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Towards a novel ontological infrastructure for chemical process simulation and optimization in the context of eco-industrial parks

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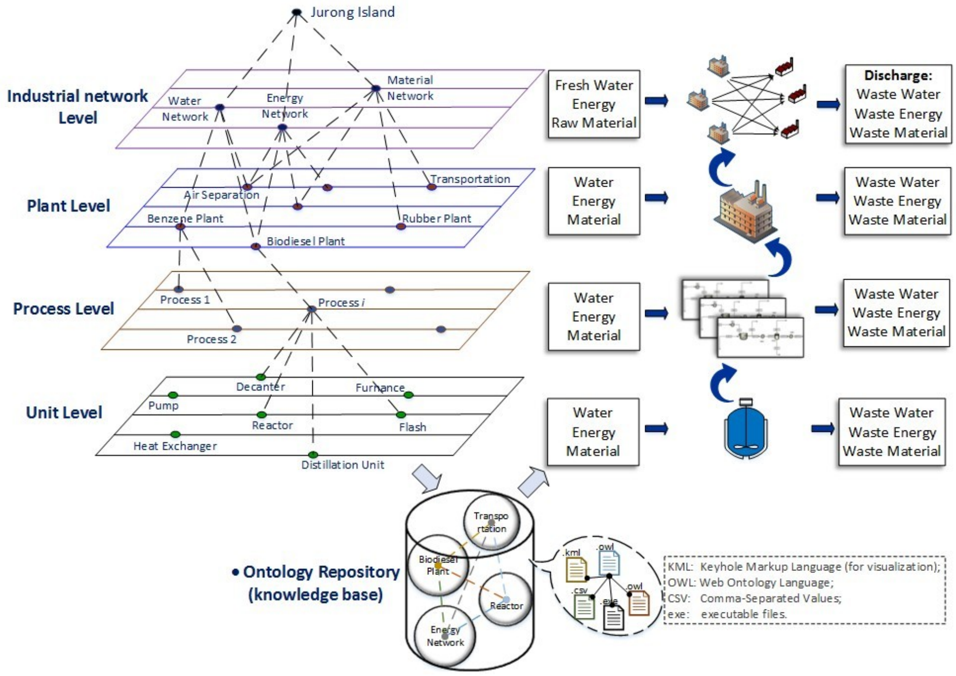
Highlights

- A ontology-based expert system called J-Park Simulator is constructed for energy and resource management of eco-industrial parks
- OntoCAPE is adapted to establish a knowledge base for a biodiesel plant
- Concepts are defined to incorporate description for executable mathematical models
- Plant-wide information query, process simulation and optimization can be carried out through J-Park Simulator

Abstract

In this paper, we introduce the concept of constructing an ontology-based expert system called J-Park Simulator (JPS) for the design and operation of eco-industrial parks (EIPs). It is inspired by Jurong industrial park in Singapore. A biodiesel plant is implemented into the system as a first step. OntoCAPE is adapted for the purposes of the biodiesel plant to establish a knowledge base, which is employed to carry out a number of applications via JPS. Firstly, information query can be performed. Information of the biodiesel plant can be extracted through natural language query. Secondly, JPS can be used to carry out process simulation. New process equilibrium can be evaluated after certain operation parameters change. Thirdly, process optimization can be realized through JPS. Optimal operation condition under different market scenarios can be obtained for the biodiesel producing process in order to reduce the energy consumption and achieve maximal plant profit. In addition, discussion on how the proposed approach can be applied to the design and operation of an EIP is also given.



Contents

1 Introduction

The study of EIPs has received great attention in the past few decades. An EIP is a cluster of businesses that collaborate with each other and the local community to efficiently share resources and reduce waste and pollution. The advantage of forming an EIP is that the combinative benefit (social, economical and environmental) achieved through the symbiosis relationships is much greater than the simple summation of the stand-alone individuals.

A great number of research works have been carried out to study EIPs, and numerous computer-aided system design and optimization methodologies have been reported to improve their performance [6, 21]. The synergistic benefit among businesses is realized by exchanges of materials, water and energy through a shared network. Currently, the reported optimization methodologies mainly focus on the optimal design of a single style network, either water, or energy, or materials. Water networks received abundant attention in the past decades resulting in a wide range of studies with this focus. A two-stage method was proposed by Liao et al. [25], where the fresh water target is determined in the first stage by solving a mixed integer nonlinear programming (MINLP) problem, and a flexible network is designed to meet the fresh water target in the second stage by solving a mixed integer linear programming (MILP) formulation. Chew et al. [9] presented two interplant water integration schemas, direct integration via pipelines versus indirect integration via centralized utility hub. They concluded that, indirect integration scheme can better perform direct integration in practicability and flexibility when a larger number of plants are involved. Lovelady et al. [27] developed an optimization method for the management of water among multiple processes. In their model, interception devices were considered as potential wastewater managing strategies, and a source-interception-sink structural representation was used. A multi-objective optimization strategy based on ε-constraint approach was developed by Boix et al. [5], taking three objectives into consideration (the fresh water consumption, the regenerated water flow rates and the number of pipe connections). This work was later extended to a flexibility analysis in Montastruc et al. [29].

In the area of energy networks integration, Chae et al. [8] proposed a mathematical model to synthesize a waste heat utilization network, including nearby companies and communities. A decision support dedicated to the optimization of industrial energy systems, named MIND method (Method for analysis of INDustrial energy systems) was developed by Karlsson [19] and applied to several case studies [20, 22]. Most recently, Nair et al. [30] presented a strategy for configuring multi-plant heat exchanger networks. The authors also proposed a practical idea of sharing central location and apportioning the capital and operating cost to participating companies based on individual savings.

Regarding the material exchanges, the materials can be of different types: products, by-products and wastes. A deterministic approach based on an MILP was developed by Cimren et al. [10] to analyze by-product synergistic networks that involve material processing and transport among companies. Haslenda and Jamalusin [17] presented a systematic framework for supply chain network integration in order to achieve optimal utilization of the by-products from crude palm oil refining processes. A bi-level linear integer programming model was developed by Tan and Aviso [39] to optimize the waste exchange between power plants, palm oil mills and bio-refineries.

The aforementioned studies decouple and optimise the systems present in EIPs. However, this approach is unlikely to reach global optimum solutions. The optimal symbiosis relation among businesses can only be achieved when different types of resources were taken into consideration. In such a case, a substantial amount of supporting data and information regarding different aspects of the potential network member need to be shared and communicated among agents. For such a knowledge-intensive task, a great amount of human interventions and expertise are required.

The described challenge may be handled using a knowledge-based system with advanced information management capabilities. The concepts and ideas of Industry 4.0 may aid developing such a system. In the future context of Industry 4.0, every technical component in the concerned system will be smart enough to perform self-evaluation, self-optimization and self-configuration [13, 18]. Automatic machine-to-machine trading will be enabled [37]. In such a case, information will need to be shared and exchanged among the relevant entities autonomously. A knowledge base that holds information for the entities and can act as a common platform to facilitate information exchange is considered as prerequisite. The information stored need to be contextualized so that it can be understood readily. Considering that the data generated by the entities is dispersed and the amount is ever-increasing, the knowledge base should be capable of handling such situations. Traditional information management technologies cannot provide adequate support to these particular needs.

Ontology technology has received great attention in the pase decade as an advanced tool to tackle these challenges. Several ontologies as well as their applications have been reported, covering chemical process engineering [3, 4, 28], electrical engineering [23, 24], pharmaceutical engineering [15, 16], building [11], transportation networks [26], etc. These ontologies can be utilized as base work to describe the engineering activities take place in an EIP (Fig. 1).

