A Semantic Web Engine for Biorefining Model Integration

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Abstract: The number of models available to the biorefining community is continuously increasing, there is a need to provide better ways for their description, categorization, discovery and integration in order to improve reusability of them. Biorefining models on the other hand are developed using heterogeneous methods, data format and various environments that makes their reuse challenging. In this paper, we describe a semantic web engine for the domain of biorefining, which enhances the description of biorefining model by using semantic web technologies in order to facilitate discovery and integration. In particular, we present how domain and web service ontologies are used in semantic mapping for the purpose of model integration, which is achieved by OWL-S (Semantic Markup for Web Services). Whilst the application has been designed and implemented for a specific domain, this novel design can be applicable to similar problems in other domains.

1 INTRODUCTION

Mathematical modelling and simulation have been widely and for long used to represent many aspects of biorefining i.e. bioenergy production systems, conversion processes, supply logistics and environmental impacts (L. Wanga et al., 2015). Those models can provide powerful tools to design a biorefining system and evaluate its technical feasibility, economics and environmental impacts.
As a result, there are a great number of models that can be shared with the biorefining community and hence reused. Model integration in biorefining is an important function, which enables model integration from unit composition to model orchestration and invocation. The highest level of integration is the supply chain integrating lower scale models in varieties of ways. To this end, biorefining models are characterized by heterogeneous methods, data format and different development environments making their reuse a challenge.

To address this problem, we introduce a semantic application to enable model sharing, discovery and integration. Main functionalities of the application include; i) *Model Registration* where detailed information on model functionality, inputs, outputs and condition of operation are acquired, ii) *Model Publishing* which gives the possibility for models to be shared, iii) *Model Discovery* which supports the C6Fermentation">based on different semantic techniques and iv) *Model Composition* where the user has the possibility to integrate his model with other biorefining models that are discovered through the application for achieving a more complex goal in his modelling. Models represent at abstraction level a biorefining process and are described semantically by their functionality, inputs, outputs and preconditions needed for their execution (Figure 1). The semantic description of biorefining models is supported by a biorefining domain ontology, as demonstrated in the following section. CAPE-OPEN initiative, a widely recognized industry standard that defines rules and interfaces in chemical and process systems community, is the only one that has given significant contribution in model reusability and interoperability (Belaud and Pons, 2002) of Computer-Aided Process Engineering (CAPE) applications or components. CAPE-OPEN interfaces, provide the opportunity that process modelling components can be assembled in process modelling environments at runtime and has a well-established communication mechanism by which software components can exchange functionality at runtime (Braunschweig et al., 2004). Beside the advantages that CAPE-OPEN offers, the semantics of interface are implicit and only human providers and users are able to decide which software component will best fit for a specific application's

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need and therefore the task of identifying the most adequate model from the libraries is a manual process (Braunschweig et al., 2004).

2 ONTOLOGY- DRIVEN APPROACH FOR SEMANTIC PUBLISHING AND DISCOVERY

Ontologies allow us to define concepts and relations in the domain of interest, which can be processed by a machine. OWL (Web Ontology Language) is a logic based ontology language, which means the semantics of the language is precisely defined by a logic. Furthermore, OWL is rich of computation properties and it is possible to perform computations automatically using tools, called reasoners (Horridge et al., 2014). The latest standard ontology languages is OWL2 (Motik et al., 2009). Reasoners are software systems that can be used for i) ontology design time to check certain desirable consequences follow from what has been stated and ii) application runtime to provide query answering capabilities, which ensures queries, such as representing knowledge is correctly answered. There are many reasoners, such as FaCT++ (Tsarkov and Horrocks, 2006) and HermiT (Shearer, 2008), that work well with OWL. A biorefining domain ontology (Koo et al., 2017) is exclusively developed to describe biorefining models for the purpose of i) registering and publishing them based on their semantic description, ii) performing the process of semantic discovery, and iii) facilitating the process of integration. The models in the biorefining domain ontology are describes in term of functionality, inputs required for the successful execution of a model, outputs generated after execution, and the preconditions of the model, as shown in Figure 1.

