rosignano (IT)
4	Nafplio (EL)
5	Lleida (ES)
6	Karmiel, Shafdan (IL)
7	Tain (UK)
8	Saint.Maurice l'Exil (FR)
9	Kalundborg (DK)

#### Table 1 ULTIMATE demo-cases identification

We analysed the technology demonstration purposes considering the digital solutions. Considering those demo-cases in which the main purposes are the demonstration of digital solutions, we analyse them transversal aspects such as accessibility to the information, the complexity of the involved processes, response level to partnership petitions, etc. At this stage of the project, the main motivation for the first case of the fast-track is the manageability but also we ensured the balance between the complexity and required time to deploy the entire ULTIMATE solutions. In this regard, the analysis and pre-selection of demo cases are available in the following table:

	CS# 1	CS# 2	CS# 3	CS# 4	CS# 5	CS# 6	CS# 7	CS# 8	CS# 9
# Technologie s	2	3	2	2	3	3	2	1	1
# Digital WISIS solutions	0	0	2	0	1	0	0	0	1
# of		>=	= 8						

Table 2 Pre-selection of ULTIMATE demo-cases for the fast-track

Considering these mentioned aspects, we decided to select the CS#2- "Nieuw Prinsenland (The Netherlands)" as the initial demo case for the fast-track (Figure 3).



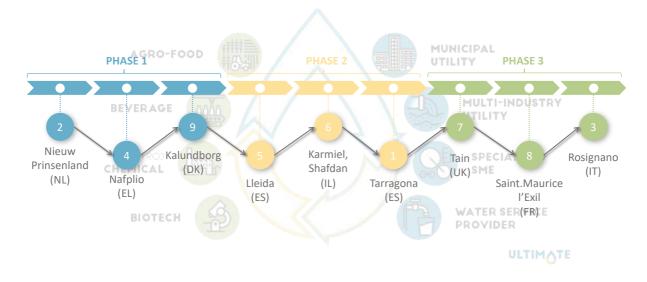


Figure 3. ULTIMATE Fast-track strategy

### 2.2. CS#2: Nieuw Prinsenland (The Netherlands)

The Nieuw-Prinsenland area is a modern agriculture and aiming food cluster at maximum symbiosis among industries (Sugar Factory Suikerunie. high-tech greenhouses. food processing, and bio-energy) water, regards with to energy, and waste. Within case study the #2 in ULTIMATE, solutions will be developed and demonstrated that will facilitate water reuse within



the greenhouses, reuse of resources (nutrients) contained in the wastewater and an energy storage solution that will support efficient deployment of sustainable energy sources for heating of greenhouses.

The water and materials aspects of the case study are performed at De Vlot (Figure 5), a wastewater treatment facility 160 hectares (60 companies) of drain water from greenhouses. The existing water treatment processes (aimed at removal of crop protection agents) are insufficient to achieve full recycling of the wastewater. ULTIMATE will demonstrate the use of membrane technology (electrodialysis) in combination with disinfection (removal of sodium and pathogens respectively) to allow for reuse of the wastewater as irrigation water in the greenhouses (zero liquid discharge). As the wastewater is

Figure 4 Nieuw Prinsenland overview



still rich in nutrients, the safe reuse of these nutrients in the irrigation water stream produced is also investigated.

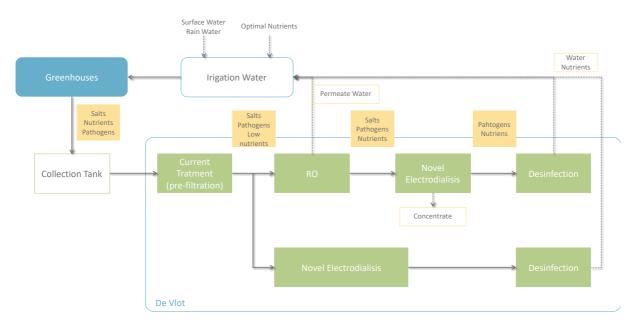


Figure 5 Greenhouses and wastewater process

The third component of the case study is the HT-ATES energy storage system (Figure 5). Greenhouses require energy for heating during winter periods. Currently, they are being heated with fossil energies. Currently, fossil free heating of greenhouses is prepared by using a geothermal source. The challenge with such a heat source is to achieve a balance in demand and supply, as heat demand is not constant throughout the year. A high temperature aquifer thermal energy storage (HT-ATES) is a possible solution to store the excess heat produced during the summer months and use it to supplement the geothermal source during times of high demand (winter).

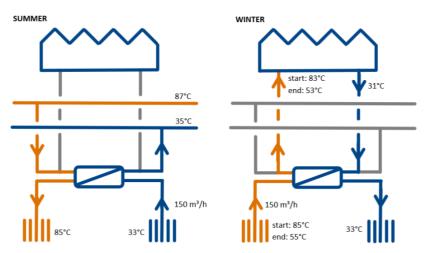


Figure 6 HT-ATES energy storage system





A detailed description of the Case Study, the baseline conditions and the technological solutions to be implemented, have been provided in Deliverable 1.1 and in the supporting information for milestones MS5 and MS9.





# $\bigcirc$

# 3. Semantic Development Methodologies & Challenges

This section focuses on the selection of a suitable ontology development methodology for the ULTIMATE project. The construction of the semantic model in ULTIMATE will comply with the envisioned requirements and, for that, we need to adopt a methodology to ensure all requirements are considered within the ontology modelling. The methodology must provide an efficient way to construct the ontology through different development cycles that comprises the development, testing and publication of the ontology.

Several methodologies have been proposed for the construction of ontologies in the semantic web domain. Among these methodologies are the predictive ontology development methodologies (e.g., Methontology [10], On-To-Knowledge [11] and NeoN [12]). Newer methodologies comprise the application of adaptive ontology development methodologies to build the ontology, based on agile (e.g., SAMOD [13]). Regarding the predictive methodologies, they are mainly focused on the use of a controlled and specific phases to elaborate the ontology. A predictive planning strategy may fail when confronted by significant project specification changes or customer modifications, but it will also be more likely to generate the anticipated result. The development starts with the requirements gathering and finishes with the ontology implementation and publication. Such ontology construction methodologies are similar to iterative software development process methodologies (Figure 7).

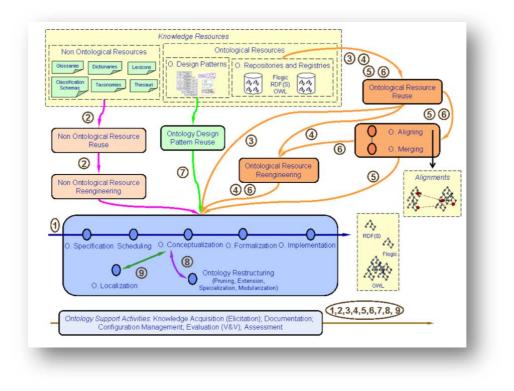


Figure 7. NeON methodology overview [12]



On the contrary, adaptive software methodologies are mainly focused on the highuncertainty in ontology development, giving short-development cycles to adapt to future customer needs. At the end, these methodologies are more susceptible to the ontology development evolution. These kinds of methodologies mainly provide for the elaboration of different cycles to build the ontology. Each cycle comprises the definition of a scenario and then their corresponding modelling based on the different user stories (requirements) generated. At the end of each cycle, a newer version of the ontology is produced, enabling an agile-based extension of the semantic model (Figure 8).

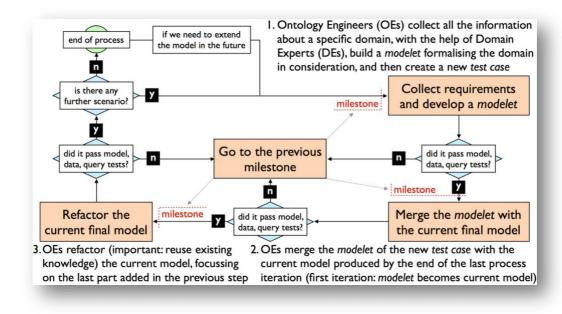


Figure 8. SAMOD methodology overview

### **3.1. Adopted Methodology in ULTIMATE**

The WISIS ontology model is envisioned with the objective of determining waste utilization potential of industries and subsequent process and systems to support industrial and process symbiosis.

The elaboration of the ontology has been performed following the SAMOD ontology development methodology [13]. This methodology is focused on applying agile methodology adapted to develop semantic models. Thus, it permits to elaborate an ontology using SCRUM technique considering sprints, user stories (requirements) and subsequent management using the model Kanban. In this regards, the SAMOD ontology development technique facilitates the elaboration of large-scale ontologies, providing for the collaboration between different teams (in this case, knowledge engineers and domain experts), reusability and the possibility of re-engineering knowledge resources, with the ability to reuse and incorporate other semantic models (e.g., SAREF4WATR, WATERP, GEOSPARQL, etc.) and other data models and schemas (e.g., Smart Water Data models). A summary of the comparison of the





chosen methodology against others considered is presented in Table 1, along certain attributes.

ULTIMATE Needs	Methontol ogy	DILIGE NT	On-To Knowled ge	NeoN	SAMOD
Collaboratio n between different teams	Partially	YES	NO	YES	YES
Inclusion of existent ontologies (or standard ontologies)	YES	NO	NO	YES	YES
Re- engineering of knowledge resources	NO	NO	NO	YES	YES
Continuous enhancemen t and evolution of the ontology	Linear	Based on user's role	Linear	Modules	Cycles
Validation methodolog y for the ontology	Evaluation based on technical elements, documentatio n, and environment (Not Detailed)	NO	Competen cy Questions and Application environme nt	Competenc y Questions, Documentat ion Validation and Technical elements of Ontology	Competen cy Questions and user- story requireme nts based on scenarios
Aligned with large	YES	YES	YES	YES	YES

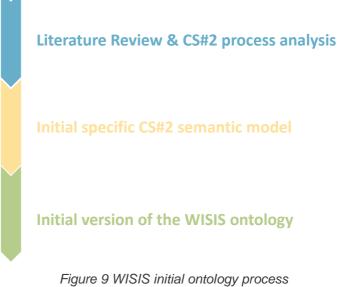




ontology construction					
Support guided ontology construction (Requiremen ts, Design, Implementati on)	YES	Based on user's Role	YES (based on processes)	YES	YES, based on cycles.

 Table 3. Comparison of Ontology development methodologies

Considering SAMOD methodology, the ontology development (Figure 9) started with the analysis of the literature to see the challenges of semantic models for industrial symbiosis. These challenges will serve to distil user stories (requirements) coming from the literature and previous works (see Section 3.2). This aspect is combined with the analysis of the fast-track demo case (see Section complement 2.2) to the corresponding user stories. With the case-study requirements and process information, we elaborated the initial semantic model for the case



study (see Section 4.6). The highlighted point of this specific implementation is to have a vision of the terms and vocabularies to be used combined with the expected interlinks of the information. Based on this information, we modelled the initial general ontology model (see Section 5). When the version of the ontology is ready, it will be merged with the rest of the semantic model. This merging is performed under a GitHub repository to facilitate conflict resolution of the code. When completed, the ontology is tested using <u>OOPS!</u> And <u>FOOPS!</u> Technology and it is documented and published and documented using the LODE technology.



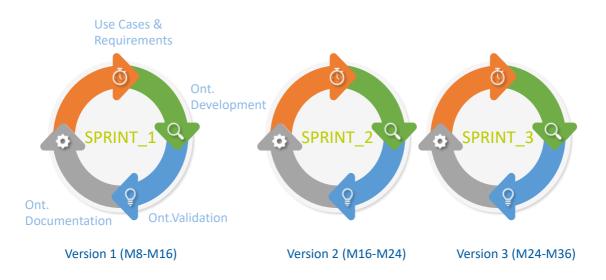


Figure 10. ULTIMATE ontology and semantic repository sprints

The described cycle corresponds to one cycle of the methodology. We envision to execute three different cycles in the framework of the ontology development. The initial two cycles (the ones that is currently described in this deliverable) corresponds to the initial version of the ontology and the semantic repository that includes the main structural aspects of the semantic model aligned with the requirements gathered from the CS#2 and also, the performed literature review (see Section 3.2). These initial cycles will comprise the following features:

Cycle 1 (M8-M16)	<ul> <li>Identification and cataloguing of industrial processes and their corresponding inputs/outputs.</li> <li>Literature review in industrial symbiosis informational modelling and ontologies.</li> <li>Alignment with FIWARE compatibility through SAREF4WATR</li> <li>Initial version of the ontology and their subsequent validation.</li> </ul>
Cycle 2 (M16-M18)	<ul> <li>Incorporation of the identified KPIs</li> <li>Second version of the ontology and their subsequent validation.</li> <li>Initial development of the semantic repository (RIOTER-cube) backed and the exposition of the OPEN-API.</li> <li>Initial development of the data visualization and exploration tool (RIOTER-eye).</li> </ul>

Table 4. Developments performed under the different cycles of the agile methodology

Continuing with the last cycle planned under the Figure 10, the main features to be implemented will be dived according to the following table:





Ontology 3 <sup>rd</sup> cycle (M24-M36)	<ul> <li>Incorporation of economic costs and information</li> <li>Incorporation of rules and semantic reasoning over the information.</li> <li>Third version of the ontology and their subsequent validation.</li> </ul>
Semantic Repository 3 <sup>rd</sup> cycle (M24-M36)	<ul> <li>Refinement of Owner and access to the different repositories</li> <li>Refinement of the automatic visualization with data dashboards and information linkage</li> <li>Incorporation of different semantic repository databases (Quad stores).</li> <li>Incorporation of needed mechanism to enable queries with reasoning.</li> <li>Other visualization of the general model</li> </ul>

Table 5. Planned features and actions to be elaborated under the last sprint cycle





### 3.2. Literature Review & Challenges

This initial stage of the SAMOD methodology is focused on the analysis of the literature in order to identify main needs and challenges in the WISIS. In this regards, we analysed over 50 articles in which we selected 16 most relevant ones according to the objectives of ULTIMATE (listed in Table 6). Mainly, the analysed articles cover the following main topics:

- Economic cost ontologies
- Waste Ontologies
- Nexus Ontologies
- Industry and process Ontologies

Complementing this literature review, we analyse in depth the processes of The Netherlands case study. From this aspect, we distil main terms and concepts to be represented in the WISIS semantic model.