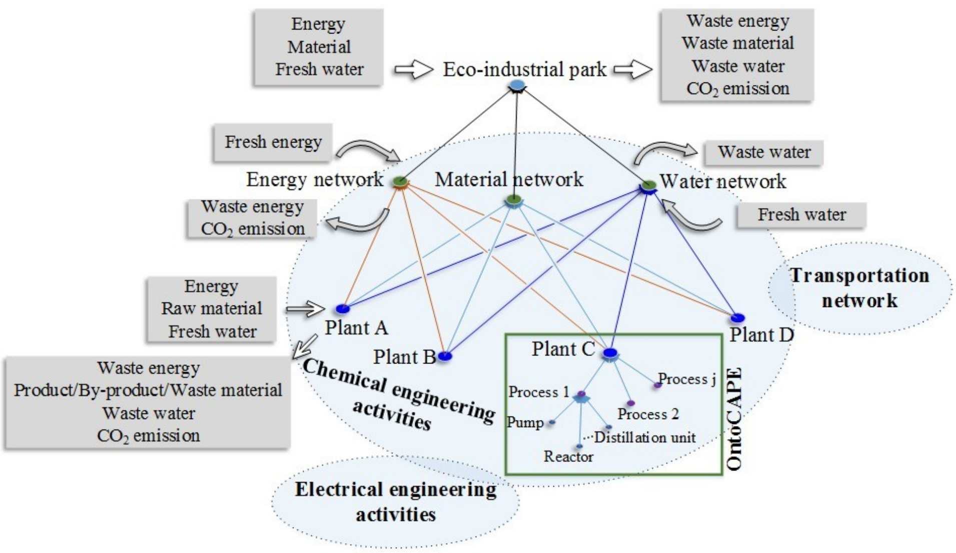


Figure 1: *Engineering activities conducted in an EIP.*

Among the reported ontologies for chemical process engineering domain, OntoCAPE [28] is the most widely accepted work. It covers the major engineering activities including the design, construction, and operations of chemical processes. Several applications were reported. It is utilized as a communication language between the interacting software agents and human users in CoGents [40], which is a multi-agent framework that supports the retrieval of desirable process modeling components from model libraries. Brandt et al [7] developed an ontology-based repository, Process Data Warehouse (PDW), for the knowledge management and integration during engineering design process. OntoCAPE was applied to annotate the electric documents generated during the design process. Recently, an ontology for process abnormal situation management, called OntoSafe, was developed by Natarajan et al. [32]. OntoSafe is an extension of OntoCAPE and is used to support a multi-agent based distributed intelligence system (ENCORE) [31]. ENCORE contains three types of agents that can cooperate with each other, including plant information manager agent, process supervision agent and user interface agent. An offshore oil and gas production process was used to test the effectiveness of the system. As the most widely accepted and field tested ontology work, OntoCAPE is employed to model the chemical processes in this work.

This paper focuses on applying OntoCAPE to construct a knowledge base for a chemical plant on Jurong Island. The developed knowledge base is then utilized to support an expert system, JPS to perform plant-wide process simulation and optimization. The rest of this paper is structured as follows. First of all, an introduction to ontology technology as well as OntoCAPE is given in the next section. In section 3, a knowledge-based expert system called JPS is presented. Section 4 introduces the development of a knowledge base for a biodiesel plant on Jurong Island, by utilizing OntoCAPE. Section 5 is dedicated to the demonstration of how the proposed approach is applied to a single chemical plant, where the establish knowledge base is used to support JPS to perform plant-wide information query, process simulation and process optimization. Section 6 discusses how the proposed approach can potentially benefit the design and operation of an EIP. Conclusion and future work are outlined in Section 7.

2 Background

2.1 Ontology technology for knowledge base construction

Ontology is a branch of philosophy that answers questions of being or existence [38]. In the past decade, it evolved in computer science for knowledge engineering. Definitions for an ontology in the literatures have been evolving over the years. Studer and colleagues [2] define it as follows:

An ontology is a formal, explicit specification of a shared conceptualization. Conceptualization refers to an abstract model of some phenomenon in the world by having identified the relevant concepts of that phenomenon. Explicit means that the type of concepts used, and the constraints on their use are explicitly defined. Formal refers to the fact that the ontology should be machine-readable. Shared reflects the notion that an ontology captures consensual knowledge, that is, it is not private of some individual, but accepted by *a group.*

Ontologies differ with respect to the richness of the internal structures and can be represented in various kind of languages. Lightweight ontologies are the ones with simple taxonomies and controlled vocabularies, while heavyweight ontologies specify relations and logical constraints between the ontological terms using expressive ontology languages [14]. A set of ontology languages have been created to implement ontologies in a computer-processable form [14]. At the earliest stage, AI-based ontology languages were developed based on first order logic. Later on, along with the boom of the Internet, web-based ontology languages were developed. The latter is also referred to as ontology markup languages (Fig. 2). Ontology markup languages are intended for publishing and sharing ontologies in the World Wide Web. It's based on the existing markup languages: XML and RDF(S).

1. XML: eXtensible Markup Language. XML was designed for store and transport data with their context information tagged. It facilitates the interoperability among human and machines, as it stores information in a both human-legible and machine-readable manner. It allows users to define and use their own tags, thus it is highly flexible and can be used for a dynamic developing process.

2. RDF: Resource Description Framework. It is a scheme for defining information on the Web. RDF encodes semantics in a subject-predicate-object format (also known as triples), where the subject, object as well as the predicate are identified by a Universal Resource Identifier (URI, which is recently extended to IRI – Internationalized Resource Identifier). Thus enables everyone to define and share new concepts.

These features can be utilized to facilitate the establishment of a decentralized information managing system, where information resources are scattered all over the Internet and/or intra-net and can be accessed through URIs (or IRIs). Moreover, ontology markup languages (ML) are based on an open standard and is platform-independent, which can be utilized to facilitate interoperability among agents.

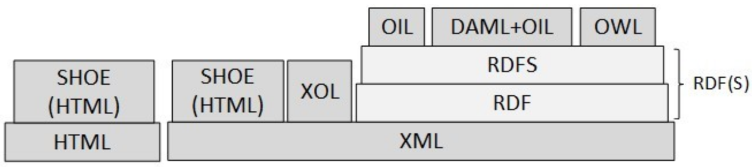


Figure 2: *Ontology Markup Languages.[14]*

2.2 OntoCAPE to model chemical processes

OntoCAPE is a formal, heavyweight ontology developed for Computer Aided Process Engineering domain (see Fig. 3 for an overview). It consists of 62 sub-ontology files organized by three structural elements: layers, partial models and modules. The topmost Meta Layer holds the most abstract and general knowledge. Fundamental modeling concepts and design guidelines are introduced on this layer. The Upper Layer specifies concepts of general systems theory to denote all types of systems, physical or abstract. The Conceptual Layer holds the core concepts for describing the Computer Aided Process

Engineering domain, while the Application-Oriented Layer extends the ontology towards desired applications. A module assembles a number of interrelated classes, relations, and axioms, which jointly conceptualize a particular topic. Modules that address closely related topics are grouped into a partial model.

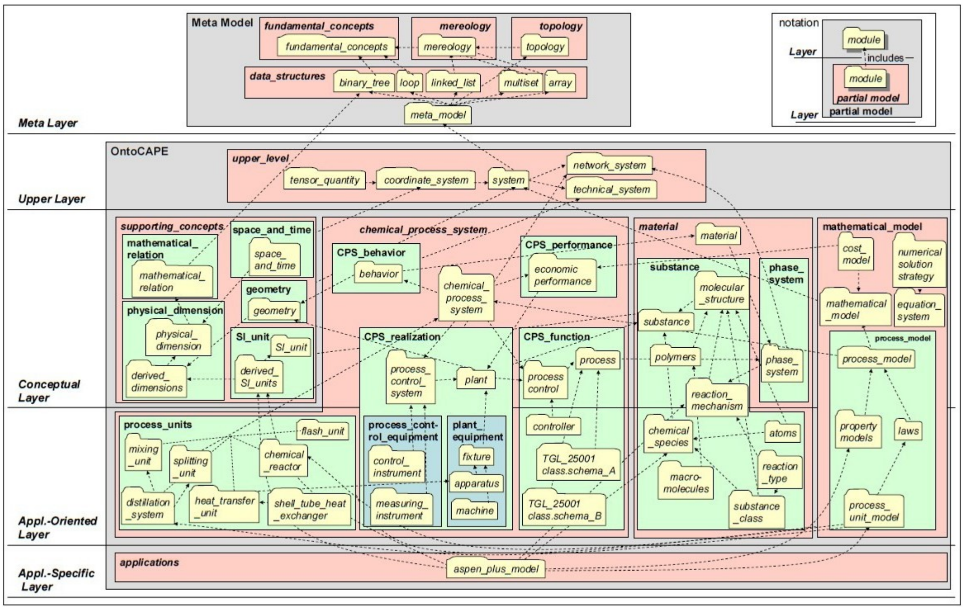


Figure 3: *Structure of OntoCAPE[28]. The ontology is organized by means of two structuring principles: abstraction layering and modularization*

A chemical process system is usually composed of a number of unit operations. Instead of describing the holistic system at once, OntoCAPE carves the composite system into subsystems and focus firstly on the description of subsystems and then the integration of subsystem information. As is shown in Fig. 4, a chemical process is described from two operation levels, unit operation level(subsystem) and chemical process level(composite system). For a better management of the system information, a single system is further decomposed into four aspect systems: function, realization, behavior and performance. Each account for a particular aspect of the system. The processing materials are modelled by partial model *material*, which is comprised of two further partial models, *substance* and *phase_system*. *substance* describes the intrinsic characteristics of a material which is context-independent, while *phase_system* represents the macroscopic thermodynamic behavior of a material. It is noted that properties that depend on the amount of a particular occurrence of matter are defined by partial model *CPS_behavior*. System related mathematical model is described by partial model *mathematical_model*.