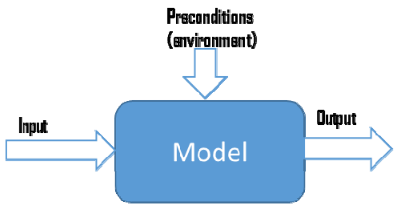


Figure 1: Representation of biorefining models.

The ontology is developed in OWL and is often enriched by adding rules using SWRL (Semantic Web Rule Language) to provide an additional layer of expression where OWL lacks expressive power.
The biorefining ontology contains all necessary concepts and relations for capturing knowledge from the biorefining domain with a special focus towards integration of models. Model class is used to collect information about a biorefining model as an instance based on functionality, input, output, and biorefining platform (Figure 2).

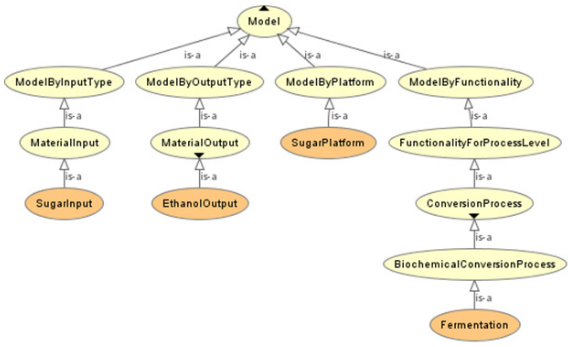
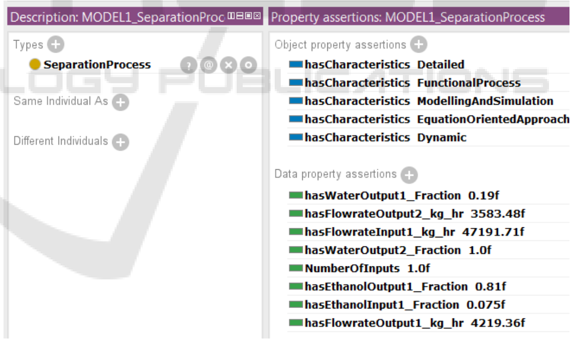


Figure 2: Illustration of the hierarchy of classes in the biorefining domain ontology.

Object and datatype properties are used to define data inputs and outputs of a model, object properties are used to further characterize a model and SWRL rules to define the preconditions which in most cases in relation to the environment where a model run. Figure 3 demonstrates an instance of a model in ontology that belongs to *SeparationProcess* class.



Description: MODEL1_SeparationProc

Types
SeparationProcess

Same Individual As

Different Individuals

Property assertions: MODEL1_SeparationProcess

Object property assertions

```
hasCharacteristics  Detailed
hasCharacteristics  FunctionalProcess
hasCharacteristics  ModellingAndSimulation
hasCharacteristics  EquationOrientedApproach
hasCharacteristics  Dynamic
```

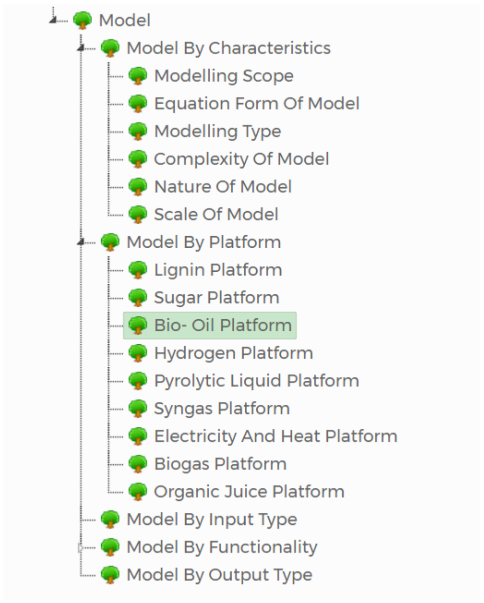
Data property assertions

```
hasWaterOutput1_Fraction  0.19f
hasFlowrateOutput2_kg_hr  3583.48f
hasFlowrateInput1_kg_hr  47191.71f
hasWaterOutput2_Fraction  1.0f
NumberOfInputs  1.0f
hasEthanolOutput1_Fraction  0.81f
hasEthanolInput1_Fraction  0.075f
hasFlowrateOutput1_kg_hr  4219.36f
```

Figure 3: Separation Process biorefining model instance.