As a result of this analyses, the main challenges and needs identified are related to the (i) combination of information and data from different infrastructure considering the Nexus; (ii) link between real information and measurements about resources with costs and economic aspects; (iii) reason about potential hindered symbiotic links between processes.



Novelty

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He, Y., Hao, C., Wang, Y., Li, Y., Wang, Y., Huang, L., & Tian, X. (2020). An ontology- based method of knowledge modelling for remanufacturing process planning. <i>Journal of</i> <i>Cleaner</i> <i>Production, 258</i> doi:10. 1016/j.jclepro.2020.1209 52	Economic cost ontologies	Remanufacturing that returns used products to a like-new condition with equivalent warranty to match is an emerging triple-win (environmental, economic and social) industry. Process planning plays a vital role in the success of remanufacturing. However, compared with traditional mass manufacturing, the design of remanufacturing process planning (RPP) is far more complex and time-consuming, heavily depending on the experiences of operators. Since each returned used product, namely the raw materials for remanufacturing, is different, a customized RPP tackling the individuality of returned used products is essential. To this end, the reuse of remanufacturing knowledge from past successful RPP could lead to efficient generation of new process planning for new arrivals.	This paper proposes an ontology-based method for knowledge modelling for RPP rapidly. Remanufacturing- ontology provides a unified framework for the management of information and knowledge from various sources. Especially, the remanufacturing knowledge modelling including problem description and problem solution is constructed via a remanufacturing semantic model; Case-Based Reasoning (CBR) method is applied to reuse the knowledge from the most similar previous successful remanufacturing case for the rapid generation of RPP, leading to considerable time and cost saving. An application program is also presented to realize the proposed method.
Zhang, J., Li, H., Zhao, Y., & Ren, G. (2018). An ontology-based approach supporting holistic structural design with the consideration of safety, environmental impact and cost. Advances in	Economic cost ontologies	Presents a holistic approach based on knowledge processing (ontology) to facilitate a smarter decision-making process for early design stage by informing designers of the environmental impact and cost along with safety considerations. The approach can give a reasoning based quantitative understanding of how the	The major contribution of the paper lies on the creation of a holistic knowledge base which links through different knowledge across sectors to enable the structural engineer to come up with much more comprehensive decisions instead of individual single objective targeted delivery.





Engineering Software, 115, 26-39.		design alternatives using different concrete materials can affect the ultimate overall performance.	
Grimaldi, M., Sebillo, M., Vitiello, G., & Pellecchia, V. (2019, July). An ontology based approach for data model construction supporting the management and planning of the Integrated Water Service. In International Conference on Computational Science and Its	Technical waste ontologies	Implementation of SINFI, the National Federated Infrastructure Information Service, whose goal is both to share information about infrastructures and underground utilities and offer a single dashboard that efficiently manages and monitors all interventions.	The aim of this paper is to propose a data model that allows measuring macro- indicators and generating interoperable datasets. An ontological approach has been used that has produced a data storage model as implemented in the Semantic Web.





Ceccaroni, L. (2001, October). Ontowedss - an ontology-based environmental decision-support system for the management of wastewater treatment plants.	Technical waste ontologies	Interdisciplinary research on artificial intelligence techniques (rule-based reasoning, case-based reasoning, ontologies and planning) applied to environmental decision-support systems. The integrated architecture's design of this applications, the OntoWEDSS system, augments classic reasoning systems (rule-based reasoning and case-based reasoning) with a domain ontology about the management of wastewater treatment plants.	The integrations of the created WaWO provides a more flexible management capability to OntoWEDSS. The construction of the OntoWEDSS decision support system is based on a specific case study but the system is also of general interest, given that its ontology-underpinned architecture can be applied to any wastewater treatment plant and, at an appropriate level of abstraction, to other environmental domains. The OntoWEDSS system improves the diagnosis of the state of a treatment plan, provides support for wastewater-related complex problem- solving, and facilitates knowledge modelling and reuse by means of the WaWO ontology.
Kultsova, M., Rudnev, R., Anikin, A., & Zhukova, I. (2016, July). An ontology-based approach to intelligent support of decision making in waste management. In 2016 7th International Conference on Information, Intelligence, Systems & Applications (IISA) (pp. 1-6). IEEE.	Technical waste ontologies	A concept of intelligent support of decision making in waste management using knowledge-based approach is presented, which is a promising way to increase efficiency of waste management system in the cities. Analysis of the domain of waste management shows that the appropriate support of decision making can be implemented using contemporary technologies of artificial intelligent such as rule-based reasoning and ontology.	A general scheme of the integration of this reasoning mechanism and ontology is suggested, as well the problems of domain knowledge representation are considered. Implementation of a prototype of intelligent decision support system in waste management using rule- based reasoning and ontology is described.



Albrecht, T. R., Crootof, A., & Scott, C. A. (2018). The Water-Energy-Food Nexus: A systematic review of methods for nexus assessment. <i>Environme</i> <i>ntal Research</i> <i>Letters, 13</i> (4), 043002.	Nexus ontologies	This paper reviews WEF nexus methods to provide a knowledge base of existing approaches and promote further development of analytical methods that align with nexus thinking. The systematic review of 245 journal articles and book chapters reveals that use of specific and reproducible methods for nexus assessment is uncommon; nexus methods frequently fall short of capturing interactions among water, energy, and food; assessments strongly favour quantitative approaches; use of social science methods is limited; and many nexus methods are confined to disciplinary silos.	This paper finds that to address complex resource and development challenges, mixed-methods and transdisciplinary approaches are needed that incorporate social and political dimensions of water, energy, and food; utilize multiple and interdisciplinary approaches; and engage stakeholders and decision- makers.
Endo, A., Burnett, K., Orencio, P. M., Kumazawa, T., Wada, C. A., Ishii, A., & Taniguchi, M. (2015). Methods of the water- energy-food nexus. <i>Water</i> , 7(10), 5806-5830.	Nexus ontologies	This article presents the key methodological results from the Water- Energy-Food Nexus (WEFN) project by the Research Institute for Humanity and Nature (RIHN). The objective of the project is to maximize human- environmental security (i.e., minimize risk) in the Asia-Pacific region by choosing policies and management structures that optimize WEF links, including water-energy (water for energy and energy for water) and water-food (water for food) connections.	The approach is based on the view that it is important for transformative, sustainable solutions to maximize human-environmental security and decrease vulnerability by optimizing the linkages within the WEF clusters. The populations that live under these natural circumstances face an elevated risk of negative impacts due to natural disasters, while also benefiting from abundant ecological goods and services. Thus, there are trade-offs and conflicts within WEF resources, as well as among the region's various resource users.





Kumazawa, T., Hara, K., Endo, A., & Taniguchi, M. (2017). Supporting collaboration in interdisciplinary research of water– energy–food nexus by means of ontology engineering. <i>Journal of</i> <i>Hydrology: Regional</i> <i>Studies, 11</i> , 31-43.	Nexus ontologies	Discussion of the effectiveness of ontology engineering approach in the process of collaborative research, and propose the way of ontology use contributing to interdisciplinary research through the experimental workshops of research development.	The introduction of ontology engineering approach will enable us to share a common language and a common theoretical basis. But the development of the new method based on ontology engineering is necessary.
Babaie, H., Davarpanah, A., & Dhakal, N. (2019). Projecting pathways to food–energy–water systems sustainability through ontology. <i>Environmenta</i> <i>I Engineering</i> <i>Science</i> , <i>36</i> (7), 808-819.	Nexus ontologies	The FEWsOnt ontology models major structural and dynamic concepts of the food–energy–water (FEW) systems from the complex system perspective by defining the emergent, nonlinear, and scale-invariant state transitions and behaviours of the network elements that result from natural and planned processes. It explicitly specifies major concepts and interactions among the FEW systems and their relations to social and natural systems, applying a network system approach and semantic web technologies and defines a formal terminology that annotates the FEW concepts from a complex and adaptive system perspective.	The processes that change the state of the system elements are modelled with a scale-invariant view across several systems' organizational levels. The processes and links among system elements are constructed based on their positive or adverse effects on sustainability. This approach will allow users to discover the dynamic interactions among the FEW systems' components through queries and optimize the trade-offs by choosing the pathways toward sustainability.





Endo, A., Kumazawa, T., Kimura, M., Yamada, M., Kato, T., & Kozaki, K. (2018). Describing and visualizing a water– energy–food nexus system. <i>Water</i> , <i>10</i> (9), 1245.	Nexus ontologies	An ontology engineering method, which is a qualitative method, was applied for the replicability of the WEF nexus domain ontology and the map, because ontology engineering is a method of semantic web development for enhancing the compatibility of qualitative descriptions logically or objectively. The WEF nexus system map has three underlying concepts: systems thinking, holistic thinking, and an integrated approach at an operational level.	nexus system and create policy options and scenarios to solve the identified nexus problems under scientific evidence and uncertainty to maximize human environmental security, with the hypothesis that the use of water resources for food and energy production in a land area affects the
Sarason, Y., & Conger, M. (2018). Ontologies and epistemologies in 'knowing' the nexus in entrepreneurship: Burning rice hay and tracking elephants. International Journal of Entrepreneurship and Small Business, 34(4), 460-479. doi:10.1504/IJESB.2018. 093602	Nexus ontologies	In order to further the understanding of the dominant assumptions of the nature of the nexus (ontology) and our understanding of the nexus (epistemology), we interpret and reinterpret a case of an entrepreneurial venture in Vietnam.	They propose that a multi-paradigm analysis in entrepreneurship will yield insights that are applicable to a more global perspective of entrepreneurship.



da:, P., & Rahman, M. M. Legal ontology for nexus: Water, energy and food in EU regulations. https://core.ac.uk/downl oad/pdf/76520246.pdf	Nexus ontologies	Objectives of the thesis are – (a) to identify the problems in water-energy- food nexus from ICT and Law point of view and to propose theoretically a legal knowledge framework for water- energy-food nexus in order to reduce those problems technologically, (b) to construct and implement legal ontology for nexus extracted from EU water, energy and food Regulations in OWL 2 language, which is a part of the grater work of implementing legal knowledge framework for water-energy-food nexus proposed through the compilation of objective (a).	Firstly two sets of evaluative criteria have been developed for twofold purposes – (a) to set standard criteria for construing legal ontology for nexus, and (b) to evaluate current legal ontology modelling perspectives and methodologies in order to find the correct one used for this research purpose. Secondly, evaluation of existing methodologies of constructing legal ontology has been performed. The findings led the necessity to develop a new and modular based methodology for legal ontology for nexus which is presented in detail.
Ghodsvali, M., Krishnamurthy, S., & de Vries, B. (2019). Review of transdisciplinary approaches to food- water-energy nexus: A guide towards sustainable development. Environm ental Science & Policy, 101, 266-278.	Nexus ontologies	This paper provides a systematic literature review to debate the current concepts and methods of the transdisciplinary research on the FWE nexus with the aim of developing a guide for socially inclusive sustainable development. Although the concept of transdisciplinary has been widely accepted by nexus research, an explicit cognition of its practicability in real- world is still lacking, and sophisticated methodological development is required.	They proposed a conceptual framework to explore the potential contribution of transdisciplinary towards linking FWE nexus practices and sustainability outcomes in real-world situations. This framework is useful in steering the management of nexus issues with integrative perspectives. Relying on the proposed framework, they made recommendations for successful transdisciplinary nexus practices.

