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Discovering Valorisation Paths in Waste Biorefineries using an Ontology Engineering Approach

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Abstract

Pectin and D-limonene from citrus peel, hydrogen gas from pulp and paper industrial by-products, peptides from dairy residues, lactic acid and biosurfactant from grape stalks, methane from MSW and biodiesel from waste cooking oil are only few paradigms exhibiting successful valorisation of waste resources. With the shortage of fossil fuels putting pressure to find alternative and sustainable feedstocks, such valorising opportunities need to be more systematically realised. However, a major shortcoming in the commercialisation of waste conversion technologies is their high capital cost requirements due to their novelty, making their investment discouraging. The integration of waste with virgin resources to be processed by existing facilities will decrease current process' environmental impact, fossil fuel dependency and benefit from economies of scale. Such practice will aid in the smoother transition from fossil fuel to a bio-based economy. Aim of this work is to bring the knowledge of the waste valorising opportunities closer to the non-expert. This goal was achieved through the combination of ontology engineering and synthesis approach.

Keywords: ontology, waste, valorisation, synthesis, biorefinery

1. Introduction

The ever increasing global waste production in combination to the scarcity of materials creates an enormous strain on our resource system (Arancon et al., 2013). The need to reduce the use of virgin resources and recover raw materials from waste give rise in research areas such as Industrial Symbiosis (IS) (Cecelja et al., 2015), waste biorefineries (Satchatippavarn et al., 2015; Yang, X. et al., 2015), waste valorisation (Tuck et al., 2012) and circular approach economies (Su et al., 2013). Tremendous amount of work has been done in the past, to identify optimal strategies for treating and minimising waste. However, given that waste is inevitable, it has started to be regarded as lucrative business and estimates show that waste market share could reach $2 trillion by 2020 (Aylott, 2013).

Waste resources can be considered abundant generated by both industrial and municipal activities. The chemistries or else known as "synthesis paths" to extract materials from waste and convert them to valuable products can also be considered abundant. If its chemical compounds are recovered, they can become standalone feedstock or be also integrated with alike material resources to be processed by existing industrial facilities

(Floudas et al., 2012; Huber and Corma, 2007; Huang et al., 2010). This is a combinatorial problem resolved by process systems engineering (PSE). Such sustainable, retrofitting practice will enlarge the process capacity, benefiting from economies of scale, improve LCA performance and cost-effectiveness originating from waste's off-market prices.

To achieve such task: a) to appropriately integrate waste resources with virgin feedstocks and b) to identify suitable synthesis paths, producing diverse products, it requires the use of a well-established research field, ontology engineering. Therefore, it is required a well-structured and flexible Knowledge Management System (KMS), achieving extensive sharing of information across various processing facilities. Such tacit knowledge comprises of chemistries, process models, technology specifications, feedstock characteristics etc. The concept has been primarily derived from Magioglou et al.'s work (2014) and it was further developed for inter-industries integration.

2. Problem Description and Methodology Overview

2.1. Problem Description

A large number of chemistries exist, converting hybrid feedstock (virgin and waste resources) to broad range of products by making use of conventional and biorefinery concept technologies. However such knowledge is available to only limited number of parties with an extended process engineering background. This is multi-discipline, combinatorial problem that is proposed to be solved by a robust and layered methodology enabled by ontology engineering.

2.2. Methodology Overview

2.2.1. Synthesis

Prior to the platform construction, various chemistries transforming a wide range of waste resources to valuable products are gathered from bibliography, pilot studies and commercial applications. Chemistries are represented as synthesis routes comprising from chemicals and conversion processes. The chemicals are further subdivided to feedstocks, intermediates and products. The synthesis paths are brought together in a network or else known as superstructure. The synthesis units are denoted by *Biomass Bipartite graph Representation* (BBR) (Kokossis et al., 2015). Consequently, after the intense investigation into a range of waste valorising paths, a broad repository of process models is formed. For the integration of models, to simulate or optimise a network of synthesis routes, a vast amount of data is required. Such prerequisite dictates the library of models to rest on a knowledge layer that provides data such as feedstock and product prices, location and seasonal availability, technical specifications, technology cost, technology CO_2 footprint etc. from heterogeneous and scattered sources.