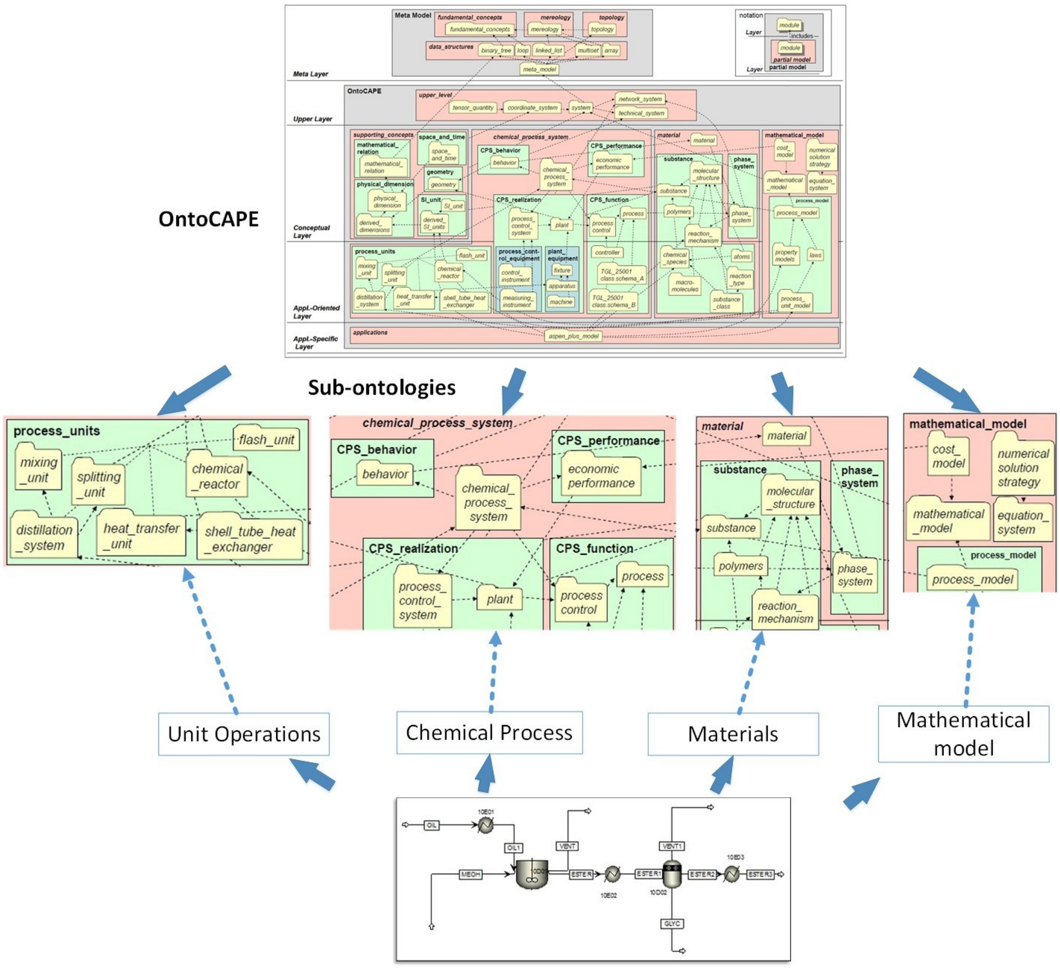


Figure 4: *Representing different aspects of a chemical process by utilizing the partial models provided by OntoCAPE.*

In this research, OntoCAPE is adopted as the base ontology due to the following reasons:

1. It has incorporated many aspects (process modelling, process simulation, process design, etc.) from engineering ontologies of related domains, and covers most of the processes for engineering activities during the life cycle.
2. It is well-organized by modules and layers. Its constituent ontologies can be reused for the development and/or extension of ontologies for other domains of interest, for example electrical engineering.
3. Among the reported ontologies for chemical process engineering domain, OntoCAPE is currently the most (re)usable ontology available to support software development. It has been field-tested in a number of software projects.

3 J-Park Simulator, a novel knowledge-based expert system for Jurong Island

Jurong Island is an artificial island with more than 100 industrial residents. It forms an important part of Singapore economy and is responsible for 30% of the total greenhouse gas emission [33, 41]. Realizing EIP on Jurong Island is beneficial to both Singapore economic growth and environmental conservation. The concept of Industry 4.0 is introduced to the system development of JPS. Industry 4.0 is the future industrial paradigm, which is also interpreted as the Industrial Internet of Things (IIoT), where a networked industrial components are formulated in the shape of Cyber-Physical Systems (CPS) [18]. In the context of Industry 4.0, the concerned physical entities in the real world will be reflected by virtual representations (avatars) in the corresponding cyber system. Moreover, the direct and indirect interdependency relationships among the physical entities will be described in the cyber system. Real time operation parameters can be autonomously communicated from the on-site producing unit to the cyber system through the implementation of sensors. Model Development Suite (MoDS), an advanced software tool [1] will be employed to build surrogate models [36] for the technical components. Smart sampling techniques [12] will be used to improve the surrogate models. The technical components in the cyber system will be equipped with advanced computing and information managing technologies, based on which, the system can perform self-evaluation, self-optimization as well as self-configuration. [13]. In this way, the resource and energy management of the EIP can be achieved effectively and efficiently. As a first step, a knowledge-based expert system, called J-Park Simulator is established by our research group.

The current architecture for JPS is given in Fig. 5, which consists of three basic parts.

1. A graphical user interface (GUI) (Fig. 6), which serves as operating platform for input and output information;
2. A knowledge base, where all the semantic description for the concerned entities as well as their interdependency relationships are stored. The construction of the knowledge base will be discussed in the following section;
3. A processing engine, which processes user input and derive solutions from it by extracting information from the knowledge base. MoDS (Model Development Suite)[1] and GAMS (General Algebraic Modeling System) [35], are embedded in the system to perform system simulation and optimization.

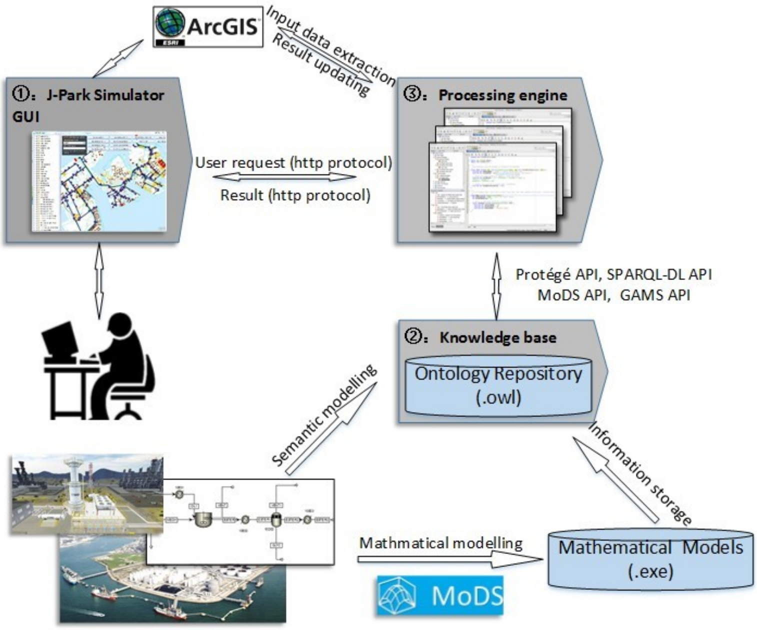


Figure 5: *Current architecture for J-Park Simulator.*

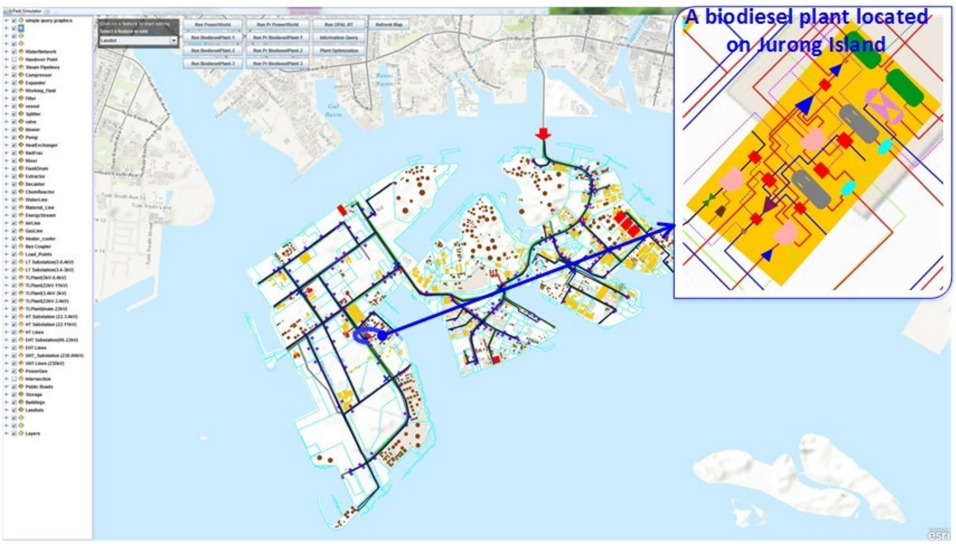


Figure 6: *Graphic user interface of J-Park Simulator, showing the map of Jurong Island and a biodiesel plant on Jurong Island.*

The system is implemented in Java programming language deployed in Eclips Integrated Development Environment. Apache TomCat is employed as the Java servlet container. The communication between the GUI and the processing engine is realized through HTTP protocol.