Table 6. Result of the literature review analysis





# 4. ULTIMATE Ontology Requirements and use-cases

The main purpose of the ULTIMATE semantic model is to interlink industrial processes and industries to better understand symbiotic pathways and resource reuse strategies. For that, we have to integrate contextual information like process information, industry location and also type of industries involved. Complementary, we need to integrate operational information about the processes covering aspects like databases, sensors, Internet of Things (IoT) devices, monitoring and control tools, etc. The proposed ontology should be able to harmonize different type of information as same time as reasoning about processes to detect complex operational events that derive in resource waste and inefficiencies. The ontology will provide a common data understanding of this information based on the context (their use). Moreover, semantic enriched data representation should be aligned with current standards from the integrated domains.

In the view of this initial required aspects, the main purpose of the WSIS ontology is to provide a complete informational understanding about the interlink and symbiotic relations between industries and processes. Another key aspect relies on the symbiotic information interlink with economic and other relevant Nexus KPIs.

#### **4.1. Scope**

The main scope of the ULTIMATE ontology is to face the main challenges identified under the literature review. Thus, the semantic model will be mainly devoted to (i) combine information and data from different infrastructure considering the Nexus: (ii) link between real information and measurements about resources with costs and economic aspects; (iii) reason about potential hindered symbiotic links between processes. These variables and information in most of the cases represent the devices and industrial systems related to process monitoring in a broad of domains (industry, farming, textile, etc.). So, one of the main aspects of the ontology is to make understandable the information collected from the different devices and harmonize such information under a common data model compatible with FIWARE. FIWARE is a curated framework of open-source platform components to accelerate the development of smart solutions [14]. This compatibility is required due to the adoption of FIWARE as a reference architecture for data ingestion, collection, knowledge discovery and visualization. Based on this, the ontology needs to follow standard definitions and terms adoptions from representative organizations (World Meteorological Organization -WMO-, OGC, INSPIRE, W3C, FIWARE, etc.).

#### **4.2. Implementation Language**

The selected implementation language for the ontology is OWL, the Ontology Web Language. The serialization format will be performed with the use of the Turtle (TTL)





language and JSON-LD serialization to expose the corresponding information and variables acquired and stored in the different data sources as the semantic repository and non-structured databases. In case required, we will explore the possibility of using semantic rules to perform ontology alignments (using SPARQL Inferencing notation - SPIN- [15], Semantic Web Rule Language -SWRL- [16]), and also model water management, energy management and material management events that occurs at operational level inside the industries (e.g. alerting about water, energy and material wastes at operational level).

### **4.3. User Groups identified for the ULTIMATE**

#### ontology

The potential end-users that will consume and explore the information modelled under the ULTIMATE semantic model are represented under the following table:

User Group (UG)	Name	Description
UG-1	Industrial Managers	Group focused on (i) managing processes inside industries; (ii) control efficiency in the process; and (iii) monitor resources wastes
UG-2	Industrial Operators	Group focused on (i) controlling the different processes; (ii) defining local parameters of the industrial processes; (iii) determining industrial process thresholds; and (iv) monitoring industrial infrastructure.
UG-3	Water Authorities	This group will be focused on: (i) elaborating water management and water quality policies; (ii) determining hazardous contaminants and spills.
UG-4	Water Managers	This group will be focused on: (i) determining water management procedures; (ii) analysing water related indicators; (iii) identifying water management alerts/anomalies
UG-5	Water Operators	This group will be focused on: (i) defining water parameters for the operations; (ii) determining water management thresholds; (iii) monitoring water infrastructure inside industries too.





User Group (UG)	Name	Description
UG-6	Risk managers	This group is devoted to (i) elaborate industrial risk plan and specially in industries with harmful materials, (ii) interlink vulnerabilities with contextual industrial information.
UG-7	Farmers	This group is devoted to (i) monitoring and control farming production; (ii) establish thresholds for ensuring the production; (iii) reuse water that permits to create an efficient production and reduce costs.
UG-8	Society/Citizens	This group is aimed at (i) exploring circular economy strategies; (ii) visualise the benefits of the industrial symbiosis and circular economy to the region.

Table 7. ULTIMATE user groups

#### 4.4. ULTIMATE Use-cases

Following the SAMOD methodology, the use-cases (or test-cases) identified are derived from the information exchange with the CS#2 and the performed literature review (see Section 3.2). The combination of these information have served to initially identify different use-cases that are presented in the following tables:

Name	Water Management Information Exchange
Description	In ULTIMATE, capturing heterogeneous information coming from water management infrastructure to analyse current scenarios of water management in urban areas and industries. This will comprise the information collection of the state of the lakes, tanks, pumps, etc. It should comprise the information collection of the supply and distribution value chain of the water infrastructure
Example-1	There is a need to represent the (waste) water tank levels
Example-2	There is a need to determine current state of the pumps

Table 8. Use-Case of Water Management





Name	Process interlink and management	
Description	In ULTIMATE, there is a need to contextualise the industries and also, to characterise the resource providers and resource consumers. In this regard, the consumption and supply of resources should be represented at both, industrial and process level.	
Example-1	Determine the type of resource inputs and outputs in the process	
Example-2	Determine the quantity of resources needed	

Table 9. Use-Cas of process interlink

Name	Energy Management Information exchange	
Description	In ULTIMATE, there is a need to contextualise the industries and also, to characterise the resource providers and resource consumers. In this regard, the consumption and supply of resources should be represented at both, industrial and process level.	
Example-1	Determine the type of resource inputs and outputs in the process	
Example-2	Determine the quantity of resources needed	

Name	Material management in the industries		
Description	Consideration of the material fluxes in the processes. In this regard, there is a need for the determination of the material supply and generated in the industrial processes		
Example-1	Consideration of material supply and consumption by each of the processes		
Example-2	Categorization of the materials at industrial level		







### 4.5. ULTIMATE Uses

Based on the different use-cases identified, we consider the following ontology uses that will serve to conform the actions to be represented inside the different types of requirements. Thus, the following uses are envisioned for the ULTIMATE ontology:

Uses	Concept	Description	
Use-1	Integrate heterogeneous information (systems)	Pull and Push information from different data sources (Sensor-based information, BBDDs, decision-making tools, thematic/general models, hydrometeorological models, wearables, etc.) coming from water infrastructure, energy infrastructure or industrial processes.	
Use-2	Standard- based serializations	Provide the information to the systems and visualization engine using standard-based serializations coming from water, energy, materials and industrial level.	
Use-3	Navigate through the information	Permit to navigate throughout the information in order to support semantic facet navigation	
Use-4	Navigate through geospatial information	Provide navigation through different maps and types of layers.	
Use-5	Determine input/outputs process resources	Provide information about the inputs and outputs of processes and industrial resources.	
Use-6	Determine symbiotic states	Determine symbiotic states between processes and industries.	

Table 12. ULTIMATE ontology uses





### **4.6. ULTIMATE Requirements**

This part of the ontology development aims at describing the functional and nonfunctional requirements that the ontology must fulfil. The identified functional requirements are represented in the form of **Competency Questions (CQs)**. These questions need to satisfy the user requirements and serve as ontology validations about the informational uses of the representative users. The non-functional requirements of the ontology describe the extra features that the semantic models need to satisfy (e.g., multi-language representation). As a result, the informational requirements of the user are identified and planned to be included in the ontology to be elaborated. This will establish the base of the entire platform and informational navigation of the semantic repository.

#### **4.6.1. Functional Requirements**

For the elaboration of the functional requirements, we adopted a bottom-up approach for a better understanding of the domain. Specifically, we have involved the different users and information throughout the ULTIMATE case-studies (specially CS#2). Also, we have involved technology providers and specialists from WP2 in the elaboration of digital tools for the WISIS (Sherwood plots, optimization tools, high visualizations and KPI tools). This involvement has been produced coming from the different online meetings from WP2 but also in offline mode by the exchange of different emails to gather information and process. The result of these actions has been translated into CQs that include, for each of the presented questions, the feature (question) and an example of the corresponding answer that should be retrieved from the system. The identified CQs are:

ld	Competency Question	Answer
UCQ-1	Which assets are involved in the water/energy/industrial infrastructure?	Water pipe, energy storage system, DAF, etc.
UCQ -2	What types of sensors are involved in the infrastructures?	Energy meter, water meter, water flows, tank level
UCQ -3	What type of actuators are involved in infrastructures?	Pumps, valves, etc
UCQ -4	What type of processes are involved in the demo-case X?	Farming Operation, Oil refining, etc
UCQ -5	What type of technology have been implemented in the industry X?	Screening, Mixing Tank, etc





ld	Competency Question	Answer
UCQ -6	What is the volume of water exiting process X?	123L
UCQ -7	What is the energy flux in process X between 01-01-2022 and 01-03-2022?	01-01-2022 200Kwh, 02-01- 2022 203Kwh, 03-01-2022 190Kwh,
UCQ -8	What are the physical parameters of measurement X?	Energy flux, water flux, etc
UCQ -9	What is the region of the industry X?	POLYGON (10,10,10,10)
UCQ - 10	What are the industries related to the industrial region X?	Resource provider X, resource consumer Y
UCQ - 11	What kind of technology takes part of industry X?	Technology A, technology B, etc
UCQ - 12	What kind of resources are needed in process X?	Water, energy, etc
UCQ - 13	How much resource are required in process X?	200kwh of energy
UCQ - 14	What kind of resources are generated by process X?	Water, energy, etc
UCQ - 15	How much resource are generated by process X?	100 m3 of water

Table 13. Competency question to enable WISIS

#### **4.6.2.Non-functional requirements**

The proposed non-functional requirements are focused on determining transversal functionalities that the ontology should fulfil. In this regard, the following table represents the non-functional requirements for the presented ontology:





ld	Non-Functional Requirement
NFR-1	The ontology needs to be compatible with water standards for information exchange as WaterML2, NGSI-LD, WoT or INSPIRE
NFR-2	The ontological terms should have their specific definition.
NFR-3	The ontology must support a multilingual information representation in the following languages: English, and case studies local languages

Table 14. Non-Functional requirements of WISIS ontology

## **5.WSIS ontology development**

This part of the WSIS ontology development comprises the formal construction and publication of the ontology. In this regard, this specific section will initially cover other relevant initiatives considered for the ontology development (Section 5.1) including relevant associations, H2020 projects and standards. These initiatives have been used to select a more relevant glossary of terms to be exposed under Section 5.2. represents the different parts of the ontology to cover the different requirements exposed within Section 5.3.

## **5.1. Relevant Initiatives**

This part of the document mainly represents relevant initiatives used for the elaboration of the glossary of terms and formal definition of the WSIS ontology. For that, we revised, apart from the performed literature review, relevant H2020 projects and standards that contain data specifications, data models and ontologies.

### 5.1.1. Standardization Activities

In relation to the standardization activities, the following table depicts the most relevant related to industrial symbiosis and also, nexus indicators:

Standardization Activities	Description
ETSI STF 534	This group launched by ETSI is devoted to the creation and maintenance of the SAREF extensions to the domains of smart cities, smart industry and manufacturing, smart agri- food, smart water and environment. All of these are under the umbrella of SAREF to integrate semantically information about vertical domains. The terms of this initiative will be





Standardization Activities	Description
	considered for the construction of AQUASPICE, specially SAREF4WATR and SAREF4ENV.
ETSI-GS-CIM-001	This standard refers to the Context Information Management specification under the so-called NGSI-LD specification. This specification is mainly devoted to allow users to provide, consume and subscribe to context information in multiple scenarios and involving multiple stakeholders. It enables close to real-time access to information coming from many different sources (not only IoT data sources).
Open Geospatial Consortium (OGC)	The Open Geospatial Consortium has defined WaterML 2.0, an information model for the representation of water observations data, with the intent of allowing the exchange of such data sets across information systems (https://www.opengeospatial.org/standards/waterml). Moreover, the latest version of WaterML 2.0 (part 3) includes the informational model called HY_FEATURES that is focused on representing hydro-science and water network topology. The latest developments comprise the elaboration of Sensor Things API (https://www.ogc.org/standards/sensorthings). Complementing this information, the OGC also offers CityGML ADE, for the representation of utility networks in 3D city models (http://www.citygmlwiki.org/index.php/CityGML_UtilityNetw orkADE)
OneM2M	IoT standard devoted to the elaboration of IoT reference architecture. This initiative contains ontological models for the elaboration of syntactic and semantic interoperability of IoT Systems. Additionally, it also includes XML schemas.
ISO/TC 184	ISO standard focused on automation systems and their integration for design, sourcing, manufacturing, production and delivery, support, maintenance and disposal of products and their associated services





Standardization Activities	Description
ISO/TC 184/SC 4	ISO standard focused on industrial data standards.