2.2.2. Transition from BBR & Superstructure Approach to Semantically Enabled Value Chain

The input-output process models along with their connections to the chemicals dictate a particular structure in the proposed Knowledge Management System (KMS). The Semantic Web technologies and ontology engineering appear to enable such challenge to be solved. Moreover, the use of ontologies is ideal for knowledge representation of the synthesis pathways, the taxonomy of the chemical components as well as for the dynamic knowledge addition. Ontology consists of classes, progressive subclasses and the entities of the class-instances. The units making up a synthesis path, they have shaped the classes of the Waste Biorefinery Ontology (WBO). Thus, as shown in Figure 1, the primary classes are *flows* and *processes*. The class *processes* was subdivided to *biorefinery* and *conventional processes*, while the flows into *feedstocks*, *intermediates* and *products*. Feedstocks are further subdivided to waste and virgin resources. An analogous secondary subclassification was not defined for products and intermediate chemicals as it was found in many cases that both, the conventional and the waste biorefinery paths share common intermediates and products. For this work, it is of great interest to further examine the class of waste resources and identify a proper taxonomy that would enable the automatic discovery of the valorisation paths. A classification of waste resources was defined based on the dominant ingredient of the waste, encompassing *cellulose & hemicellulose*-, *sugar*-*lignin*-, *triglycerides*- and *protein*-waste class. Figure 1 depicts the overall taxonomy of the Waste Biorefinery Ontology.

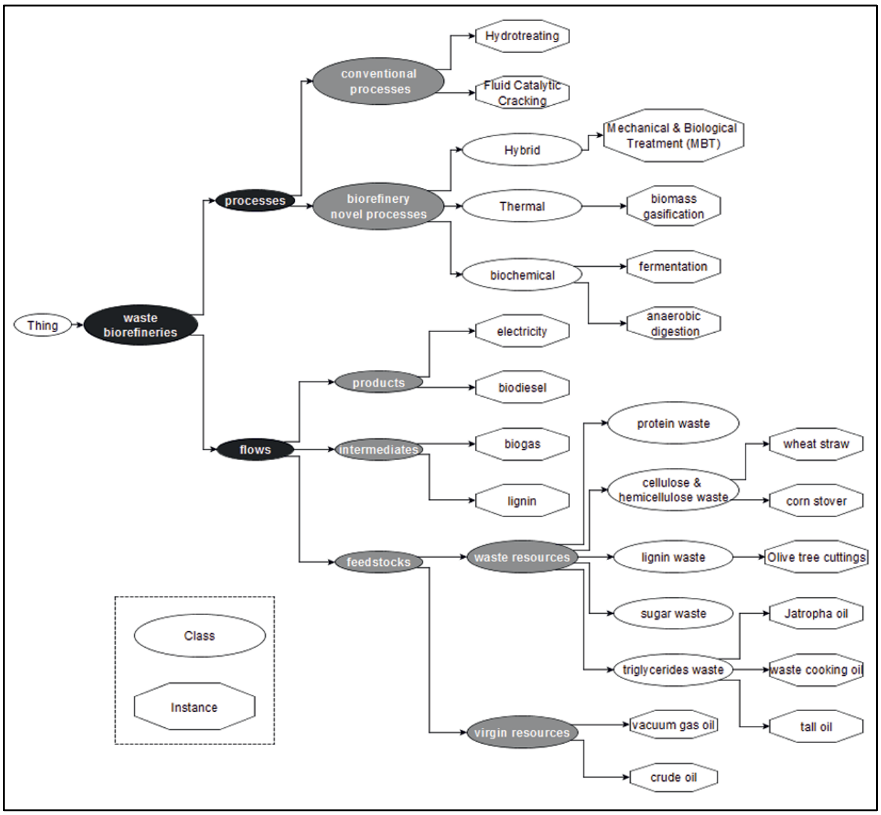

Figure 1: Waste Biorefinery Ontology

2.2.3. Querying & Retrieval: a method to suggest valorisation paths

The key insight of this work is that not all waste resource classes are connected to all valorising processes. Table 1 clearly illustrates some of the suitable primary valorisation processes for waste feedstocks possibly integrated with compatible virgin resources.

Table 1: Suitable primary conversion technologies for different classes of waste

Waste Resources	Virgin Resources	Primary Valorisation Processes
Cellulose & Hemicellulose waste		enzymatic conversion, hydrolysis, anaerobic digestion, acid/oxidative dehydration, hydrogenation
Lignin waste	Wood, Coal, Char	gasification, pyrolysis, plasma arc gasification, liquefaction, torrefaction
Sugar waste		fermentation, ABE fermentation
Triglycerides waste	Gas Oil, Crude Oil, Palm Oil, vacuum gas oil (VGO) etc.	transesterification, fluid catalytic cracking, hydrotreating, thermal depolymerisation
Protein Waste		anaerobic digestion, Mechanical and Biological treatment (MBT), hydrotreating, solvolysis (depolymerisation)

