Waste Streams Property Characterisation in Biorefinery Systems Engineering Using an Ontology Approach

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Abstract

The aim of this work is to advance the currently available repositories for a waste biorefinery by adding a new layer of detail within the ontology concerning stream chemical and properties characterisation. The work offers a systematic approach to the collection, classification, repositories and ontology building for organic waste streams, and includes the necessary methodologies and workflows for expanding the current repository. The work consists of a detailed literature review and industrial data collection for the classification of the streams according to processing technologies. A detailed repository of models to describe all the properties of the involved streams is included as well.

Keywords: organic waste, property models, ontology engineering, repository

1. Introduction

The challenges regarding energy, food, water and environmental impact faced by our society, demand a better valorisation of (bio)resources in all industrial areas. At the global level, there is a high interest in implementing strategies to "close the loop" of products life cycle from across all industrial activities, which are reflected in new policies and legislation and an increased focus in R&D activities for recycling and re-use of waste products in order to implement a full-scale circular economy system (Gonzalez-Garcia et al., 2018). All these efforts are materialised in development of waste biorefineries focused on waste recovering and valorisation or renewable biorefineries which are integrating virgin resources with recycled ones for production of added value products (e.g. fuels, chemicals or other type of products) (Barla et al., 2016). Such PSE (process systems engineering) problems involving many different technologies and sources of information needed for solving different type of problems (e.g. selection of processing pathways for a new product or using a new feedstock, location-dependent product and process synthesis, etc) are not easy to be handled and they need a systematic approach (Bertran et al., 2017). In the recent years, ontologies as means of information/knowledge representation are expanding across different domains, including PSE and they are used for solving different types problems such as process synthesis for different applications (Bertran et al., 2017; Kokossis et al., 2016; Roh et al., 2016), supply chain modelling and design (Muñoz et al., 2011), decision-making for environmental impact minimisation (Cecelja et al., 2015), or computer-aided process engineering applications (Morbach et al., 2007). All these types of problems are encountered within domains such as (waste) biorefinery. In the RENESENG project, repositories including technologies and flow instances for biorefineries and waste biorefineries were created (Siougkrou et al., 2018b). The aim of the current work is to expand the Biorefinery Systems Engineering (BSE) ontology and repository with a new level of detail for waste streams/flows classification and characterisation in terms of chemical composition and physio-chemical properties by providing appropriate data and models. The work follows a systematic approach for the ontology structure and repository data and model collection and integration.

2. Ontology/repository structure and description

The workflow of expanding the BSE ontology and repository followes a series of steps: (1) classification of waste streams within the ontology, (2) collection of waste stream data form literature and industry, (3) repository building by importing pure component database, collecting models and afferent parameters for the method database, (4) collection of algorithms needed for the user services. Once steps 1-4 are finalized, all the data will be added to the BSE repository following the previously used methods (Siougkrou et al., 2018b).

2.1. Ontology waste flow classification

The available ontology for BSE contains already two main classes: technologies and flows, with each class being organised on different subclasses such as feedstock, intermediates and products for the flows (Siougkrou et al., 2018b). The waste flows are included within the feedstock subclass. In the current work, the waste flows are further classified based on provenience, type, stream phase, and composition, as it is presented in Figure 1. More subclasses can be included if necessary at a later stage of ontology development.

2.2. Repository data

In order to be able to provide all the necessary information of the flow/stream characterisation, besides the flows database, following databases should be available within the repository: pure components properties, models and algorithms.

The flows database includes entries for each flow/stream available. The data is collected from literature or from industry. For each stream, the data is collected according to a pre-defined datasheet (see Table 1) which is saved as an independent file, and which includes the following:
(i) general information - the name, flowrate, temperature and pressure of the streams are provided along with the technology connection within the ontology;
(ii) composition – stream composition can be given as detailed composition (flowrate of each chemical component), or as general composition where the composition for main class of components is specified (e.g. 40% water, 50% triacylglycerols, 10% fatty acids). The user can provide as well the composition ranges within the stream can variate. This is helpful in later stapes for process synthesis and detailed modelling;
(iii) properties - cover a wide range of physio-chemical properties (e.g. phase, density, viscosity, specific heat, etc.), where the user can provide the experimental data. The

calculated values of the properties are saved as well. The last calculation result for each property is saved together with the name of the calculation method/model used.
(iv) other – includes price information of the stream, location of the stream, availability (e.g. seasonal, all year), and user notes where observations or other data can be stored.