Table 15. WSIS Standardization activities

#### 5.1.2. Association initiatives

In terms of EU and international associations, the ones that are related to WSIS and IoT systems are the listed in the following table:

Association Initiatives	Description
ΑΙΟΤΙ	The Alliance for Internet of Things Innovation (AIOTI) is a multi-stakeholder platform for inspiring IoT Innovation in Europe that combines large and small companies, academia, start-ups and scale-ups, end-users, policy makers and representatives of society in an end-to-end approach (https://aioti.eu/). Two of the AIOTI working groups are relevant for three works: Smart Water Management, Manufacturing and IoT Standardization (semantic interoperability)
Water Europe	The Water Europe (http://watereurope.eu/) mission is to foster collaborative, innovative and integrated European research and technologies development, to ensure the European growth and competitiveness of the water sector, to provide global answers to global challenges for the next generations, and to address the challenges of integrated and sustainable management of water resources.
ICT4WATER cluster	The ICT4Water cluster is a hub for EU-funded research and innovation projects developing digital innovations for the water sector (https://www.ict4water.eu/). It brings projects together supporting them to exchange information and best practices, disseminate and exploit project outputs, contribute to defining digital water strategies, and contribute to policy development in the digital and water domain.
IWA	The International Water Association (IWA) is an open platform in which both innovators and adopters of new technologies and approaches can generate creative friction; it is a place for diffusion, benchmarking and evidence





Association Initiatives	Description
	(https://iwa-network.org/). The IWA develops research and projects focused on solutions for water and wastewater management, organizing events that bring the latest science, technology and best practice to the water sector at large, and working to place water on the global political agenda and to influence best practice in regulation and policymaking.
Corss-Synergies	The cross-synergy working group is the alliance of the latest H2020-SC5-11 projects to elaborate common actions on ontologies and data models, sensors, AI data-driven models, business and communication and dissemination activities. Concerning WSIS ontology, interests are on the Smart Data Models (https://www.fiware.org/developers/smart-data-models/) alignment with the reference architecture and the ontology.
EFFRA	The Made In Europe partnership will be the voice and driver for sustainable manufacturing in Europe. It will boost European manufacturing ecosystems towards global leadership in technology, circular industries and flexibility. The Partnership will contribute to a competitive, green, digital, resilient and human-centric manufacturing industry. It will be at the centre of a twin ecological and digital transition, both a driver and subject to these changes.
ONTOCOMMONS	OntoCommons is an H2020 CSA project dedicated to the standardisation of data documentation across all domains related to materials and manufacturing. OntoCommons lays the foundation for interoperable, harmonised and standardised data documentation through ontologies, facilitating data sharing and pushing data-driven innovation, to bring out a truly Digital Single Market and new business models for European industry, exploit the opportunities of digitalisation and address sustainability challenges.
BRIDGE	BRIDGE wants to provide field experience, feedback and lessons learned from the participating projects to help overcome the barriers to effective innovation. It aims at gathering coordinated, balanced and coherent recommendations to strengthen the messages and maximize their impacts towards policy makers in view of removing barriers to innovation deployment.





Table 16. WSIS Standardization activities

#### **5.1.3. European projects Initiatives**

In terms of EU project activities, we revised and selected the following projects and their relevant outcomes related to the ontology objectives and scope:

EU project Initiatives	Description
H2020-SIM4NEXUS	SIM4NEXUS (https://www.sim4nexus.eu/) aims to predict society-wide impacts of resource use and relevant policies on sectors such as agriculture, water, biodiversity and ecosystem services through a model-based analysis. This project aims to adapt existing knowledge and develop new expertise on the Nexus; to reduce uncertainty, and to show the implementation by a network of regional and national cases.
H2020-B-WATER- SMART	B-WATER-SMART (https://b-watersmart.eu) aims to speed up the transition to water-smart economies and societies in coastal Europe and beyond. To achieve this, it will adopt a large-scale systemic innovation approach to select, connect and demonstrate tailored solutions for multiple users and sectors. It will further create new business models based on circular economy and water-smartness
H2020- FIWARE4WATER	This project began in June 2019 and intends to link the water sector to FIWARE© by demonstrating its capabilities and the potential of its interoperable and standardized interfaces for both water sector end-users (cities, water utilities, water authorities, citizens and consumers), and solution providers (private utilities, SMEs, developers).
LIFE-eSymbiosis	The project aimed to develop a knowledge-based service that will promote, demonstrate and advance Industrial Symbiosis (IS) in Europe.
H2020-EMMC-CSA	EMMA-CSA aimed at establishing current and forward- looking complementary activities necessary to bring the field of materials modelling closer to the demands of manufacturers (both small and large enterprises) in Europe. The ultimate goal is that materials modelling and simulation will become an integral part of product life cycle management in European industry, thereby making a strong contribution to enhance innovation and competitiveness on a global level





Table 17. WSIS European projects initiatives

#### **5.1.4. Relevant Ontologies related to WSIS**

In consideration with relevant ontologies, the following table shows the ones related to ULTIMATE ontology:

Ontology Initiatives	Description
WAWO+ ontology	Waste Water Ontology (WaWO) (http://www.cs.upc.edu/~loliva/OntoWAWO+.owl ) has been developed to model information about wastewater treatment tasks through the definition of the basic terms and relations comprising the vocabulary of the wastewater treatment area. It is the demonstration of a shared understanding of the wastewater domain that is agreed among several agents: mainly, experts in chemical, environmental and engineering. The main aim of the WaWO ontology is to design a model that: presents a vocabulary for the wastewater domain that all agents can jointly use and understand by describing the meaning of each term in an as unambiguous and precise manner as possible.
SAREF4WATR	This ontology is mainly focused on representing water infrastructure and the corresponding measurements. Despite this focus, the ontology considers water quality monitoring and also, the alignment of different water quality events with different types of waters.
SAREF4ENVI	SAREF4ENVI has two main aims: on the one hand, to be the basis for enabling the use of SAREF in the environment domain and, on the other hand, to exemplify how to enable interoperability between environmental devices in cooperation.
SAREF4INMA	SAREF4INMA focuses on extending SAREF for the industry and manufacturing domain to solve the lack of interoperability between various types of production equipment that produce items in a factory and, once outside the factory, between different organizations in the value chain to uniquely track back the produced items to the corresponding production equipment, batches, material and precise time in which they were manufactured
SAREF4ENER	SAREF4ENER focused on extending SAREF to the representation of energy management in buildings and other infrastructures. It was the initial ontology in which part





Ontology Initiatives	Description
	of the ontology have derived on the ontology today we know as SAREF.
OFIS	The ontological framework for Industrial Symbiosis (IS) exploits semantic knowledge modelling and enables structural data transformation for identification of potential synergies between various industries and hence formation of one to one and complex symbiotic networks.
e-Symbiosis	A new ontology framework for Industrial Symbiosis by pioneering the use of ontology engineering in the field. Semantics are used to model Industrial Symbiosis flows, to model enabling technologies and to systematise the development of a matching service.
MODA	A web portal devote to the categorization of models equations and simulations in relation to industrial symbiosis and process modelling.
CHADA	A data management portal and framework devoted to material characterization based on datasets that covers (i) sample, (ii) method, (iii) raw data and (iv) data analysis as the main component of the metadata associated to any characterization experiment.

Table 18. WSIS ontology initiatives

#### **5.1.5.Other initiatives**

In this part of the document, we describe the directives and other industrial reports that are relevant for the formal specification of the WSIS ontology.

Ontology Initiatives	Description	Description
INSPIRE	Directive	The INSPIRE Directive aims to create a European Union spatial data infrastructure for EU environmental policies or activities which can have an impact on the environment (http://inspire.ec.europa.eu/). This European Spatial Data Infrastructure will enable the contribution of environmental spatial information among public sector organizations, providing public access to spatial information across Europe and assisting in policy-making across boundaries.
EU WFD	Directive	The EU Water Framework Directive (WFD), adopted in





		2000, requires effective water management and helps Member States prepare for extreme weather events which, due to climate change, are becoming more frequent and cause tremendous damages (http://ec.europa.eu/environment/water/water- framework/).
WISE	Data Repository	The Water Information System for Europe (WISE) is a partnership between the European Environment Agency and European Commission (DG Environment, Joint Research Centre and Eurostat) (https://water.europa.eu/). It is a collective database created around the subject of water management in Europe that holds all the significant information on this matter, hence composing a new, comprehensive, shared EU data and information system for water, with river basins. It presents water-related information and data organized in four broad areas: projects, policy, links, themes, and data.
GEOSS	Data Repository	The Global Earth Observation System of Systems (GEOSS) is a collection of independent, coordinated, Earth observation, information and processing systems that relate and provide access to heterogeneous information for a huge range of users in both private and public sectors (http://www.geoportal.org/).
Copernicus	Data Repository	Copernicus is a European system for controlling the Earth and is coordinated and maintained by the European Commission (https://www.copernicus.eu/). The development of the observation infrastructure is processed under the aegis of the European Space Agency for the space segments and by the European Environment Agency and EU countries for the in-situ component. It is a collection of complex systems which gather data from different sources: earth observation satellites and in situ sensors such as airborne sensors, sea-borne sensors, and ground stations.

Table 19. Other initiatives relevant for WSIS

## 5.2. Glossary of Terms

After the compilation of the information from the mentioned initiatives, this section describes main glossary of terms and their alignment with existing ontologies, data





models, vocabularies, and standards. Hence, the following table compiles the primary study about the vocabulary used during the definition of the competency questions. This used vocabulary has also been used in the design and modelling of the WSIS ontology:

Concept	Terms	Ontology/Data Model
	The word 'period' appears	
A reference to time appears	Some of the following expressions appear: 'how many times', 'how often'	Time Ontology
	Some of the following nouns appear: 'date', 'hour', 'minute', 'second', etc.	
A reference to	The word 'sensor', 'device' or 'system' appears	
digital systems and their corresponding measurements appears	Some of the following expressions appear: 'indicators value', 'observations', 'measurements', 'indicators', etc	SAREF4WATR/S AREF4ENV/SARE F4ENVI
	Some of the following nouns appear: 'observes', 'observedProperty', etc	
Industrial Symbiosis Concepts and terms	Some of the following expressions appear: "Resource Provider", "resource consumer", "Industry", "Process"	OFIS/eSymbiosis
	The word "Industry" appears	
Units and Geographical	Some of the following expression appears: 'measures located in', 'events in indicators/scenarios'	QUDT, W3CGeo, GeoSPARQL
information	Some of the following aspects are considered: 'units attached measures'	

Table 20. Glossary of terms for the WSIS ontology

## 5.3. WSIS Ontology: Formal description

This section is mainly devoted to the presentation of the WSIS ontology. The work comprises the development of the ontology focuses on the design of the ontology and the subsequent implementation in OWL format.





The construction of the WSIS ontology considers the identified requirements (Competency Questions) depicted in the Section 4.6. As mentioned, main challenge and innovation relies on the (i) combination of information and data from different infrastructure considering the Nexus; (ii) link between real information and measurements about resources with costs and economic aspects; (iii) reason about potential hindered symbiotic links between processes.

Based on these aspects, the entire ontology model is presented in Figure 11. This ontology represents main digital and physical assets related to the representation of industrial processes and also, the resources interlink with each of the process. Therefore, the presented ontology makes a representation about the industrial digital systems with interlink with materials management and specification, water infrastructure and also, energy infrastructure. For enabling this representation, it is indicated the provenance ontologies (e.g. WISIS ontology -wsis- or SAREF4WATR - s4watr-). The elaborated ontology, mainly incorporates terms and resources from the following standard semantic models:

Prefix	Namespaces
dcterms	http://purl.org/dc/terms/>
Owl	http://www.w3.org/2002/07/owl#
Rdf	http://www.w3.org/1999/02/22-rdf-syntax-ns#
Xsd	http://www.w3.org/2001/XMLSchema#
Rdfs	http://www.w3.org/2000/01/rdf-schema#
saref	https://saref.etsi.org/core/
s4city	https://saref.etsi.org/saref4city/
Vann	http://purl.org/vocab/vann/
s4syst	https://saref.etsi.org/saref4syst/
Time	http://www.w3.org/2006/time#
geosp	http://www.opengis.net/ont/geosparql#
Sf	http://www.opengis.net/ont/sf#
schema	http://schema.org/
s4watr	https://saref.etsi.org/saref4watr/
Om	http://www.ontology-of-units-of-measure.org/resource/om- 2/
Wsis	https://w3id.org/def/wsis/
ultimate	https://w3id.org/def/wsis/examples/ultimate/

Table 21. WSIS ontology prefix

For the description of the ontology figures and shapes, we used arrows to represent the relationships between classes (object properties). These relationships represent RDF, RDFS, OWL constructs and object properties. Precisely:

• <u>Plain arrows</u> with a white triangle represent the rdfs:subClassOf relation between two classes. The origin of the arrow is the class to be declared as a subclass at the destination of the arrow.