4 Constructing a knowledge base for a biodiesel plant on Jurong Island based on the enhanced OntoCAPE

In this section, OntoCAPE is employed to develop a knowledge base for a biodiesel producing plant on Jurong Island.

Figure 7 gives the detailed flow sheet of the biodiesel plant built in Aspen Plus. A feedstock of palm oil (OIL: 30 kmol/hr, 30 °C, 1 bar) is preheated (10E01) and mixed with a methanol stream (MEOH: 180 kmol/hr, 30 °C, 1 bar). The mixed stream is then fed to a Continuous Stirred-Tank Reactor (CSTR, 10D01), in which the palm oil and methanol are converted into biodiesel and glycerol in the presence of sodium hydroxide as the catalyst. The product stream (ESTER) is then heated and separated in the downstream heating (10E02) and flashing unit (10D02). The flashing unit separates the remaining methanol from the product stream, which is then sent to a distillation column (10D06). Excess methanol is added to assist in quick conversion. The unreacted methanol is recivered in the distillation column and sent back to a second reactor (10D03) for reuse. After that, the product stream is sent to a decanting unit (10D02D), where most of the byproduct glycerol (GLYC) is separated. The rest of the product stream which still contains unreacted palm oil is heated and sent to the second CSTR (10D03) for further biodiesel producing. Methanol, glycerol and water are separated from the product stream of the second CSTR in the following separating process (flashing: 10D04, Decanting: 10D03D, Extracting: 10D07). After that, the product stream is refined in a distillation column (10D08), from which a final product stream (FINALPRD) is produced. Water (RE-WATER: 233.15 kmol/hr, 30 °C, 1 bar) is pumped into a boiler (BOILER: 4 bar) to generate low pressure steam for the biodiesel producing process.

4.1 Applying advanced mathematical modelling methods to describe and optimize the biodiesel producing process

In this research, surrogate models are adopted to provide an accurate and fast-to-evaluate approximation of expensive mathematical models for the technical components in high dimensions. Experimental data, production data as well as data generated by commercial software packages can be used to construct surrogate models to describe the relation between input variables and response values of a system.

For the performance of the biodiesel producing process, six state variables are chosen as the independent variables. A number of objective values are considered, including molar flowrate (F), molar purity (y) and temperature (T) of the final product, Utility requirement of the unit operations. Table 1 shows the ranges of the six input variables. Second order polynomial (Eq. 1) is adopted as the modeling method, where $I = \{1, 2, 3, 4, 5, 6\}$, K = {"mole flowrate of biodiesel", "molar purity of biodiesel", "temperature of biodiesel", "heat duty of 10D01", "heat duty of 10D03", "heat duty of 10D02", "heat duty of 10D04", "heat duty of 10D06 - condenser", "heat duty of 10D06 - reboiler", "heat duty of 10E03", "heat duty of 10D03D", "heat duty of 10D02D", "heat duty of 10E05" }. Table 2 gives the detailed surrogate model for the biodiesel plant.

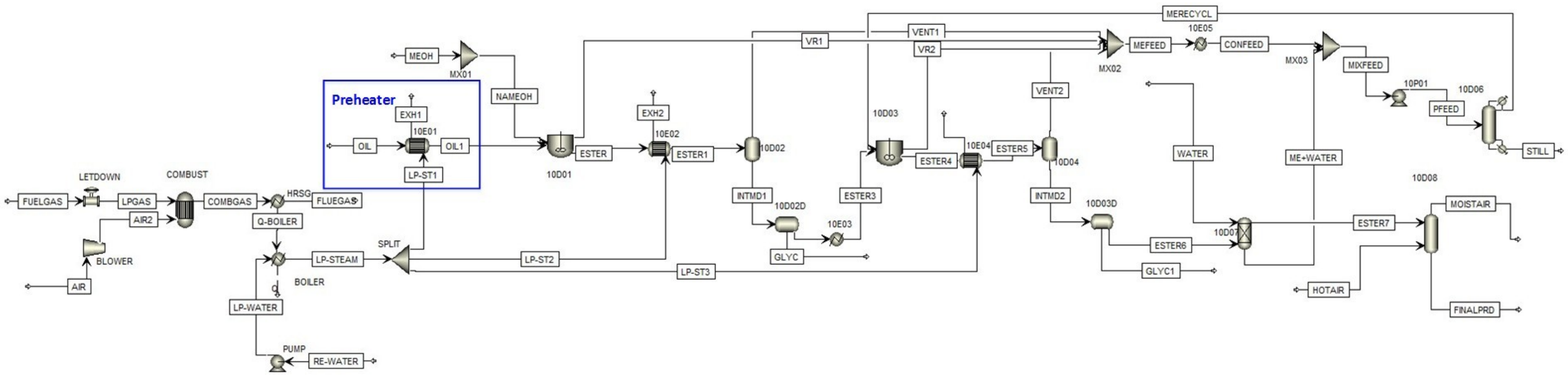


Figure 7: *Flowsheet of the biodiesel producing process built in Aspen Plus.*

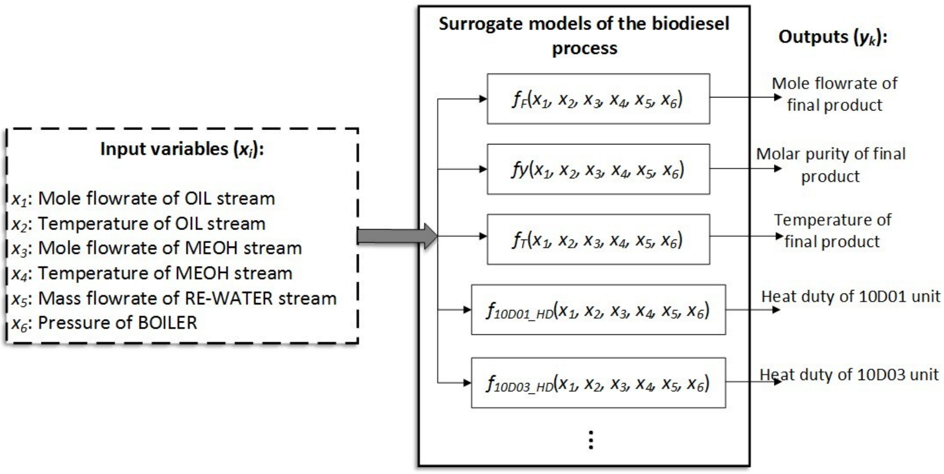


Figure 8: *Describing the biodiesel producing process as a black-box model with surrogate formulations.*

$$y_k \quad = \quad f^k(x_i) \qquad \forall \ i \in I, \ \ k \in K \tag{1}$$

Table 1: *Ranges of input parameters for surrogate modeling of the biodiesel plant.*

Parameters (x_i)	Lower bound (X_i^{lb})	Upper bound (X_i^{ub})	Current state
x_1 Mole flowrate of OIL stream (kmol/hr)	27	33	30
x_2 Temperature of OIL stream (°C)	27	33	30
x_3 Mole flowrate of MEOH stream (kmol/hr)	162	198	180
x_4 Temperature of MEOH stream (°C)	27	33	30
x_5 Mass flowrate of RE-WATER stream (kg/hr)	209.835	256.465	233.15
x_6: Pressure of BOILER (bar)	3.6	4.4	4

Note: X_i^{lb} – lower bound of x_i, X_i^{ub} – upper bound of x_i.