2.1 Registration and Publishing

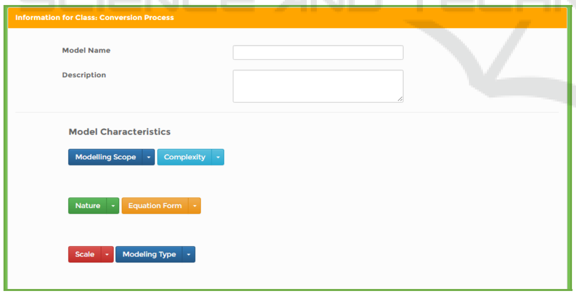
For publishing and sharing a model, the users will initially have to register the model by accessing the semantic web application. In technical terms the ontology is parsed and checked for consistency by Hermit reasoner and all classes are given to the user in the form of a tree (Figure 4a). Figures 4a-c provides a reduced view of the platform to demonstrate the operation of the repository to support the process of registration of the biorefining models and data.



- Model
  - Model By Characteristics
    - Modelling Scope
    - Equation Form Of Model
    - Modelling Type
    - Complexity Of Model
    - Nature Of Model
    - Scale Of Model
  - Model By Platform
    - Lignin Platform
    - Sugar Platform
    - Bio- Oil Platform
    - Hydrogen Platform
    - Pyrolytic Liquid Platform
    - Syngas Platform
    - Electricity And Heat Platform
    - Biogas Platform
    - Organic Juice Platform
  - Model By Input Type
  - Model By Functionality
  - Model By Output Type

Figure 4a: (Step 1) Model classification.

In step 1 (Figure 4a), user register a model under a predefined category by browsing a taxonomy presented in a form of tree. Every class in the ontology is correlated with a number of datatype and object properties, mainly in terms of its functionality input, output and precondition, which is presented in Figure 4b and c to complete the model registration process.

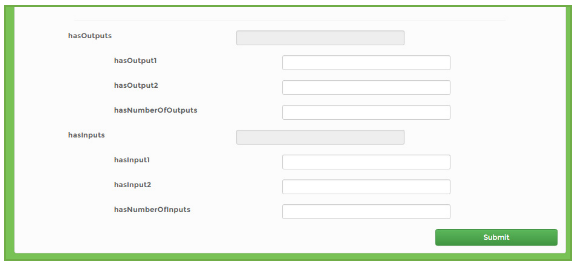


Information for Class: Conversion Process

Model Name	
Description	

Model Characteristics

Figure 4b: (Step 2) Name and description the model with annotations and object properties.



hasOutputs	
hasOutput1	
hasOutput2	
hasNumberOfOutputs	
hasInputs	
hasInput1	
hasInput2	
hasNumberOfInputs	

Figure 4c: (Step 3) Complete inputs and outputs of the model by giving value to the data properties.

Illustration of the registration process under ModelbyFunctionality category in the biorefining domain ontology is given in Figure 5. Together with reasoner, fermentation model is registered in terms of platform, as well as input and output type.

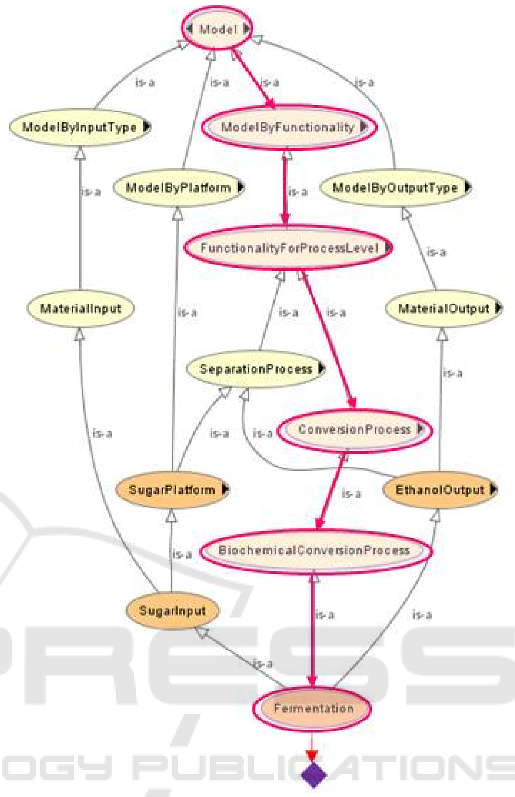


Figure 5: Registration of a fermentation model in the biorefining domain ontology.