The specific chemicals and processes, are connected by ontological object properties as presented by Magioglou et al. (2014): *has input, has output, is processed with, is produced by, can lead to* etc.; therefore, achieving to convert knowledge found in literature on valorisation paths to a readable and processable form by ontology engineering tools. Consequently, the object properties represent the connectivity between processes and chemicals, composing a synthesis route. The retrieval of valorisation paths, when a waste is selected, is achieved by querying the ontological properties (*has input, has output* etc.) using SPARQL standards. Precisely, when the user chooses certain waste(s) in order to discover integrated valorisation paths, the particular waste (instance) is connected by object properties with compatible primary valorisation technologies as illustrated in Table 1. The technologies are linked with intermediate chemicals and the chemicals are further connected to secondary technologies. The establishment of connections is continued until the path is reached to a chemical identified as a 'product'. The retrieval of paths is achieved by posing natural language inquires to the ontology such as 'What can be produced from the selected feedstock/intermediate?', 'From which feedstock/intermediate can I produce the specific product?', 'Which technology can process specific feedstock/intermediate?' and 'Which technology can produce the selected product/intermediate?' Based on a long sequence of such linked-queries, the user can discover full synthesis paths produced from selecting specific waste feedstocks as well as integrating with compatible virgin raw materials. The platform exploits the results of each single SPARQL query and constructs data structures. Respectively, a sequence of linked-queries creates sets of such data structures. Based on these sets, the server constructs all possible paths.

2.2.4. Data Integration & Platform Architecture

The platform uses Linked Data, involving RDF links, to integrate data from different sources. Employing appropriate software tools, all data gathered from heterogeneous sources such as relational databases, text files, Microsoft Excel files, semantic sources etc. are transformed into the desirable RDF format and stored in a selected triple store for potential data retrieval.

A PHP framework, using the model-view-controller architecture, is established to provide the platform the required information extracted from data layers where the semantics lie. At the front end, a dynamic HTML, CSS and JavaScript interface is implemented so that the non-expert user can interact with the platform. User's input selection is passed as a natural language pattern, while the output is a graphical visualisation of the appropriate synthesis paths, using dynamic JavaScript graph library. At the back end, the web server invokes and processes the ontology information, thus rendering the web page with the corresponding pathways.

3. Illustration

The methodology is illustrated by investigating the scenario of discovering the valorisation paths of five different types of waste: olive tree cuttings, wheat straw, waste cooking oil, tall oil and black liquor. Figure 2 does not aim to provide the valorising paths from bibliography and pilot cases but to demonstrate how the knowledge found in the overall waste valorising value chain can be customed to the natural language queries posed by users. For instance, the user could be more interested into specific products with identified high demand in the regional market or the paths valorising particular waste resource which might be available locally. The user could also be interested to discover only integrated synthesis paths, only conventional routes or even only biochemical processes due to policy restrictions. Such qualitative restrictions are taken into consideration by the ontological platform, allowing the discovery of valorising paths to be accomplished through a filter search matching the needs of the user. This feature aids in the rigorous navigation through the different options even upon value chain expansion.

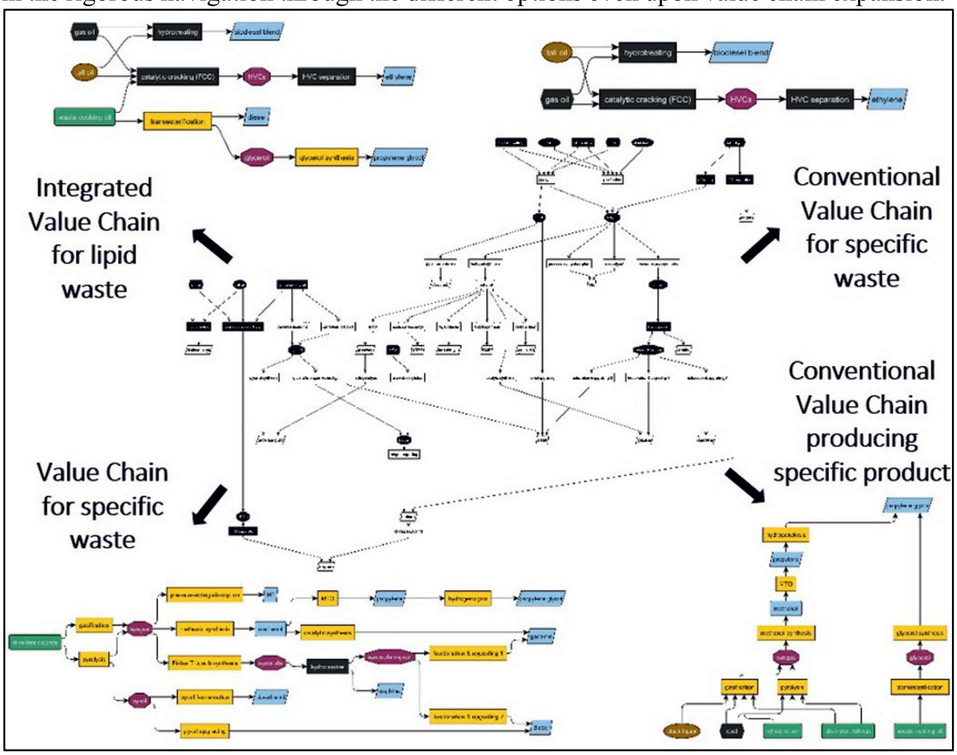

Figure 2: The waste value chain can be custom-made to the natural language queries of the user