Table 2: *Detailed surrogate models of the biodiesel process.*

Coefficients	F	y	T	U 10D01	U 10D03	U 10D02	U 10D04	U 10D06_Reboiler	U 10D06_Condensor	U 10E03	U 10D03D	U 10D02D	U 10E05
C	86.6324	0.978	49.1	1.0795	0.3656	-0.0025	0.0043	4.838	4.657	0.562	0.6868	1.1808	1.224
A_1	7.8633	-0.0052	-0.7668	0.0857	0.065	-0.0013	-0.0248	-0.2150	-0.2287	0.0549	0.0729	0.1070	-0.1913
A_2	0.0139	0	-0.0014	0.0010	0.0001	0	0.0002	0.0849	-0.0142	0	0.0001	0.0002	-0.0003
A_3	0.6275	0.0038	-0.0134	0.0209	-0.0295	0.0031	0.0306	0.3307	0.324	0.0011	-0.0059	0.0106	0.246
A_4	0.0107	0	-0.0010	0.0137	0	-0.0001	0	-0.0689	0.0069	0	0.0001	0.0001	-0.0004
A_5	0.0184	0	-0.0018	0.0012	0.0001	-0.0031	-0.0299	-0.0504	0.0039	0.0001	0.0002	0.0003	-0.0002
A_6	-0.0049	0	0.0006	0	0	0	-0.0006	0.1424	0.0272	0	0	0	0.0003
$A_{1,1}$	-0.0892	-0.005	0.044	-0.005	0.0014	0.0005	0.0112	-0.1756	-0.0281	0.0002	0.0003	-0.0005	0.0038
$A_{1,2}$	-0.0361	0	0.0039	0.0016	-0.0002	0.0002	0.0002	0.0278	0.0124	-0.0002	-0.0003	-0.0005	0.0012
$A_{1,3}$	0.2003	0.001	-0.0017	0.0079	-0.0031	-0.003	-0.0303	0.0422	0.0476	0	-0.0006	0.002	-0.0055
$A_{1,4}$	-0.0002	0	0.0002	0.0001	0.0002	0.0005	-0.0002	-0.0168	-0.0014	0	0	0	0.0005
$A_{1,5}$	-0.0366	0	0.0038	0.0019	-0.0002	0.003	0.0293	0.0293	0.0376	-0.0003	-0.0003	-0.0005	0.0009
$A_{1,6}$	0.0363	0	-0.0036	0.0005	0.0002	0	0.0009	-0.015	-0.0383	0.0003	0.0003	0.0005	-0.0013
$A_{2,2}$	-0.0073	0	0.0007	-0.0011	0.0001	-0.0002	0.0001	0.1544	-0.0018	0	0	-0.0001	-0.0003
$A_{2,3}$	0.0177	0	-0.0019	0.0001	0.0002	-0.0002	0.0001	0.0481	0.0216	0.0001	0.0002	0.0002	-0.0012
$A_{2,4}$	-0.0008	0	0	-0.0001	0.0002	0.0002	0.0002	-0.2243	-0.0328	0	0	0	-0.0012
$A_{2,5}$	0.0238	0	-0.0024	-0.0018	0.0003	0.0001	0	-0.143	-0.0113	0.0002	0.0002	0.0003	-0.0007
$A_{2,6}$	-0.0201	0	0.0021	-0.0003	-0.0003	0	-0.0004	0.2809	-0.0083	-0.0001	-0.0002	-0.0003	0.001
$A_{3,3}$	-0.0948	0.0006	0.0021	-0.0041	0.0018	0.0055	0.0184	-0.1312	0.0255	-0.0002	0.0003	-0.0012	0.0018
$A_{3,4}$	0.0029	0	-0.0003	0.0015	0.0004	-0.0003	0.0002	-0.0133	0.0021	0	0	0	-0.0004
$A_{3,5}$	0.0222	0	-0.0021	0.0001	0.0003	-0.0078	-0.0391	0.062	0.0741	0.0002	0.0002	0.0003	-0.0008
$A_{3,6}$	-0.0022	0	0.0005	0	-0.0003	0	-0.0003	0.0245	-0.0046	0	0	0	0.0014
$A_{4,4}$	0.0049	0	-0.0004	0	0.0004	-0.0001	-0.0006	0.0166	-0.0212	0	0	0	0.0002
$A_{4,5}$	-0.0224	0	0.0021	-0.0003	-0.0001	0.0003	-0.0006	0.0932	-0.0142	-0.0001	-0.0002	-0.0003	-0.0004
$A_{4,6}$	-0.0255	0	0.0024	-0.0005	-0.0004	0.0001	-0.0001	-0.2303	-0.0051	-0.0002	-0.0002	-0.0003	0.0002
$A_{5,5}$	0.0042	0	-0.0004	-0.0015	0	0.0054	0.0176	-0.0635	-0.0132	0	0	0	0.0004
$A_{5,6}$	-0.0142	0	0.0015	-0.0003	-0.0002	0.0001	0.0009	-0.1595	0.0056	-0.0001	-0.0001	-0.0002	0.0008
$A_{6,6}$	-0.0126	0	0.0011	-0.0004	0.0002	0	0.0002	0.2615	-0.0204	0	0	-0.0002	-0.0005

Note: F – mole flowrate of final product, y – molar purity of final product, T – temperature of final product, U – Utility demand.

The surrogate model (Eq. 1) is used to formulate a mathematical programming model for the biodiesel process. The objective is to find the optimal process operating condition (x_i) in order to maximise the overall profit (*Obj*) of the plant, which equals to the product revenue minus the operational cost. For the operational cost, utility cost and raw material cost are considered at the present stage. The model can be easily extended to take other possible cost into consideration. The mathematical programming model is given as below:

$$\begin{aligned} \max \ \ Obj = P^{\mathrm{pd}} \times \sum\nolimits_{k'} y_{k'} - P^{\mathrm{u}} \times \sum\nolimits_{k''} y_{k''} - \sum\nolimits_{i} P_i^{\mathrm{rm}} \times x_i \\ \forall \ \ i \in I^{'}, k^{'} \in K^{'}, k^{''} \in K^{''} \end{aligned} \tag{2}$$

$$\begin{aligned} s.t. \quad & Eq.(1) \\ & X_i^{\mathrm{lb}} \leq \quad x_i \leq X_i^{\mathrm{ub}} \qquad \forall \ \ i \in I \end{aligned} \tag{3}$$

where P^{pd} denotes the price of product, P^{u} represents the utility price, and P^{rm} denotes the price of raw materials, $I^{'}$ = $\{1, 3\}$, $K^{'}$ = {"mole flowrate of biodiesel"}, $K^{''}$ = {"heat duty of 10D01", "heat duty of 10D03", "heat duty of 10D06 - condenser", "heat duty of 10D06 - reboiler", "heat duty of 10D04", "heat duty of 10D02", "heat duty of 10E03", "heat duty of 10D03D", "heat duty of 10D02D", "heat duty of 10E05" }.

4.2 Applying ontology technology to describe the biodiesel producing process

4.2.1 Modeling the unit operations

The biodiesel producing process is composed of 24 unit operations. Each can be modeled individually as a subsystem. Fig. 9 illustrates the model of the preheater 10E01. On this modeling level, detailed information including the operating status, process flowsheet, and equipment design parameters are covered. As is shown, 10E01 is constructed to heat raw material flow (OIL) by utlizing utility stream LP-ST1. The current mass flowrate of the raw material stream is 24220 kg/hr, while the current heat duty of 10E01 is 510.7 kW. The raw material stream refers to material OIL, whose intrinsic characteristics (C51H98O6) as well as thermodynamic behavior (1 bar, 30 °C) are specified.

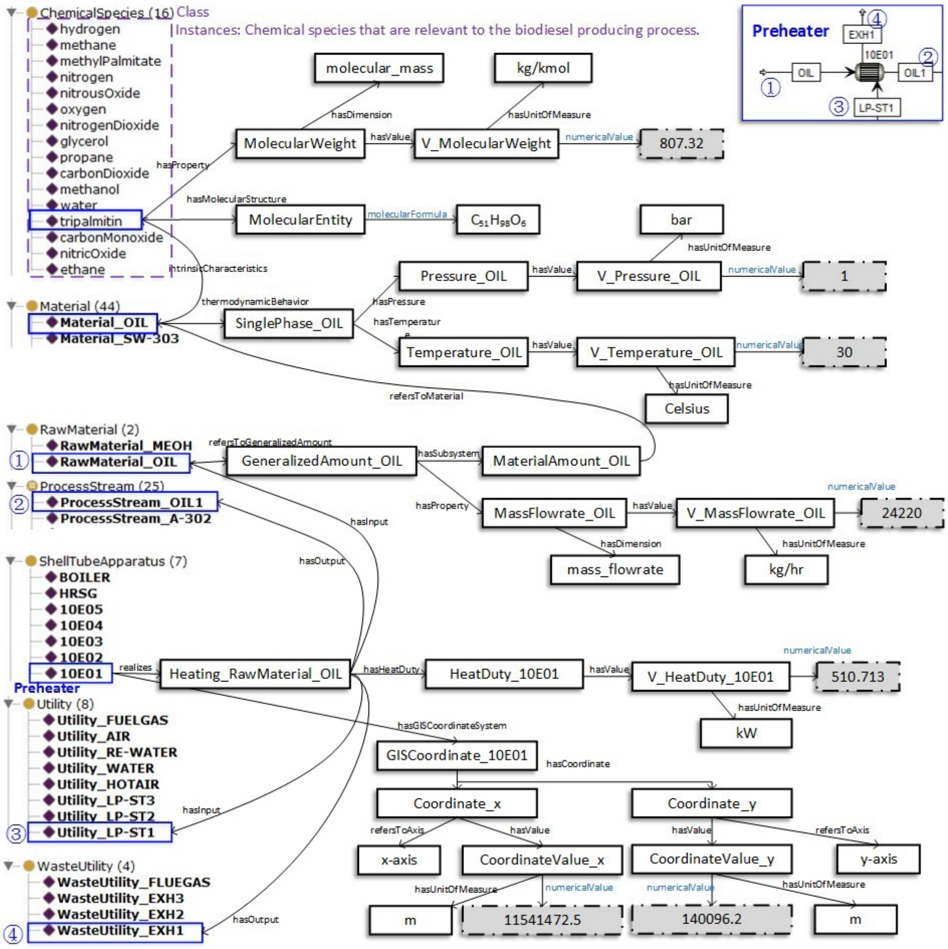


Figure 9: *Describing the preheater in the biodiesel producing plant by employing the ontology structure provided by OntoCAPE.*

4.2.2 Modeling the biodiesel plant as a composite system

Modelling of the chemical process is more straightforward, which is shown in Fig. 10. As the detailed operation and designing information are already reflected in the model of its subsystems, it is omitted on this modeling level. Yet, it can be easily obtained via the relationship between the composite system and its subsystems. The corresponding code generated by Protégé is shown in Fig. 11. It is proposed to associate each technical component with its own executable mathematical models (surrogate model and/or mathematical programming model) together with their solving strategies, so that the mathematical models can be readily evaluated by the software packages integrated in the system.