- <u>Dashed arrows</u> between classes indicate a local restriction in the origin class. More frequent restrictions refer to object properties that can be instantiated between the classes in the origin and the destination of the arrow. The identifier of the object property is indicated within the arrow.
- <u>Dashed arrows</u> with no identifier are used to represent the rdf:type relation, indicating that the element in the origin of the arrow is an instance of the class in the destination arrow.

In the diagrams, <u>datatype properties</u> are denoted by attributes (rectangles) adhered to the classes in a UML oriented notation. Dashed boxes represent local restrictions in a class (e.g., datatype properties that can be applied to the class it adheres to).

Individuals (or ontology instances) are denoted by rectangles in which the identifier is underlined.





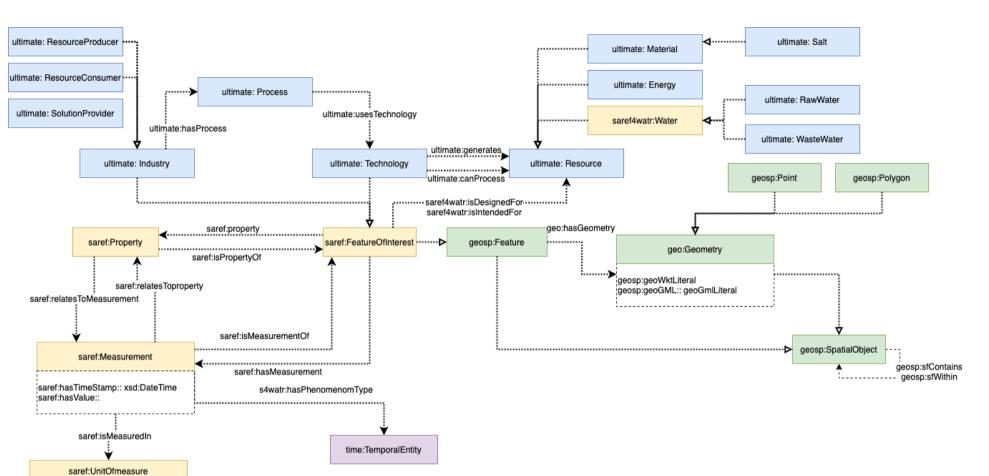


Figure 11. WSIS ontology core-module





#### 5.3.1. Digital and measurements representation

As it is depicted in Figure 12, the representation of industrial systems, their connections and the subsequent observations and measurement are performed using the ontological patters resented on the SAREF and SAREF4WATR ontology standards. To avoid duplication in the documentation of the standards SAREF4WATR, specific details can be shown inside the <u>documentation</u>. In an overview, SAREF and SAREF4WATR follow up the <u>Observation and Measurement</u> pattern for the representation of temporal measurements.

Under this pattern, specific measurements (<u>saref:Measurements</u>) are interlinked with specific Devices (<u>saref:Device</u>) to catalogue the specific digital system that performs the observation procedure. Both devices and measurements refer to a specific property (<u>saref:Property</u>). This property refers to the specific types of measurement (e.g., water flow, temperature, energy flows, etc). These properties and subsequent measurements are observed in real elements or feature of interests (<u>saref:FeatureOfInterest</u>). These real objects normally are related to a geospatial representation (<u>geosp:Feature</u>) that covers points or specific areas (e.g., polygons, multi-polygons, etc).

The measurements are specified by a temporal specification (<u>time:TemporalEntity</u>) and a unit of measure (<u>saref:UnitOfMeasure</u>). There exists a special measurement related to the feature of interest to measure specific general indicators over a region.

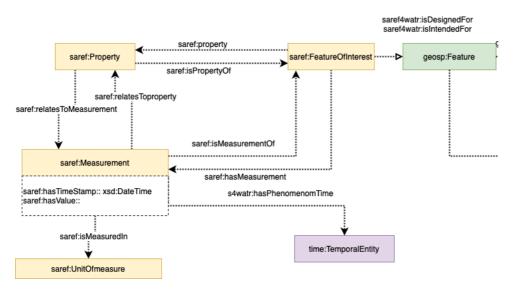


Figure 12. Observation and Measurement standard pattern

#### **5.3.2.Resource interlink management**

One of the core elements of the ontology relies on the identification, cataloguing and representation of the different industrial resources that could be exchanged (see Figure Figure 13). For that, we used a case-driven material cataloguing. Under this vision, we focused on the interrelation between specific technology (<u>wsis:Technology</u>) and the generation (<u>wsis:generates</u>) and processing (<u>wsis:canProcess</u>) of specific



resources (<u>wsis:Resource</u>). The resource are categorized into water (<u>s4watr:Water</u>), energy (<u>wsis:Energy</u>) and material (<u>wsis:Material</u>). An important aspect is the alignment of the measurements and physical aspects with the corresponding resources to associate the different flows, volumes with each associated resource.

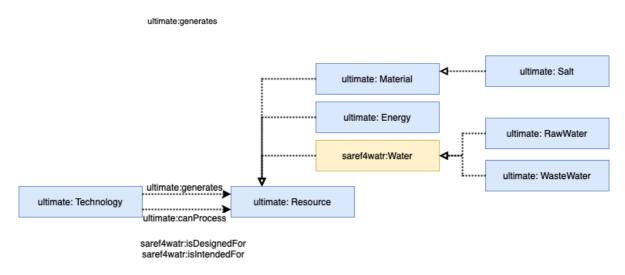


Figure 13. Resource Management representation

### 5.3.3. Industrial symbiosis representation

This part of the ontology (Figure X) is mainly devoted to represent industries and the process and technology involved. Thus, the industry (wsis:Industry) can be resource producer (wsis:ResourceProducer), resource consumer (wsis:ResourceConsumer) and also, solution provider (*wsis:SolutionProvider*). This types of industries contains (wsis:hasProcess) several processes (wsis:Process) to the generation of products. (*wsis:usesTechnology*) one or several technologies This processes uses (wsis:Technologies) to process the resources and also generate new resources. Finally, the technology is also located in specific region and location and also, perform specific generation and processing of resources (measurement). For that, technologies are also feature of interest inside the ontology а (saref:FeatureOfInterest).

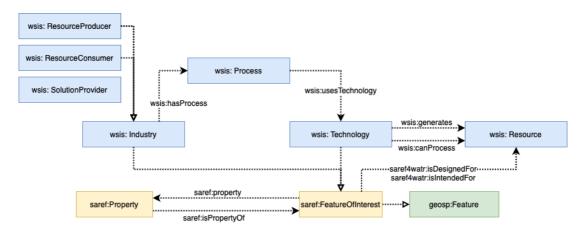
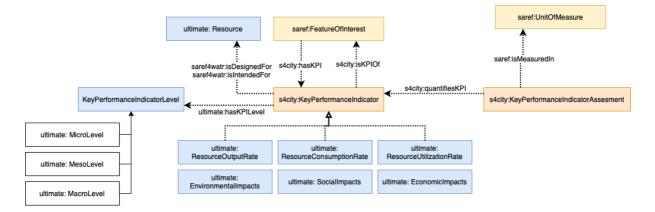


Figure 14. WSIS representation of the industrial symbiosis



### **5.3.4. Key Performance Indicators at different scales**

This representation is mainly focused on incorporation of different key performance indicators at different scales aligned with the resources or the impacts measured in specific locations (saref: FeatureOfInterest). In this regards, the introduced key performance indicators are catalogued in different levels (wsis:KeyPerformanceIndicatorLevel). This levels are divided into micro-level (wsis:MicroLevel), meso-level (wsis:MesoLevel) and macro-level (wsis:MacroLevel). Complementing the different scales, the Key performance indicators have been catalogued in resource output rate (wsis:ResourceOutputRate), resource consumption (wsis:ResourceConsumptionRate), rate resource utilization rate (wsis:ResourceUtilziationRate), environmental impacts (wsis:EnvironmentalImpact), (wsis:SocialImpact) social finally. EconomicImpacts impact and (wsis: EconomicImpacts). To complement the representation of the KPIs, we established an interrelation between the KPIs (s4city:KeyPerformanceIndicator) and also, KPIs assessment (s4city:KeyPerformanceIndicatorAssessment).



# 6. WSIS Ontology Validation and Testing

This section is mainly focused on describing the ontology validation and testing. For that, this part of the document initially validates the core ontology to ensure correctness in the ontological schema and representation (Section 6.1). With this validation, we followed up with the testing of the elaborated ontology according to the use case of Agricola (Section 6.2). Thus, we performed unit test over the ontology to ensure the alignment with the Competency Questions (Section 4.6).

## 6.1. WSIS ontology validation

The evaluation of the ontology is a process to ensure good practices in the representation of ontology resources. For that we initially, we used <u>OOPS!</u> Tool for ensuring the correctness of the following aspects among other relevant ones:





- The domain or range of a relationship is defined as the intersection of two or more classes. This warning could avoid reasoning problems in case those classes could not share instances.
- No naming convention is used in the identifiers of the ontology elements. In this case the maintainability, the accessibility and the clarity of the ontology could be improve.
- A cycle between two classes in the hierarchy is included in the ontology. Detecting this situation could avoid modelling and reasoning problems.

Thus, the initial step has been to ensure the correctness of the core ontological models using OOPS! Tool (Figure 15). After executing the tool, we received two recommendations inside the evaluation report. Summarising the evaluation results, we received the following comments:

Evaluation Result	Problems & Solutions
CRITICAL	<ul> <li>PROBLEM-NAMESPACE HIJACKING. It refers to reusing or referring to terms from another namespace that are not defined in such namespace. This is an undesirable situation as no information can be retrieved when looking up those undefined terms. This pitfall is related to the Linked Data publishing guidelines provided in [11]: "Only define new terms in a namespace that you control" and to the guidelines provided in [5]. This pitfall appears in the following elements:</li> <li>http://purl.org/vocab/vann/preferredNamespacePrefix</li> <li>http://purl.org/vocab/vann/preferredNamespaceUri</li> <li>http://www.w3.org/1999/02/22-rdf-syntax-ns#comment</li> <li>For detecting this pitfall we rely on TripleChecker. See more results at TripleChecker website. Up to now this pitfall is only available for the "Scanner by URI" option.</li> <li>SOLUTION. We put it same URI inside the ontology for their consistency.</li> </ul>

As an evidence of the result, the following image depicts the entire document validation report after executing the validation (Figure 15):





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	ontOlogy Pitfa	all Scanner!			
		detect some of the most common pitfalls appearing wh to the text field above. A list of pitfalls and the element		be displayed	
	Scanner by URI: https://w3id.org/def/wsis/ Example: http://oops.linkeddata.es/example/swc_2	000.05.00#	Scar	mer by URI	
	Example: http://oops.iinkeodata.es/example/swc_z	009-05-09-10			
	If you just include the RDF c extension, P37. Ontology not	ode here, the following Pitfalls will not be checked: P36. U t available, P40. Namespace hijacking	RI contains file		
	Scanner by direct input:		Scanner by RDF		
	Uncheck this checkbox if you don't want us to ke	ep a copy of your ontology.		Go to advanced evaluation	
	Evaluation results				
	It is obvious that not all the nitfalls are equally impo	rtant: their impact in the ontology will depend on multi		nt to help?	
	pitfall has an importance level attached indicating ho			Suggest new pitfalls	
	<ul> <li>Important <sup>Q</sup>: Though not critical for ontology f</li> </ul>			rovide feedback	
	<ul> <li>Minor <sup>O</sup>: It is not really a problem, but by corre [Expand All]   [Collapse All]</li> </ul>	scong it we will make the ontology nicer.	Do	cumentation:	
	Results for P04: Creating unconnected ontol	ogy elements.	4 cases   Minor 🦳 🔒	titfall catalogue	
	Results for P08: Missing annotations.			lser guide lechnical report	
	Results for P10: Missing disjointness.		ontology*   Important 9	echnical report	
	Results for P11: Missing domain or range in	properties.	33 cases   Important  Rel	ated papers:	
	Results for P13: Inverse relationships not ex	plicitly declared.	19 cases   Minor 🔍	JSWIS 2014	
	Results for P40: Namespace hijacking.			KAW 2012	
	According to the highest importance level of pitfall for You can use the following MTML code to insert the ba	ound in your ontology the conformace bagde suggester edge within your ontology documentation:	is "Critical pitfalls" (see below).	ISWC 2012 Demo Intoqual 2010 CAEPIA 2009	
		href="http://oops.linkeddata.es"> <img src="http://oops.linkeddata.es/resource/i</img 	mage/cops_critical.png"	b services:	
	CRITICAL PITFALLS				
	CRITICAL PITTALLS	alt="Critical pitfalls were found" height			
	CATTOR, PITTRUS			veloped by:	

Figure 15. WSIS validation by OOPS!