2.2 Discovery

By registering and publishing the models with the necessary semantic annotation, biorefining models are stored in a semantic repository and many experts in the field can make use of them. Next important step is to discover the models that the semantic repository maintains. For discovering the required model the user can choose among four options:

i) *List of all models by different categories*: Browse the models as they are listed based on different categories (i.e. by functionality, by output etc.)

ii) *Search* for the desired model using two filters: a) functionality and b) output of the model.

iii) Write a *SPARQL* query to filter the required models and run it through the application.

iv) *Semantic matching* between a set of requirements, which is set by the input of a requesting model and the list of models in the semantic repository as candidate models that meet the requirements. This method is developed with an intention to achieve the purpose of model integration and is further detailed in Section 2.3.

The first and the second techniques are keyword based queries. The SPARQL editor is made available by employing jOWL (Decraene, 2007), a jQuery plugin for OWL-RDFS documents and is intended to be used by users who are familiar with knowledge based systems and SPARQL querying language.

2.3 Semantic Matching

Discovery of candidate models that fully or partially matches the requirements of a requesting model is a very important step for a successful model integration. The requirements of a requesting model are a set of inputs that the requesting model needs which has to correspond to the outputs that a model in the semantic repository has in order to be a candidate model for integration. This way the process of matching will result in the process of comparing the input requirements that the requesting model has with the outputs that candidate models offer.

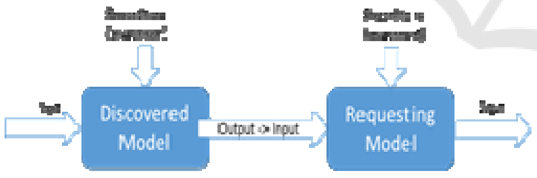


Figure 6: Model input/ output matching.

In our work we have used input/output matching approach introduced by Cecelja et al. (2015) that undergoes three-stage matching phases: i) elimination, where all models that do not satisfy the critical criteria are excluded from the selection list, ii) semantic matching by calculating similarity measures which defines the level of compatibility between the requested model and the candidate models and iii) ranking of the candidate models by similarity measure. The critical criteria is defined by the user during the formulation of the requesting model. Semantic matching process calculates the semantic relevance between the requesting model and the models published in the repository. This is calculated as an aggregated value (Algorithm 1) of *distance measure* (Algorithm 2) and *property similarity* (Koo et al., 2017). Distance measure signifies the semantic similarity where the ontology is processed as a graph structure and is calculated by finding the shortest distance between concepts in the ontology where paths has different weights. The quantified distance measure is normalized with the longest path between concepts in the ontology. Property similarity is calculated by the average of cosine and Euclidian similarity using the values of the properties characterising the models as a vector.

Algorithm 1: Semantic Matching.

```
Input: O an ontology, M_r the requesting
model which is instance of O
Output: S, a set of models ordered
based on the semantic matching
    For all models in the repository
      Eliminate (O, M_r)
    For all models in O after
    elemination
      CalculateSemanticSimilarity(O[M_i
     ], M_r)
      CalculatePropertySimilarity(O[Mi
     ], M)
      S[i]←DefineMatchingMatching(Ss,
     Qm)
     Print S in descanted order
```

Algorithm 2: CalculateDistanceMeasure.

```
  Input: O an ontology with the
reduces number of instances after the
elimination, the requesting model M_r
  Output: K, a number representing the
semantic matching
     For all models in the repository
      findShortestPath(O, M_r)
      findLongestPath(O)
      CalculateK(findShortestPath(O,
     M_r),findLongestPath(O))

     Print K
```

3 SEMANTIC WEB SERVICE FOR INTEGRATION

One main reason of reusing models in biorefining is to generate new knowledge from the integration of heterogeneous data, methods and tools. Semantic web technologies are considered as the best method to the support model integration as they use graphical method to describe data models that handle unstructured data. The approach we propose to achieve the model integration in biorefining is adopted form the semantic web services integration methodology and the input/output matching. We consider each biorefining model is an instance of the domain ontology as a web service and semantically described with the OWL-S. OWL-S is a well-established framework with respective service ontology which, in this case, facilitates a full automation of model integration. In practical terms, OWL-S framework (Martin et al. 2004) is implemented as an ontology with three interconnected sub-ontologies (Figure 7); Service Profile (Profile.owl), Process Model (Proces.owl), and Process Grounding (Service.owl). Typically a semantic web service has interlink to all the .owl files in Table 1.