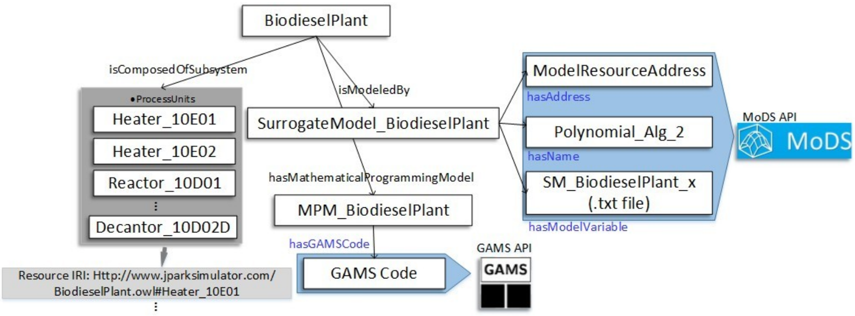


Figure 10: *Modeling the biodiesel plant as a composite system by utilizing the enhanced ontology structure.*

```
<!-- http://www.jparksimulator.com/BiodieselPlant.owl#BiodieselPlant --> ①

<owl:NamedIndividual rdf:about="http://www.jparksimulator.com/BiodieselPlant.owl#BiodieselPlant">
    <rdf:type rdf:resource="file:/C:/OntoCAPE/OntoCAPE/upper_level/system.owl#CompositeSystem"/>   ②
    <system:isModeledBy rdf:resource="http://www.jparksimulator.com/BiodieselPlant.owl#SurrogateModel_BiodieselPlant"/>
    <hasMathematicalProgrammingModel rdf:resource="http://www.jparksimulator.com/BiodieselPlant.owl#MPM_BiodieselPlant"/>
    <system:isComposedOfSubsystem rdf:resource="http://www.jparksimulator.com/BiodieselPlant.owl#Decantor_10D02D"/>   ③
    <system:isComposedOfSubsystem rdf:resource="http://www.jparksimulator.com/BiodieselPlant.owl#Flash_10D02"/>
    <system:isComposedOfSubsystem rdf:resource="http://www.jparksimulator.com/BiodieselPlant.owl#Heater_10E01"/>
    <system:isComposedOfSubsystem rdf:resource="http://www.jparksimulator.com/BiodieselPlant.owl#Heater_10E02"/>
    <system:isComposedOfSubsystem rdf:resource="http://www.jparksimulator.com/BiodieselPlant.owl#Reactor_10D01"/>   ④
                            ⋮

<!-- http://www.jparksimulator.com/BiodieselPlant.owl#SurrogateModel_BiodieselPlant -->

<owl:NamedIndividual rdf:about="http://www.jparksimulator.com/BiodieselPlant.owl#SurrogateModel_BiodieselPlant">
    <rdf:type rdf:resource="file:/C:/OntoCAPE/OntoCAPE/model/mathematical_model.owl#SurrogateModel"/>
    <p5:hasAddress>C:\apache-tomcat-8.0.24\webapps\ROOT\BiodieselPlantSim</p5:hasAddress>⑤
    <p5:hasName>Polynomial_Alg_2</p5:hasName> ⑥
</owl:NamedIndividual>

<!-- http://www.jparksimulator.com/BiodieselPlant.owl#MPM_BiodieselPlant -->

<owl:NamedIndividual rdf:about="http://www.jparksimulator.com/BiodieselPlant.owl#MPM_BiodieselPlant">
    <rdf:type rdf:resource="file:/C:/OntoCAPE/OntoCAPE/model/mathematical_model.owl#MathematicalProgrammingModel"/>
    <mathematical_model_extended:hasGAMSCode>*this project is built for the optmization of the biodiesel plant in J-Park Simulator
*author Li ZHOU 23/08/2016
Set
   i        set of independent variables  /1,2,3,4,5,6/                ⑦
   j        set of user defined parameters /Biodiesel, PalmOil, Methanol, Utility/
   k        full set of dependent variables
   /FinalProduct_Flow_Total_Mole,FinalProduct_Purity_Molar_Mole,FinalProduct_Temp,10D01_Heat_Duty,10D03_Heat_Duty,10D06_Condenser_Heat_
   ty,10D04_Heat_Duty,10D02_Heat_Duty,10E03_Heat_Duty,10D03D_Heat_Duty,10D02D_Heat_Duty,10E05_Heat_Duty/
   sk(k)    subset for unit operations that consum utility
   /10D01_Heat_Duty,10D03_Heat_Duty,10D06_Condenser_Heat_Duty,10D06_Reboiler_Heat_Duty,10D04_Heat_Duty,10D02_Heat_Duty,10E03_Heat_Duty
   t_Duty,10E05_Heat_Duty/
   b        index for variable bounds        /lo,up,initial/

alias (i, is);

parameter
   price(j)   user defined price

$if not set gdxincname $abort &apos;no include file name for data file provided&apos;
$gdxin %gdxincname%
$load price
$gdxin
display price;
                            ⋮
```

Figure 11: *Biodiesel plant's ontological representation in the OWL format. ①-IRI for the information resource of the biodiesel plant, through which the IRI for its surrogate model (②), mathematical programming model (③) as well as the unit operations (④) can be obtained. Further information about the surrogate model (⑤ and ⑥) as well as mathematical programming model (⑦) can be reached.*

5 Utilizing the constructed knowledge base to support J-Park Simulator in information query, process simulation and process optimization

In this section, the established knowledge base of the biodiesel producing process is tested under the framework of JPS.

5.1 Process information query

Logical rules provided by an ontology can be used to infer the information stored on the knowledge base through a wide range of query languages. A query architecture is developed and deployed, which is presented in Fig. 12. A query interface is built to enable users to pose queries and display their results. The query handler is used to: 1) extract keywords from user requests and convert it to SPARQL-DL query; 2) receive query results, reassemble the information pieces and return it to the query interface. The query handler and the query interface are implemented in Java programming language. A snapshot of the query interface is shown in Fig. 13.

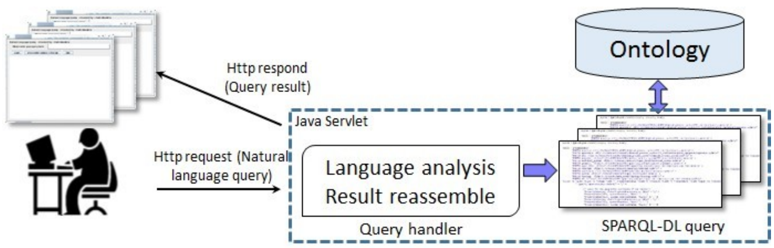


Figure 12: *Current architecture for the ontology-based information query service of JPS.*