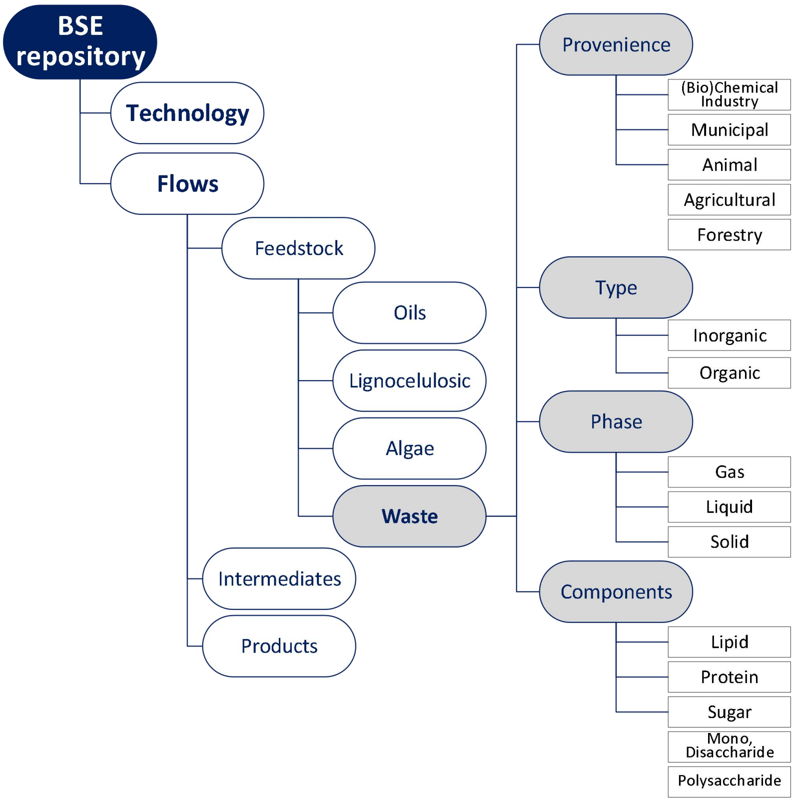

Fig.1 Biorefinery Systems Engineering ontology representation with emphasis on waste resources based on the work from Siougkrou et al., 2018.

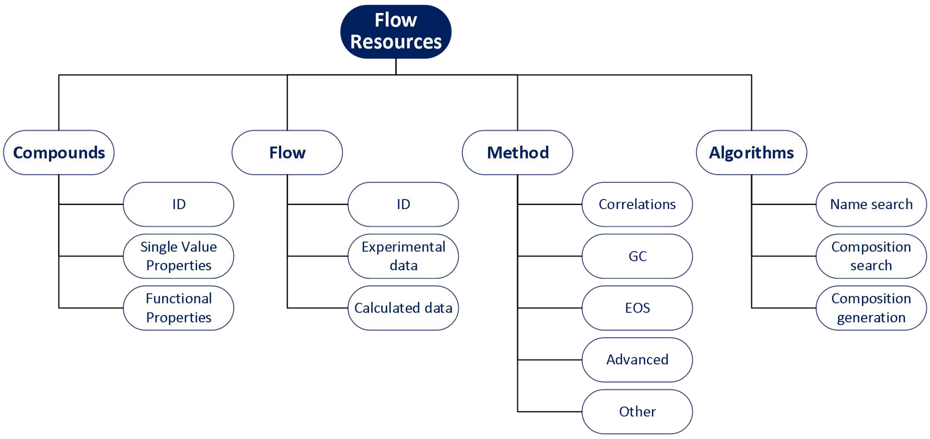

Fig 2. Resources needed for Flow characterisation.

Table 1 Flow input-output characterisation within the BSE repository.