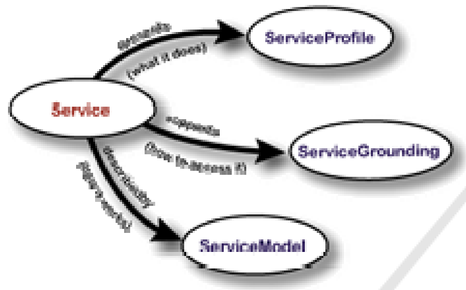


Figure 7: OWL-S upper layer ontology (Martin et al. 2004).

Table 1: C6Fermentation model as OWL-S service.

C6FermentationService.owl	Service instance
C6FermentationProfile.owl	Profile
C6FermentationProcess.owl	Process model
Grounding.owl	*Grounding instances*
Grounding.wsdl	*WSDL definitions for grounding*

Within the OWL-S framework, Service Profile delivers a way to describe services, in our case, models (Martin et al., 2004) and contains two different types of information i) contact information of the model provider and ii) functional description of the model in terms of inputs required by the requesting model, outputs generated from the candidate model, preconditions for execution and expected effects from the execution (IOPE). Below is part of the content of the service and profile .owl files of the C6Fermentation model described by OWL-S. By taking advantage of OWL-S profiles structure and their references to OWL concepts of the biorefining domain ontology, the discovery process find those models that are most likely to satisfy the needs of a requesting model (Martin et al., 2007).

C6FermentationService.owl

```
…………
<service:Service
rdf:ID="C6Fermentation">
<!--  Reference to the C6Fermentation
Profile  -->
<service:presents rdf:resource="URI
C6FermentationProfile.owl#Profile_C6Fer
mentation "/>
<!--  Reference to the C6Fermentation
Process Model  -->
<service:describedBy
rdf:resource="URI\C6FermentationProcess
.owl#C6Fermentation_Process"/>………………
</service:Service>
```

C6FermntationProfile.owl

```
…………
<!--  reference to the service
specification  -->
<service:presentedBy
rdf:resource="URIC6FermentationService.
owl#C6Fermentation "/>
<!--  reference to the process model
specification  -->
<profile:has_process
rdf:resource="URIC6FermentationProcess.
owl#C6Fermentation_Process"/>
<profile:serviceName>C6Fermentationt</p
rofile:serviceName>…………………………………….
<profile:contactInformation>
<actor:Actor rdf:ID="C6Fermentation ">
<actor:name>C6Fermentation Process
</actor:name>
<actor:phone>67668788</actor:phone>
<actor:fax>412 268 5569</actor:fax>
<actor:email>email@domain.com
</actor:email>
…………………………………
<!--  Descriptions of IOPEs  -->
<profile:hasInput
rdf:resource="URIC6FermentationProcess.
owl#TotalFlow"/>
<profile:hasInput
rdf:resource="URIC6FermentationProcess.
owl#Temperature"/>
<profile:hasInput
rdf:resource="URI/C6FermentationProcess
.owl#Pressure"/>
…………………………………………………..
<profile:hasOutput
rdf:resource="URI/C6FermentationProcess
.owl#ComponentFractionEthanol"/>…………………
```