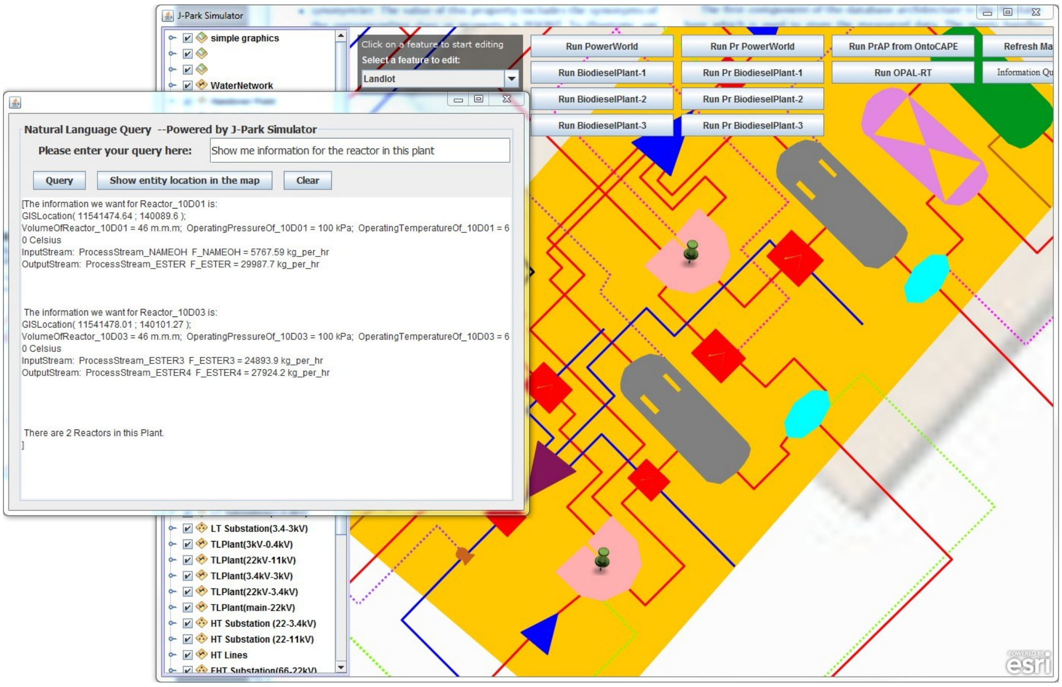


Figure 13: *User interface of the ontology-based information query service of JPS showing the query result for reactor.*

5.2 Process simulation

In this section, the information of the executable surrogate model is extracted to perform process evaluation. Figure 14 shows snapshot of performing process simulation for the biodiesel plant on JPS, where the feeding flowrate of palm oil was increased from 30 to 33 kmol/hr. After simulation, the biodiesel producing rate increased from 86.6 to 94.3 kmol/hr.

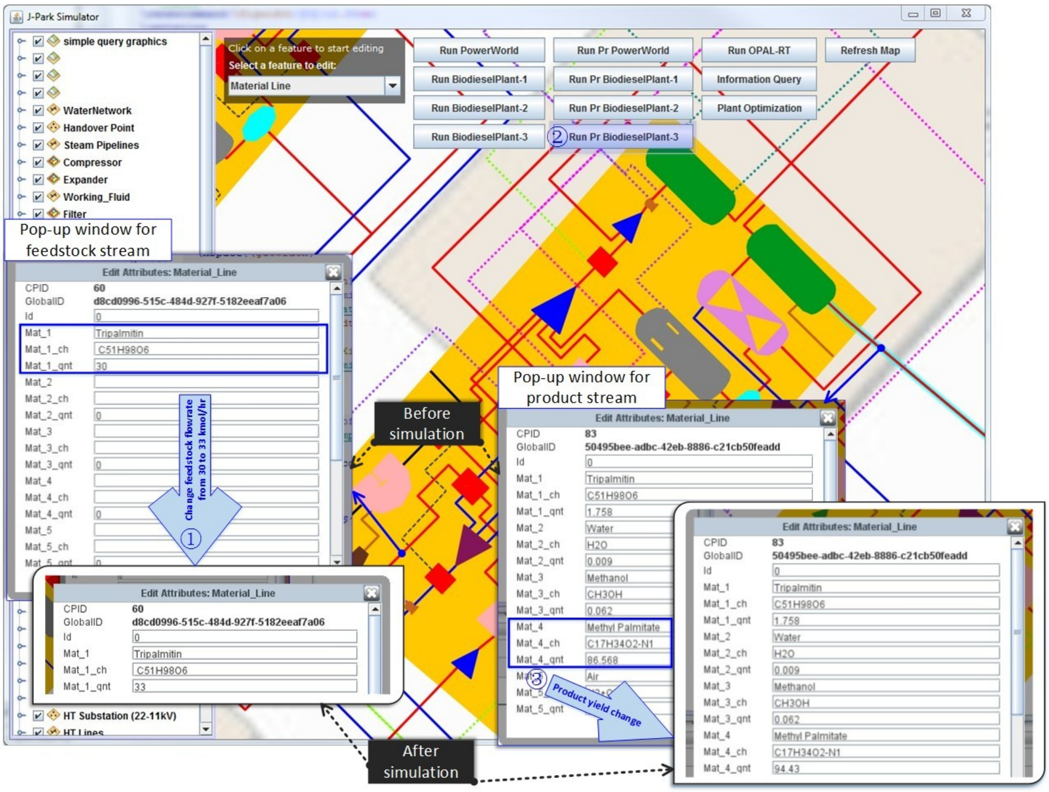
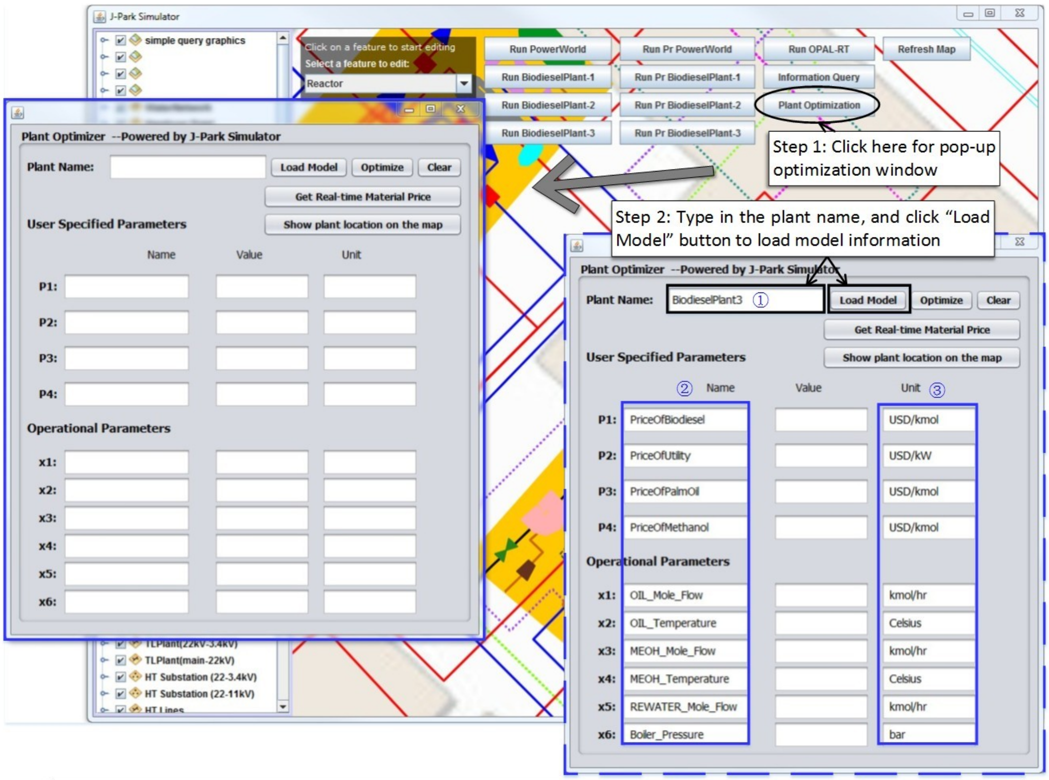


Figure 14: *Snapshots of the ontology-based process simulation service of J-Park Simulator, showing the steps and results for process simulation of the biodiesel plant.*

5.3 Process optimization

The information of the mathematical programming model stored on the knowledge base can be extracted and utilized for process optimization. An optimization interface is developed, which is shown in Fig. 15.