After the validation of the ontology structure, the second validation performed relates to the FAIR principles in relation to ensure the reusability principles of the ontology. For that purpose, we used <u>FOOPS! Tool</u>. This tools permit to provide the means for researchers to assess whether a vocabulary (OWL or SKOS) conforms or not to the best practices for publishing ontologies on the Web.

The execution of the FOOPS! Tools revealed (Figure 12) that the ontology is almost aligned with the principles in a (72%). Indeed, the ontology needs to revise during the next version, the following aspects:

- 1. Check the IRI version in some of the description.
- 2. Make public the prefix of the ontology.
- 3. Check some ontology metadata to ensure the annotations and comments for better understanding of the terms and relations.





	URI			
https://w3	id.org/def/wsis/			
Example: ht	tps://w3id.org/example (click here to en	nter this ontology)		
		RUN		
		KON		
Title:	Water Smart Industrial Symbiosis (W	VSIS) Ontology		
URI:	https://w3id.org/def/wsis/			
License:	https://opensource.org/licenses/ISC	0		
	72%		Findable (609) Beunable (632/9) Interspenable (3/0)	
		Findable		~
F1: (me	a)data are assigned a glot	Findable bally unique and persistent ider	ntifier	^

Figure 16. WSIS validation with FOOPS!

As a conclusion of the ontology validation, WSIS ontology accomplish with FAIR principles in the majority despite it needs to solve several aspects like accessibility and versioning. These aspects will be corrected in the final version of the ontology. In terms of semantic modelling, the ontology needs to define annotations and potential properties ranges and domains.

## 6.2. WSIS ontology testing

Ontology testing has been performed over the CS#2 as depicted in the section 2.2. Over this case study we initially semantically model and introduce data to the resultant ontology specification for the case study (Section 6.2.1). After this, we elaborated several tests suit according to the competency questions defined (see Section 6.2.2).

#### 6.2.1.CS#2 Semantic modelling

Base on the analysis performed over the literature and the case study description, the semantic model elaborated (see Figure 11) covers both process depicted under Section 2.2: The water reuse from the wastewater for greenhouses and agriculture purposes (see Section 6.2.1.1); and (ii) the heating and cooling system energy recovery implemented in the case-study (see Section 6.2.1.2). The entire complete model for the case-study can be shown under the Figure 21.



#### 6.2.1.1. Waste-Water Reuse process

This main purpose of this process is to describe the resource inputs and outputs in relation to water and agriculture information. In this regards (Figure 17), the elaborated ontology model is aimed at describing the different processes of the wastewater treatment plant considering the incoming water from greenhouses and their corresponding transformation until return a treated water with nutrients coming back for the agriculture process of the greenhouses. As seen in the image, the process mainly generates different types of waters with different concentrations of salts, nutrients and other components that also need to be modelled. Moreover, the processes also generate different salts as result from the treatment processes. Finally, the red line in the image represents the process interlink based on the interrelation of the different intermediary resources.

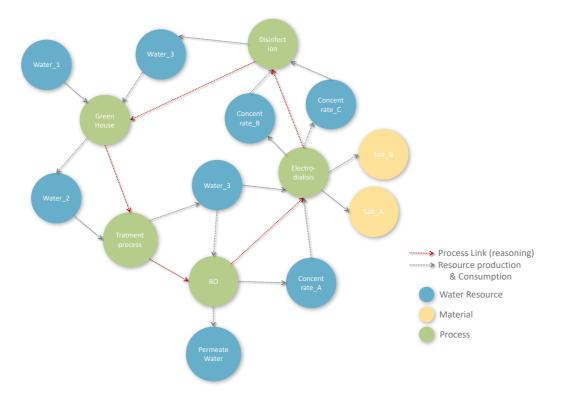


Figure 17. Simplified ontology model of the process

Based on this simplified model, the complete model for this process of the industry is the one depicted in the Figure 18.



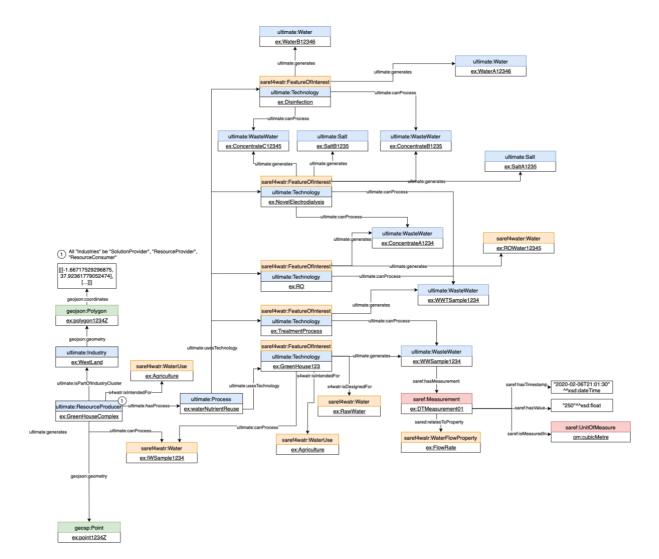


Figure 18. Complete model for Waste water reuse in CS#2

#### 6.2.1.2. Heating and Cooling System

Similarly as the previous example, the heating process (Figure 19) represents the heating and cooling process applied to the different greenhouses. Therefore, the following simplified ontology model represents the different energy fluxes of the heating and cooling system.





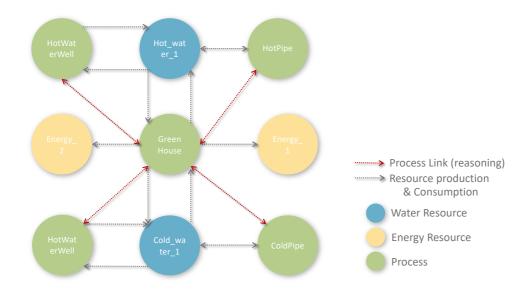


Figure 19. Simplified model for the Heating and Cooling process in CS#2

Similarly as the previous example, the complete semantic model for this second process is the one represented in the Figure 20.

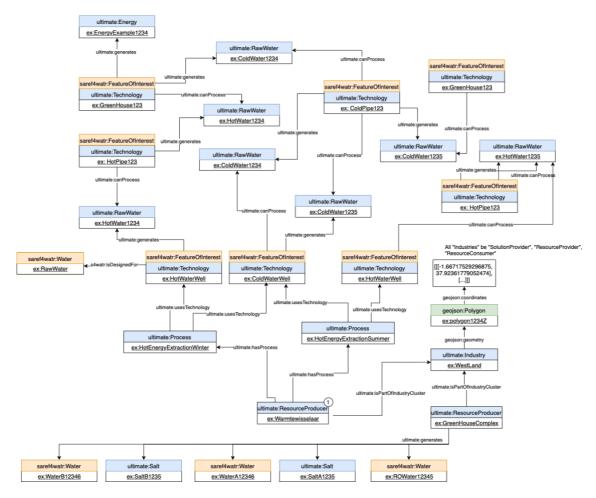
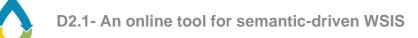


Figure 20. Complete semantic model for the heating and cooling process in CS#2





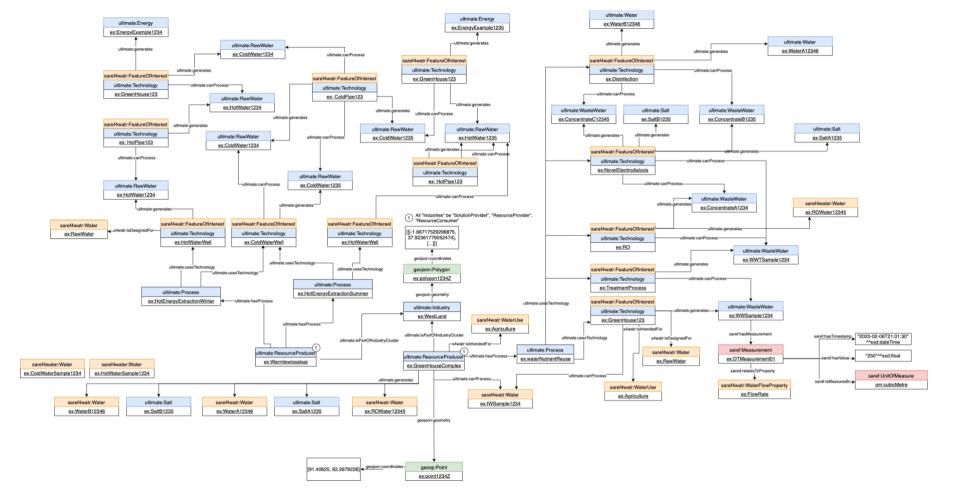


Figure 21. Complete WSIS instantiation for the CS#2





### 6.2.2.WSIS testing using CS#2 information

Based on the built semantic model constructed for CS#2, the work has been focused on translating this diagram into an ontology instances based on the core model described (Figure 22). Considering this meta-model, we elaborated specific data sets of the information to be introduced publicly in <u>Triply</u>. Triply is a web-based semantic store that permit and facilitate static data sharing. This triple store enables a SPARQL endpoint over your information to query the data. Thus, it will permit us to test the ontology considering a triple store and SPARQL end point.

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⊞	Table			294 statements Uploaded 2 minutes				<u>↓</u> ×	
/>	SPARQL			opioaded 2 minutes	ago				
و	Graphs	1							
	Services	1							
	Assets	0							
	Insights								
				Documentation	Triply				
				Getting started API reference	About Contact us				
2	Copy dataset			Javascript Client	General terms		0		
	<			Yasgui	Privacy policy	9	0	info@triply.cc © 2022 Triply B.V. All rights reserved.	

Figure 22. WSIS information from CS#2 loaded in Triply

Once the data is publicly available, the next step has been to elaborate a program in Node.js to perform the unit test. For that purpose, the program mainly uses the following libraries:

- <u>Jest</u>. For testing and elaborating unit-test over the remote triple-store repository.
- <u>SPARQL ENDPOINT</u>. SPARQL library to query and endpoint at manipulate the corresponding information.

Based in these libraries, we performed the implementation of the 15 Competency Questions described in the Table 13. This implementation mainly focuses on the elaboration of the corresponding SPARQL query and the execution of the SPARQL wrapper for getting the result. Once the result obtained, it has been checked to ensure their correctness:

test ('UCQ-15. How much resource are generated by process X?', async () => {





const sparqlQuery =`PREFIX rdf: <http: 02="" 1999="" 22-rdf-syntax-ns#="" www.w3.org=""></http:>
PREFIX rdfs: <http: 01="" 2000="" rdf-schema#="" www.w3.org=""></http:>
PREFIX wsis: <https: def="" w3id.org="" wsis=""></https:>
PREFIX geosp: <http: geosparql#="" ont="" www.opengis.net=""></http:>
PREFIX s4watr: <https: saref.etsi.org="" saref4watr=""></https:>
PREFIX saref: <https: core="" saref.etsi.org=""></https:>
SELECT ?technology ?resource_needed ?value WHERE {
?industries rdf:type wsis:ResourceProducer .
?industries wsis:usesTechnology ?technology .
?technology wsis:generates ?resource_needed .
?resource_needed saref:hasMeasurement ?measurement .
?measurement saref:hasValue ?value .
} LIMIT 10`;
const bindingsStream = await myFetcher.fetchBindings(
'https://api.triplydb.com/datasets/aitorcorchero/ULTIMATE/services/ULTIMATE/sparql',
sparqlQuery
);
<pre>sparqlPromise = await new Promise ((resolve, reject) =&gt; {</pre>
let chunks = [];
bindingsStream.on('data', (triple) => chunks.push(triple));
bindingsStream.on("end", () => resolve(chunks));
bindingsStream.on("error", error => reject(error));
});
return expect (sparqlPromise.length > 0).toBeTruthy();
});

Based on this definition of the test, we executed the test and obtaining as a result that 3 test failed (Figure X). After a detailed understanding of the test and the information requested, we noticed that the main cause were by the lack of semantic reasoning. In detail, the triple store that stores the information do not have any reasoning capabilities and for that, several information of the knowledge graph is missed.