The Process Model describes a model in the sense of how it works, the tasks it performs, the sequencing of this tasks, the intermediate inputs and outputs and the transformation that happens in each stage. A part of the C6FermentationProcess.owl file code is presented below, which expresses the process model.

```
   C6FermentationProcess.owl
   ………………….
<process:AtomicProcess
rdf:ID="C6Fermentation">
<rdfs:comment>
Get inputs for successfully running the
model.
</rdfs:comment>
<process:hasInput>
<process:Input rdf:ID="Get_Input_S1">
<process:parameterType
rdf:datatype="http://www.w3.org/2001/XM
LSchema#anyURI">
anyURI/BiorefiningConcepts.owl#ModelFun
ctionality </process:parameterType>
</process:Input>
</process:hasInput>
………………………
<process:hasOutput>
</process:parameterType>
</process:Output>
</process:hasOutput>……….
<process:inCondition>
<expr:SWRL-Condition>
<rdfs:label>hasPlatform</rdfs:label>
<expr:expressionObject>
<swrl:AtomList>
<rdf:first>
<swrl:IndividualPropertyAtom>
<swrl:propertyPredicate
rdf:resource="#hasPlatform"/>
<swrl:argument1 rdf:resource="#GAMS"/>
</swrl:AtomList>
</expr:expressionObject>
</expr:SWRL-Condition>
</process:inCondition>
```

OWL-S Grounding contain all necessary details for invoking a model (Pedrinaci et al., 2011) and the main function is to show how the inputs and outputs of process are defined concretely as messages, which carry those inputs and outputs in some specific transmittable format. To achieve this purpose OWL-S makes use of the Web Services Description Language (WSDL) which is a well-defined language for the purpose.

The model integration phase in the application starts at the stage of model discovery. The user owns a model (the requesting model) and tries to discover other models that could be integrated with his model, such as models that fully or partially match the requirement of the model. This phase is supported by input/output matching approach explained in section 2.3. The user is given a rank of available models that are matching fully or partially to the requesting model. Based on the criteria, user then selects one of the candidate models. Automation of the candidate model selection and composition is avoided to give to the user flexibility of choosing different pathways. Selection of the most suitable model will call the composition and invocation process to apply the model and data integration. Figure 8 gives the model composition layered architecture where: i) Base layer handles model registration and invocation ii) Atomic model layer contains the so called atomic models (simple model) and serves as the base for planning and invocation of models iii) Composite service layer contains composite models (complex model that can be further decomposed in atomic models) iv) Service abstraction layer serves as the basis of model composition v) Model Composition layer composes models based on their semantic description vi) Model planning layer provides the sequence of models to be invoked based on a planning algorithm vii) Model Invocation layer invoke models based on the sequence generated from the previous layer.

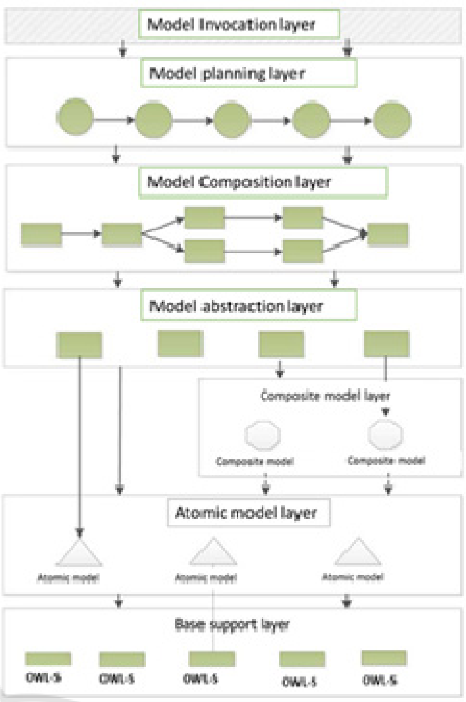


Figure 8: Layered model composition architecture adopted from Xiang et al 2015.