General information	Composition	Properties	Other
Name	General composition	Experimental data	Price
Flow type[1]	Detailed composition	(Calculated data)	Location
Technology connection[2]	Composition ranges		Availability
Flowrate			User notes
Temperature			
Pressure			

[1] From classification within the ontology; it can be part of different classes (see Fig. 1)
[2] From the technology connectivity: IsProducedBy/IsProcessedWith; it can have different connections (Siougkrou et al., 2018b)

The pure component database includes all the necessary information for pure compounds found in (waste) streams/flows (e.g. identifiers, primary and secondary properties values, functional properties correlations and their parameters). The database is imported from other sources using an ontology reuse method (Trokanas and Cecelja, 2016) and it is updated by user input when new data is available.

The method database includes all the necessary calculation models organised in different sub-classes: thermodynamic methods (e.g. GC, EOS, Advanced) to describe phase properties, and other methods needed to characterize the streams (e.g. oxygen demand, LCA indicators, etc.). Each method is organised into two sections: models and parameters. The models section includes files with the mathematical formulation of the method, while the parameters section includes files with parameters needed for a specific method (e.g. binary interaction parameters for equation of state models, R, Q and group-group binary interaction parameter for group contribution models, etc.).

The algorithm database includes all the algorithms necessary to provide the user service, as described in the following section.

2.3. User services

Different direct services can be accessed by the user regarding the flows: (i) browse within the flows ontology, (ii) search after a name, (iii) search after a composition, (iv) generate detailed composition from general composition to match a certain type of stream, (v) calculate properties for a given composition. The steps followed by the user for each case is presented in Figure 3. When finishing an enquiry, the user can choose to end or to continue with another problem such as process synthesis based on the identified flow and its afferent technological connections and which can further can continue with an optimisation problem (Siougkrou et al., 2018a).

Other services for the user that can be implemented are data validation and/or reconciliation for a flow/stream (e.g. composition, experimental property data vs calculated) or for a set of flows/streams connected to the same process/technology (e.g. mass balance check, experimental property data from different sources vs. calculated data with different models).

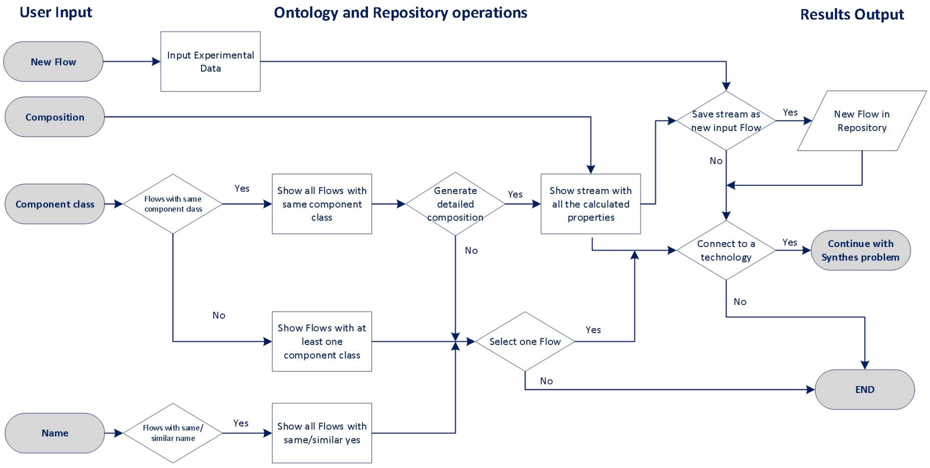

Fig 3. User experience with (Waste) Flows operations.

3. Conclusions

The extension of available BSE ontology and repository for (waste) flow classification and characterisation has been proposed. The work focuses on waste streams, but it can be expanded for any other type of stream within the BSE ontology. Sub-classes following different classification criteria for waste flows are included within the ontology. The associated repositories needed for detailed flow/stream characterisation include four categories of data: pure component, flow, methods and algorithms. The user can add, compare or search data through available services.

The future work should be focused on expanding the data available within the flow and model repository. The performance of available thermodynamic methods for waste streams calculation should be testes, and if necessary, models reparameterization should be considered.

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