✓ UCQ−1. Which assets are involved in the water/energy/industrial infrastructure? (366 ms	;)
VUCQ-2. What types of sensors are involved in the infrastructures? (205 ms)	
<ul> <li>UCQ-3. What type of actuators are involved in infrastructures? (195 ms)</li> </ul>	
$\times$ UCQ-4. What type of processes are involved in the demo-case X? (202 ms)	
$\sim$ UCQ-5. What type of technology have been implemented in the industry X? (202 ms)	
<ul> <li>UCQ-6. What is the volume of water exiting process X? (199 ms)</li> </ul>	
× UCQ-7. What is the energy flux in process X between 01-01-2022 and 01-03-2022? (204 ms)	
<ul> <li>UCQ-8. What are the physical parameters of measurement X? (209 ms)</li> </ul>	
<ul> <li>UCQ-9. What is the region of the industry X? (195 ms)</li> </ul>	
$\times$ UCQ-10. What are the industries related to the industrial region X? (202 ms)	
<ul> <li>UCQ-11. What types of sensors are involved in the infrastructures? (205 ms)</li> </ul>	
<ul> <li>UCQ-12. What kind of resources are needed in process X? (199 ms)</li> </ul>	
<ul> <li>UCQ-13. How much resource are required in process X? (205 ms)</li> </ul>	
<ul> <li>UCQ-14. What kind of resources are generated by process X? (198 ms)</li> </ul>	
✓ UCQ-15. How much resource are generated by process X? (206 ms)	

Figure 23. WSIS ontology tests

As a conclusion of the ontology testing, WSIS ontology almost accomplish most of the test defined and therefore, it is highly aligned with the user requirements. However, special efforts are still needed in terms of reasoning and their subsequent validation.

# 7. Ontology publication

The WSIS ontology has been published using <u>Ontoology</u> tool in order to gather a public URI but also, ensure the reusability of the terms and vocabulary by the community. The corresponding documentation and version code of the ontology can be found the following link:

#### https://aolite.github.io/WSISOntology/

The documentation of the ontology has been performed by using an external tool called <u>WIDOCO</u>. This tool permits to automatically generate the documentation of the ontology-based on the labels defined in the semantic model. Despite directly using this tool, we preferred to use a continuous integration methodology for ontology documentation and publication. Hence, this procedure will involve once the ontology model is published on GitHub, tests are passed and the ontology is published using WIDOCO tool.

Considering this aspect, the main annotations used in the ontology development for documentation purposes are:

Annotation	Description
Dc:contributor	Definition of the contributors of the ontology
Dc: creator	Definition of the creators of the ontology
Dc: description	Description of the ontology (indicating main purpose)





Dc:source	Tags of the ontology
Dc:title	Title of the ontology
Dc:created	Date of creation
Dcterms:license	Licence determined for the ontology
Dcterms:modified	Date of the last modification
versionInfo	Version of the ontology
Comment	Description of the main entities and classes
label	Human readable label for the classes and the properties (optional)

Table 22. WSIS documentation annotations

After the end of each of the continuous integration processes, we have the ontology published in a custom landing page that could be increased with other ontologies if we work on the same repository. To ensure accessibility, we used a public link and URL under the W3C domain (Figure 24. WSIS landscape portal)

			-	y landing page
Ontology	Serialization	License	Language	Description
WSIS Ontology Example of CS2 from ULTIMATE project	ť.	https://opensource.org/licens	en	An example of the usage of the WSIS ontology performed under the ULTIMATE project
WSIS Ontology Example at industrial level considering AQUASPICE-AGRICOLA Case Study		https://opensource.org/licens	en	An example of the usage of the WSIS ontology performed under the AQUASPICE project.
Water Smart Industrial Symbiosis (WSIS) Ontology	TURTLE	https://opensource.org/licens	en	An ontology as a catalyst for Water Smart Industrial Symbiosis (WSIS), in which water/wastewater plays a key role within a dynamic socio-economic See more
Page created with VocabLite Built with Bootstrap Latest revision March, 2022	a (Ontology Engin	eering Group)		Vite

Figure 24. WSIS landscape portal

From the landscape portal, we can also access to the detailed documentation by clicking on the "Water Smart Industrial Symbiosis (WSIS) ontology). Then, we can access to the WIDOCO template for the ontology (Figure 25)





CA	D I	aolite.github.io/W	SISOntology/OnTool			x-en.html		P O O 🚊 🗯
								languag
ULTIMATI	WISIS (	Ontology						
Release 20	21-07-05							
11010430 201	1-07-00							
This version:								
Revision:	atewater.eu/wis	<u>sis/v0.0.1/</u>						
v0.0.1								
Authors:								
Aitor Corch	ero							
Publisher:	atewater.eu/							
Download seria								
		XML Format N Triple	S Format TTL					
License:			100 C					
License http	://opensource.org/	/licenses/ISC						
Cite as:				trieved from: ht	ps://ultimatewater	.eu/wisis/v0.0.1/		
Aitor Corch	ero. ULTIMATE	WISIS Ontology. F	Revision: v0.0.1. Re					
		WISIS Ontology. F	Revision: v0.0.1. Re					
Aitor Corch		WISIS Ontology. F	Revision: VO.O.1. He		20 			
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Aitor Corer Provenance of it Abstract A WISIS ontolog Table of cor • 1. Introduc • 1.1. • 2. ULTIMA • 3. ULTIMA • 4. Cross re	is page from exploring tents ion amespace dec TE WISIS Ontol TE WISIS Ontol ference for ULT	g and interlinking in	dustrial process va	riables between				
Altor Corer Provenance of th Abstract A WISIS ontolog Table of cor • 1.1.1 • 2. ULTIMA • 3. ULTIMA • 4.1.0	is page from exploring tents ion amespace dec TE WISIS Ontol TE WISIS Ontol ference for ULT	and interlinking in larations ogy: Overview ogy: Description IMATE WISIS Onto	dustrial process va	riables between				

Figure 25. WSIS WIDOCO documentation

As a conclusion of the ontology documentation we ensured that the ontology is well documented and the semantic vocabulary is ready to be reused under the following link:

https://aolite.github.io/WSISOntology/





# 8. A WSIS Semantic Repository: RIOTER

This part of the document is mainly devoted to depict the semantic repository for exploring WSIS information. In this regards, this part of the document will describe the implementation performed in the both main elements of the online tool: the backend (called Rioter-cube) (see Section 8.1) and the frontend (called Rioter-eye)(see Section 8.2).

## 8.1. Rioter-Cube: A backend to expose semantic

## enhanced data

The Rioter-eye (see Figure 27) corresponds to the backend service to retrieve and expose the linked data information gathered from a defined SPARQL endpoint. This system expose all the information through a defined Open API (through Swagger).

In terms of an architecture (see Figure 26) the system is mainly is constructed using the model-view-controller pattern in which the queries (REST operations) are separated from the modules in charge of collecting the data and the data representation. This model-view-controller has been implemented using <u>Nest.js</u> framework.

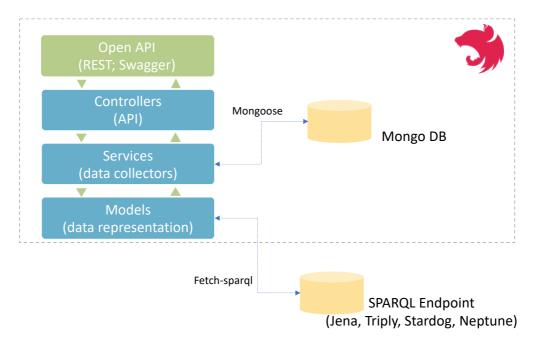


Figure 26. Rioter-cube overall architecture

Under this framework the system exposes the operations (REST-API) through an Open API (see Figure 27) that permit to acquire information and expose using a common vocabulary (serialized in JSON-LD). Once a request arrives to the system,





the system is in charge of gathering the corresponding dataset configuration from a MongoDB database. Under this database, the stored information corresponds to the following items:

- 1. <u>User configuration</u>, roles and accessibility to the system.
- 2. <u>Dataset information</u> that includes endpoint adhered and some cached data from the SPARQL endpoints.
- 3. <u>Endpoints configuration</u> that includes the SPARQL endpoint, the way to access it and the needed information (e.g. user, password, inferences) to establish the strategy to query linked data information.

In terms of the Linked data information, it is gathered from external triple/quad stores that expose the information through a SPARQL endpoint (e.g Fuseki-jena, Stardog, Virtuoso, Neptune, etc). Finally, the information exposed follows up the rules established in the models (for those information stored in the MongoDB) and, JSON-LD serialization of the instances that follows the rules of standard ontologies (e.g. WSIS ontology for ULTIMATE).

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↓         C         ♠         □         Image: Control of the second	₽ ● O m + □ Ξ
Rioter-Cube Open API 🚥 🚥	
This open API is mainly devoted to the elaboration of a semantic data cube with the harmonization capabilities for NGSI-LD and WoT	
Semantic Repository	~
default	^
POST /auth/login	~
GET /profile	$\sim$
GET /classes	$\sim$
GET /facets	$\sim$
Datasets	^
GET /datasets Get All Datasets	$\sim$
POST /datasets Create a new dataset into the platform	$\sim$
GET /datasets/{id} Get One Dataset specified by id	$\sim$
PUT /datasets/{id} Create a new dataset into the platform	~
DELETE /datasets/{id} Delete User	~
GET /datasets/(id)/endpoints Get Endpoints by the specified Dataset	$\sim$

Figure 27. Open API exposed by the Rioter-cube

In terms of the operations, the Open API exposed (REST-API) contains the following information divided into the different tables:

Users			
URL	Operation	Response	Description
/users	GET	USER[]	Operation to obtain all users





/users	POST	USER	Operation to create users
/users/{:id}	GET	USER	Operation to obtain a user by id
/users/{:id}	PUT	USER	Operation to modify users
/users/{:id}	DELETE		Operation to remove a user

Table 23. User operations described in the Open-Api

Auth					
URL	Operation	Response	Description		
/auth/login	POST	AUTH	Operation to obtain a token from the platform based on user/password credentials		
/profile	GET	USER	Based on the defined token, obtention of the user profile.		

Table 24. Authoritation operations described in the Open-Api

Endpoint					
URL	Operation	Response	Description		
/endpoints/{:id}	POST	Endpoint	Creation of an endpoint		
/endpoints/{:id} /server/graphs	GET	JSON	Obtention from SPARQL endpoint the different graphs.		
/endpoints/{:id} /graphs	GET	Endpoint	Obtention from the Endpoint class the defined endpoints		
/endpoints/{:id} /graphs	POST	Endpoint	Creation of graphs inside an endpoint.		

Table 25. Endpoint operations described in the Open-Api

Dataset	Dataset						
URL	Operation	Response	Description				
/datasets	GET	DATASET[]	List of datasets available for an specific user (by token)				
/datasets	POST	DATASET	Create da dataset for a user (by token)				
/datasets/{:id}	GET	DATASET	Obtain a dataset by id				
/datasets/{:id}	PUT	DATASET	Modify a dataset by id				





/datasets/{:id}	DELETE		Remove a dataset by id.
/datasets/{:id}/ endpoints	GET	ENDPOINT[]	Obtain endpoints for a specific dataset
/datasets/{:id}/ classes	GET	CLASS[]	Obtain classes for a dataset
/datasets/{:id}/ classes	PUT	CLASS	Create/Modify classes for an specific dataset
/datasets/{:id}/ classes/{:idCl}	GET	CLASS	Obtain information from specific class
/datasets/{:id}/ classByUri	GET	CLASS	Get class by URI name
/datasets/{:id}/ describe	GET	JSONLD	JSONLD describing the class information (specific instance)
/datasets/{:id}/ browseData	GET	JSONLD	JSONLD with the overall class information (instances data)
/datasets/{:id}/ endpoints	POST	ENDPOINT	Create enpoints into the system
/datasets/{:id}/ classes/{:idCl}/ relations	GET	JSONLD	Get all relations (object properties) established between classes
/datasets/{:id}/ classes/{:idCl}/ facets	GET	JSONLD	Get all facets (data and object properties) for specific class.
/datasets/{:id}/ classes/{:idCl}/ count	GET	CLASS	Get a class with the number of instances.
/datasets/{:id}/ classes/{:idCl}/ instances	GET	JSONLD	Get all instances for an specific class
/datasets/{:id}/ classes/{:idCl}/ facets/{idFacet }/ranges	GET	JSONLD	For each facet of a class, obtain all ranges.
/datasets/{:id}/ classes/{:idCl}/ facets/{idFacet }/ranges/{idRan ge}values	GET	JSONLD	For each facet of a class, obtain all ranges values.

Table 26. Dataset operations defined in the open-API





Rioter-cube (semantic repository) is mainly **devoted to the data gathering and** harmonization of the information coming from different endpoints. Thus, it contribute to link WSIS data coming from the different processes and different industries.