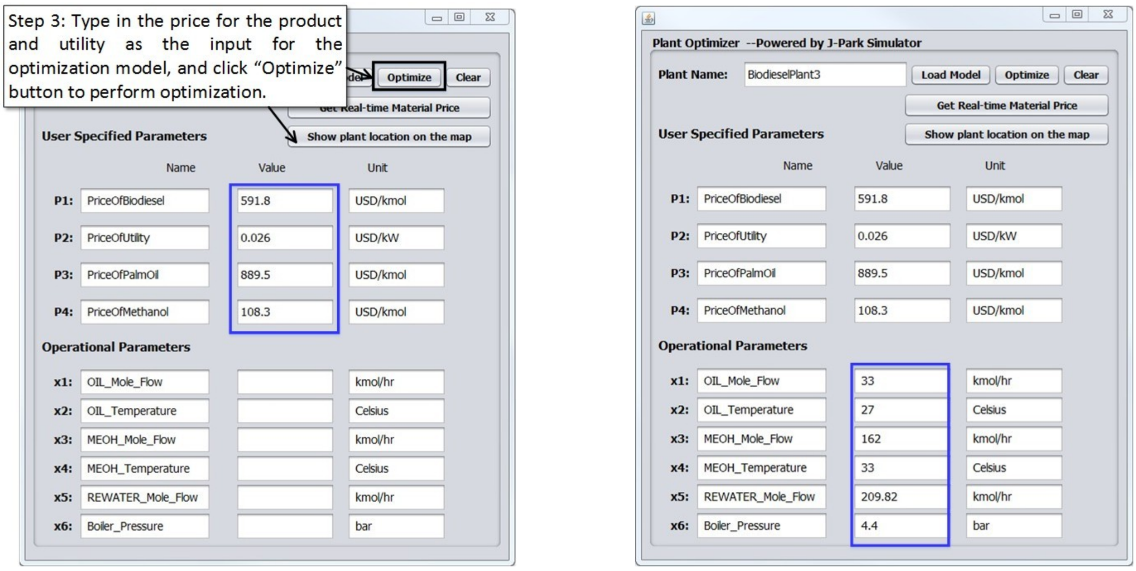
Java code for loading the model information:

```
                                  ①: Locate the process information resource via the plant name.
String uri = "File:/C:/apache-tomcat-8.0.24/webapps/OntologyFiles/"+ PlantName + ".owl";
OWLModel owlModel = ProtegeOWL.createJenaOWLModelFromURI(uri);

/**associating the Parameters to a JAVA OWLIndividual variable*/
OWLIndividual P = owlModel.getOWLIndividual("http://www.jparksimulator.com/"+ PlantName + "#ModelParameter_P");
String[] PName = P.getPropertyValue(owlModel.getOWLProperty("system:hasName")).toString().split("#");
ModelInformation.add(PName[1].split(" ")[0]);② Extract the names of the model parameters.
String[] Punit = P.getPropertyValue(owlModel.getOWLProperty("system:hasUnitOfMeasure")).toString().split("#");
ModelInformation.add(Punit[1].split(" ")[0]);  ③ Extract the units of the model parameters.
                                  ⋮
```

Figure 15: *User interface of the ontology-based process optimization service of JPS, showing actions required to load the mathematical programming model for the biodiesel plant and the relevant Java codes.*

A user is required to provide input parameters including real time price of the product (biodiesel), utility and raw material (palm oil and methanol). The optimization command will trigger the establishment of a GAMS job in the back end by extracting the stored GAMS code from the knowledge base. The optimization result obtained by the GAMS job is then sent back to the optimization interface (Fig. 16). Table 3 gives the comparison between the obtained optimal operational condition and the base case, where the product flowrate increased 8%, while the total energy requirement decreased 8.5%.



(a) *Specify values for model parameters.* **(b)** *Process optimization result.*

Figure 16: *User interface of the ontology-based process optimization service of JPS, showing actions required to perform process optimization for the biodiesel plant after model loading (a) and the optimization result (b).*

Table 3: *Comparison between the optimal operational condition and the base case.*

Cases	x_1	x_2	x_3	x_4	x_5	x_6	F	Total energy requirement (kW)
Base case	30	30	180	30	233.15	4	86.63	14595.5
Optimized case[a]	33	27	162	33	209.8	4.4	93.65	13355.2

[a] *The price information is collected from: http://www.icis.com/chemicals/channel-info-chemicals-a-z/*

In the future, this process will be automated. The acquisition of real time commodity price will be automatically extracted from the market website. The optimization job will be automatically formulated and solved as soon as the commodity prices change. The optimized operating parameters can be utilized to guide the real-site producing via a control system.

6 A bottom-up hierarchical framework for resource management in EIPs

In the previous section, a biodiesel plant is implemented as a proof of methodology to show how the semantic knowledge as well as the mathematical models of a single technical system can be utilized. The other technical components in the concerned system can be implemented in a similar way to construct the expert system for the energy and material management. As is shown in Fig. 17, the technical entities can be organized into a four-level modelling framework (unit level, process level, plant level and industrial network level) [34]. Information of different type (semantic information, surrogate model, mathematical programming model, etc.) for the individual components will be collected and structured by ontology technique, resulting in an ontology repository for the industrial park. The ontology repository then serves as knowledge base to facilitate the process of system evaluation, optimization, network design, and more. Furthermore, the ontology repository is designed to be constructed in such a manner that the interdependencies among entities are clearly specified, facilitating the (potentially) correlated entities to ”communicate” with each other. For example, the designing and configuration of a resource network (a node on the industrial network level, which can be a water network, an energy network or a material network) relies heavily on the information from the potential participants (nodes from the adjacent plant level, which represents the chemical plants that are likely to join the network and exchange resources with the community). The evaluation of each node is handled by an agent, which can access the knowledge base of the node itself (read and write access) as well as the correlated nodes (read access only). The knowledge base not only provide information for node service (query, simulation, optimization), but also serves as an exchange platform to support bottom-up information passing. In such a way, information can be exchanged among organizations, and the overall energy management can be better achieved.

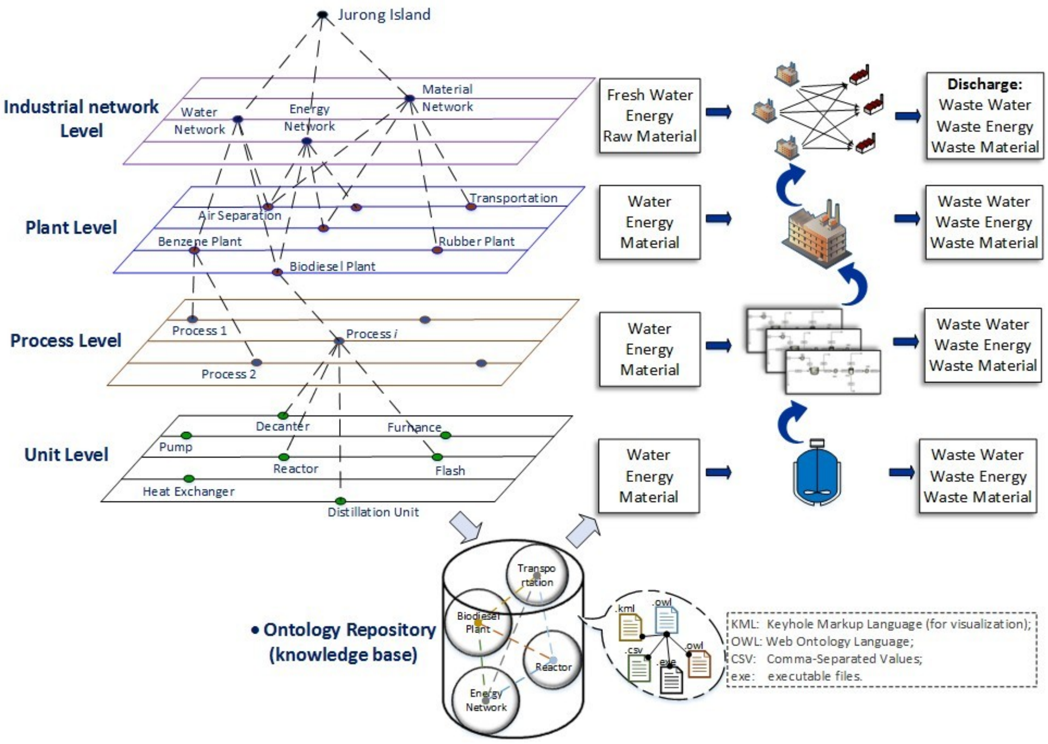


Figure 17: *Bottom-up hierarchical framework for resource management in EIPs.*

7 Conclusion and future work

In order to realize EIP on Jurong Island, an expert system called JPS is designed. OntoCAPE is enhanced and applied to a biodiesel plant on Jurong Island, as a first step towards semantically modelling the overall industrial park. The biodiesel producing process is modeled on two different operation levels, unit operation level and process level. Semantic information as well as executable mathematical models are associated to the corresponding technical system. The established ontology model is then used to support JPS in several applications. 1) Information query: process information of the biodiesel plant can be extracted through natural language query via JPS. 2) Process simulation: JPS can evaluate the process performance after certain operation parameters change. 3) Process optimization: JPS can be used to determine the optimal operation condition for the biodiesel plant in order to reduce the energy consumption and achieve maximal plant profit under different market scenarios.

Plant-wide system information managing, simulation and optimization are the starting steps to establish the expert system for the industrial park. The long term goal is to model every technical component in the system, capture the interdependent as well as the symbiotic relationship among the entities and to realize the resource and energy management of the industrial park. To that end, future work will include:

1. Establish an ontology to describe the symbiotic relationship between chemical plants. OntoCAPE only covers conceptualization of the intra-plant producing activities. In order to fully model an EIP, resource network design and management need to be considered.

2. Extend OntoCAPE to model the activities of other domain, for example, electric power system, transportation system, etc. Define the cross-domain interdependency relationships.

3. Integrate sensor model to the current semantic model and extend the current ontology to store observation data for real-site production, such as pressure and temperature to the knowledge base. The data can then be used for process supervision, process analysis, mathematical model developing and adjusting.

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