4 APPLICATION IMPLEMENTATION

The application is mainly developed using semantic technologies but is also supported by other web technologies. Figure 9 displays the semantic application architecture which is conceptualized in three main pillars; i) Back end or Service Layer ii) Middleware and iii) Front End. At the back end, the semantic web services and the domain ontology are stored. The core part of the system is developed in Java and represents the middleware layer, which is responsible for i) reasoning and interacting with the knowledge domain ii) match making engine and iii) interaction of front end interface and services. The Front End, being a web application, will be accessed through any browser and this part of the system has been developed using Bootstrap and Java Server Pages technologies. Through this interface the users can i) *search* for specific models based on specific criteria (i.e. the functionality of the model or output of the model or for a set of criteria) ii) *registration* of a model and iii) *composition* (Figure 10) of the requesting model with the models found in the repository (candidate models). As the knowledge base expands the system is updated in real time with the new knowledge and services. At the middleware layer a key role plays OWLAPI (Horridge and Bechhofer, 2011), a Java library for manipulating OWL ontologies. In collaboration with the reasoner (i.e. HermiT) and other supporting Java classes, OWLAPI, are checking the domain knowledge for consistency, parsing the inferred ontology for passing it to further elaboration from the front end, expanding the knowledge base with new instances of models or integrated models. As the highest aim of the repository is model integration the input/output matchmaking module is a crucial component and a processor step to our end use, the model integration. For the development of the match maker OWL-S Java API for parsing, serializing, validation, reasoning, and execution services for OWL-S (Sirin and Parsia, 2004).

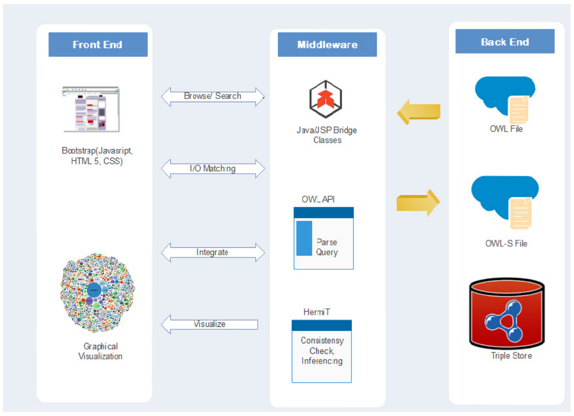
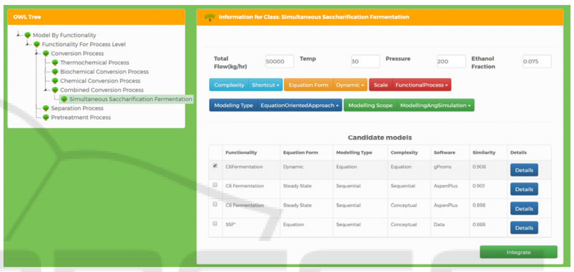


Figure 9: Application architecture.

The Semantic matching algorithm makes use of the JENA library (Dickinson et al., 2004), especially for measuring distances between concepts (*findShortestPath()*). Figure 9 shows the stage of the application where a list of biorefining models is offered to the user. The user can decide to test the integration of his model by choosing any of the candidate models even if the matching between his model and the candidate ones are not full matching (100%). Another instrument that can support the user in his decision in the *"Details"* section for every candidate model, where a justification of the semantic similarity is given. Justification is given by emphasising matching and non-matching properties between the requesting and candidate model and the semantic relevance that the requesting model has with each of the candidate models.



Total Flow(kg/hr)	Temp	Pressure	Ethanol Fraction
50000	30	200	0.075

Candidate models

	Functionality	Equation Form	Modelling Type	Complexity	Software	Similarity	Details
☑	C6Fermentation	Dynamic	Equation	Equation	gProms	0.908	Details
☐	C6 Fermentation	Steady State	Sequential	Sequential	AspenPlus	0.901	Details
☐	C6 Fermentation	Steady State	Sequential	Conceptual	AspenPlus	0.898	Details
☐	SSF*	Equation	Sequential	Conceptual	Data	0.888	Details

Figure 10: Part of the application where a list of candidate models is presented to the user for proceeding with the selection and integration steps.

5 CONCLUSIONS

A semantic web engine for supporting the biorefining community in model sharing and reuse has been introduced. Semantic web technologies are used to describe biorefining models semantically in order to assure model discovery and integration based on the content, instead of just syntax. All the models are described by the biorefining domain ontology and further treated and instances of OWL-S ontology. Users of the application can be experts of the biorefining community with different levels of expertise. The application is a complex one and build upon advanced technologies but this complexity is hidden to the user and they can benefit only from the advantage of it. The datatype properties, inputs and outputs of a biorefining model, are given by the owner of the model during registration stage. In some cases the user might need to test the integration for different data inputs. Future work will be focused on designing an intelligent algorithm that will facilitate the integration of biorefining models with dynamic data properties.

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