## 8.2. Rioter-Eye: An Exploration and Visualization

### tool for Linked Data

Rioter-eye (see Figure 28) corresponds to a data exploration and visualization tool (online tool). This tools is mainly focused on interacting with the RIOTER-eye to visualise the contained information in the different WSIS datasets (SPARQL endpoints). This module has been programmed using Angular and the main modules refers to:

- Authentication and User Administration. This part of the application is mainly devoted to log in/log out users and also, manage different users (in case of being administrator) or the profile (in case being user).
- **Dataset/Endpoint Definition**. This set of views corresponds to the definition of the datasets, endpoints and selection of the graphs to be queried.
- **WSIS graph overview**. This view is devoted to the overall visualization of the datasets.
- **WSIS navigation and exploration**. This set of views corresponds to the information navigation and filtering based on the relations and data properties the graph has defined

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Figure 28. Landing page of the RIOTER-eye online tool



Similarly as the case of RIOTER-cube, the RIOTER eye is also programmed using a Model-view-controller pattern applied to the visualization (see Figure 29). In this case, the controllers corresponds to the elements (data collectors to the Open API) that permit to visualise the information in the webpages (HTML and CSS). The Models are the data representation of the information to be visualised.

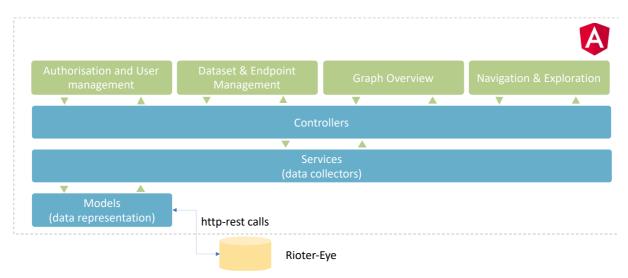


Figure 29. Rioter-eye main architecture

#### 8.2.1. Authentication and User Administration

This part of the visualization is mainly focused on the definition of the visual parts to log in into the application (Figure 30). For that, we decided to access to the platform using user/password authentication to generate a token that permit to identify the user and access to the definition of datasets and endpoints.

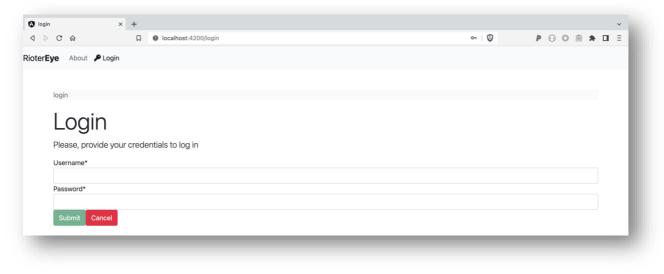
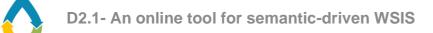


Figure 30. Login visualization into the platform





Once the introduced credentials are correct, the next visualization is the main menu of the application (Figure 31). This part of the application is devoted to easy access to the information available in the system.

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datasets			
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ULTIMATE			
Query Service -	Update Service -	Hexplore Details	
	Showing 1 out of 1 dataset		
-			

Figure 31. Main view of the online tool when logged

If we go to the administration part of the platform, the main visualisation part is the list of available users (Figure 32).

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1 D C ଲ	localhost:4	200/users		er   🕲	P 🛛 O 🖻 🛪	3
oterEye About [	Datasets • Administration •	🕒 admin i Logout				
users						
Create User						
<u>admin</u>						
Username admin		Details				
		St	owing 1 out of 1 admin			

Figure 32. Visualization part of the list of users

In this part of the application, we can create new users into the platform (Figure 33) in order to provide newer access to people of the potential community or case-studies.





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oter <b>Eye</b> About Da	tasets 👻 Administration 👻 🕒 admin 🔓 Logout		
users / new			
Username*			
Email*			
Password*			
Submit Ba	ack		

Figure 33. User creation form in the platform

We can see to the details of the crated users to able to modify their information or remove them from the database (if the logged user is the administrator) (Figure 34).

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users / aolite			
aolite			
Username			
aolite			
Back Edit D	elete		

Figure 34. Users detail view

#### 8.2.2. Dataset/Endpoint Definition

Once the users are defined, they are able to create their own datasets (Figure 35). This part starts with the definition of main information of the dataset that includes the name, the accessibility and the type of query to be performed.





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	March 1		
	datasets / new		
	Dataset Details Endpoint Details Dataset Graphs		
	Name*		
	ULTIMATE	~	
	Access		
	Private		
	Query Type		
	Optimized		
	"Optimized" is recommended for large datasets, "Detailed" enables network overview.		

Figure 35. Definition of the dataset

To the dataset we can include several endpoints (Figure 36). The information required to the endpoint definition corresponds to the type of server (e.g. Generic, Fuseki, Stardog, Neptune), the URL to the SPARQL endpoint and also, the required timeout to stop the query in case the server delays in their answer.

0 D C Q	Iocalhost:4200/datasets/ULTIMATE/edit	o. 0	₽ 0 0 🖻 🗯 🖬
oterEye About Datasets -	Administration - 🛛 admin 🔒 Logout		
	datasets / ULTIMATE / edit		
	Dataset Details Endpoint Details Dataset Graphs		
	SPARQL Server type		
	Generic		
	SPARQL Query Service URL*		
	https://api.triplydb.com/datasets/aitorcorchero/ULTIMATE/services/ULTIMATE/sparq	✓	
	SPARQL Service Timeout*		
	300000		
	Long timeouts recommended, in milliseconds. 300000 corresponds to 5 minutes.  Endpoint password protected		
	Endpoint writable		
	Submit Cancel		

Figure 36. Endpoint definition in the dataset

The final part of the definition of the dataset corresponds to the selection of the graphs to query the information (Figure 37). In the case of ULTIMATE, we have created a default graph that contains the WSIS ontology (for inference purposes) and the graph that includes the CS#2 information. Hence, we selected only case-study graph to visualise the information.

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	Dataset Graphs		
	https://triplydb.com/aitorcorchero/ULTIMATE/graphs/NewPrinseland		
	https://triplydb.com/aitorcorchero/ULTIMATE/graphs/ontology		
	Submit Cancel		

Figure 37. Definition of the graphs to be queried

#### 8.2.3.WSIS graph overview

With the dataset defined, we are able to explore the graph and visualise the contained information (Figure 38). This view is mainly divided into two main parts. The initial part





is devoted to search terms and classes. The second part is the word cloud of the containing information.

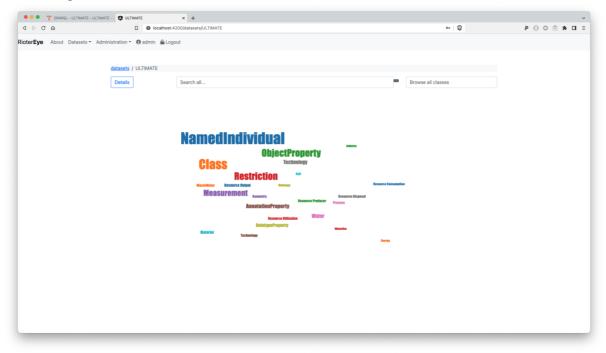


Figure 38. ULTIMATE CS#2 overview of the information

#### 8.2.4.WSIS navigation and exploration

Last part of the visualization corresponds to the details of the information (Figure 39). This view, initially list the classes and permit to filter it through the different defined facets (elements that are on the left part of the screen).





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Facets	Instances	S				
Search all facets values	٩	https://triplydb.com/.well-knov	vn/genid/263a7a8072be5f23	3e83ec21c1a0a02	<u>6c</u>	
asWKT		https://triplydb.com/.well-known	n/genid/2e59555d9c4eb8f4	6aae50cb966315	<u>3b</u>	
		https://triplydb.com/.well-know	n/genid/318f9a997a78b9ba	4d482862dd7a3a	<u>cb</u>	
canProcess		https://triplydb.com/.well-know	m/genid/3d4b30556ada1b3f	941b4a65c76679	<u>e1</u>	
canProcess		https://triplydb.com/.well-known	/genid/521840e40aad3da80	)6e98302879326	<u>d7</u>	
		https://triplydb.com/.well-knowr	n/genid/60f0920c2298880c	46af5d8006b50e	<u>81</u>	
canProcess		https://triplydb.com/.well-know	/n/genid/6dbf6294d6a421fd	1364960ce41eca	<u>49</u>	
		https://triplydb.com/.well-known	n/genid/d249b55e768a5d99	29b65ba38bbff9	<u>eb</u>	
canProcess		https://triplydb.com/.well-know	wn/genid/eacf1ece018ec931	fb34db0806f383	<u>69</u>	
		https://w3i	d.org/def/wsis/examples/ulti	mate/newPriscela	nd	
creator		1 2				
description		Showing 10 out of 20 instance	ces filtered from 20			

Figure 39. Faceter view of the CS2 measurement information

When we click into a measurement, the detailed information is displayed (Figure 40). Under this visualization, the information displayed corresponds to all data properties and data ranges defined for the specific instance inside the knowledge graph.

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A ▷ C ŵ	🛛 🕒 localhost:4200/datasets/ULTIMATE/ultimate:measurement/resource?uri=https:%2F%2Ftriplydb.com%2F.we 🕶 🛛 🞯	P 🛈	0	ē 1	
oterEye About Datasets -	Administration 👻 😫 admin 🔒 Logout				
datasets / ULTIMATE /	ultimate:measurement / resource				
	https://triplydb.com/.well-known/genid/263a7a8072be5f23e	83ec210	:1a0a	<u>026c</u>	
hasTimestamp: 2022-0		83ec210	: <u>1a0a</u>	<u>026c</u>	
hasTimestamp: 2022-0 hasValue: 95.0		83ec210	<u>:1a0a</u>	<u>026c</u>	
-	3-06T21:01:30	83ec210	<u>:1a0a</u>	<u>026c</u>	

Figure 40. Detailed information of one measurement of the CS2

Rioter-eye (semantic repository) is being constructed to understand WSIS knowledge graph based on the case study information. It main innovation relies on the facet navigation and exploration of the information distributed along different SPARQL endpoints.







## 9. Conclusion & Future Work

This final section of the deliverable is mainly focused on the description of the different conclusions and results obtaining during the execution of the Task 2.1 entitled as "*Creating a common semantic representation for WSIS*" (see Section 9.1). This task started on M6 (November-2020) and it will finalise on M36 (May-2023). Despite there is no other deliverable envisioned for Task 2.1, the newer results and outcomes performed during this last year will be included into the rest of WP2 deliverables. Hence, the future work (Section 9.2) will be focused on the continuous enhancement of the ontology and also, the refinement of the online tool to explore the information.

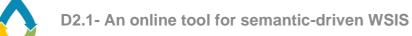
## 9.1. Conclusions

The present deliverable has described the advancements performed in ULTIMATE on the elaboration of the WSIS ontology and also, the semantic repository (called RIOTER). Considering main results obtained, WSIS ontology has been published for being reused or extended by the community. Despite their publication, the WSIS ontology will be maintained and matured during the rest of the project live span and beyond. It will continue to be enhanced following the case-based definition. That means, the ontology will continue with their maturity using case-studies evidence and the needs to identify and interlink processes and industries. As a highlight point, WSIS ontology provides response to the (i) combination of information and data from different infrastructure considering the Nexus; (ii) link between real information and measurements about resources with costs and economic aspects; (iii) reason about potential hindered symbiotic links between processes.

In consideration of the semantic repository (RIOTER), it has been presented an initial version of the online tool. In the one hand, the rioter-cube (backed) provides the innovation in reduction of time to serve the information thanks to the cached overall information, especially for large knowledge-graphs. From the part of the rioter-eye, the visual tools permit to navigate to the knowledge graph without having any experience with ontologies and semantic information. Also, the system permits to filter and explore the information using the relations defined in the knowledge graphs (facets). As a highlighted point, this visual environment could give support on the elaboration of WSIS strategies through an understanding of the information.

Both developments to the consecution of the objectives established for the Task 2.1 referring to: (i) elaborate an ontology to determine waste utilization potential of industries and subsequent processes and systems to support WSIS; and (ii) n online tool that will be compatible with the KPI tool (T2.4) and would allow interested industries to register their own water-related waste streams and identify promising opportunities for reuse at an industrial cluster and/or regional scale.





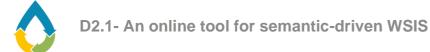
## 9.2. Future Work

T2.1 will continue their development until M36 (May 2023). Within this period, we will continue with the development of the ontology and the semantic repository as follows:

Ontology 3 <sup>rd</sup> cycle (M24-M36)	<ul> <li>Incorporation of economic costs and information</li> <li>Incorporation of rules and semantic reasoning over the information.</li> <li>Third version of the ontology and their subsequent validation.</li> </ul>
Semantic Repository 3 <sup>rd</sup> cycle (M24-M36)	<ul> <li>Refinement of Owner and access to the different repositories</li> <li>Refinement of the automatic visualization with data dashboards and information linkage</li> <li>Incorporation of different semantic repository databases (Quad stores).</li> <li>Incorporation of needed mechanism to enable queries with reasoning.</li> <li>Other visualization of the general model</li> </ul>

Table 27. Future work to be performed in relation to WSIS ontology and semantic repository





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