

J-Park Simulator: Roadmap to Smart Eco-Industrial Parks

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released: 26 Oct 2016

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Preprint No. 174



Keywords: Industry 4.0, Eco-Industrial Park, OntoCAPE, cross-domain ontology, surrogate model, Semantic Web, Internet of Things

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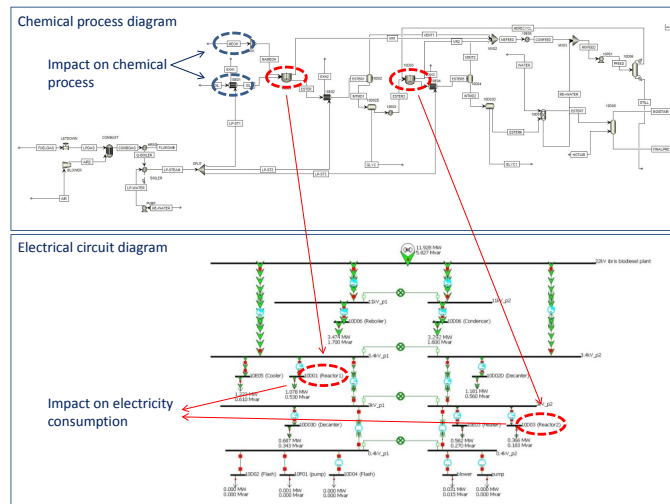


Highlights

- The J-Park Simulator is presented as a virtualisation of an Eco-Industrial Park
- Semantic Web inspired machine-to-machine communication is implemented
- Surrogate modelling is employed to conduct real time simulations
- A cross-domain ontology is applied to carry out cross-domain simulations
- A cross-domain ontology is used to answer semantic queries

Abstract

This paper presents the J-Park Simulator (JPS), a virtualisation of an Eco-Industrial Park (EIP). The JPS combines concepts of machine-to-machine (M2M) communication inspired by the Semantic Web and Industry 4.0, and advanced mathematical modelling to create a modelling platform for designing, computer-aided process engineering (CAPE) and managing an EIP. The overall aim is to reduce carbon footprint and maximise resource efficiency by taking advantage of symbiotic inter-company exchanges of material and energy. The paper outlines system architecture, supporting infrastructure, and its components such as database, data processing, data editing and visualisation, and system modelling tools. A cross-domain ontology is used to represent the wealth and complexity of data at multiple levels and across domains united in a shared data and information hub that provides real-time situational awareness of industrial processes. Networks of fast-to-evaluate surrogate models are employed to conduct real time simulations that quantify CO₂ emission reduction using, for example, waste heat recovery (WHR), and carry out cross-domain simulations both at steady-state and in transient operation. The cross-domain ontology is furthermore used to answer semantic queries. The approach and some of the benefits of this platform are demonstrated in several case studies. We find that there is significant scope to realise as yet unexploited potential for energy savings.



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1 Introduction

The Semantic Web refers to knowledge representation in machine-readable formats to better enable computers and people to work in cooperation. Industry 4.0 extends this concept to machine-to-machine (M2M) communication in industrial processes.

EIPs as clusters of industrial processes have been widely studied over the past decades by both academic groups and the private sector as converting an industrial park to an EIP is associated with potential savings derived from conserved finite resources, reduced production costs, improved productivity and competitiveness, and enhanced environmental performance. There were possibly more than 20,000 industrial parks in operation around the world in 2011 [28] that provide the potential for savings of material, energy, and waste.

Several definitions of an EIP have been reported in the literature. A widely cited study by Chertow [7] defined it as an industrial park in which businesses cooperate with each other and the local community to reduce waste and pollution, efficiently share resources and minimise environmental impact to increase business success. Recently Kastner et al. [17] reviewed the literature on EIP in which metrics and quantitative tools were developed to identify and compare EIP designs and activities.

The most studied example of an EIP exists in Kalundborg, Denmark, see Figure 1. Established in 1959, it set up its first exchange of material in 1972. The EIP is centred around Asnæs Power Station, a 1500 MW coal-fired power plant, and linked to the local community and several other companies.

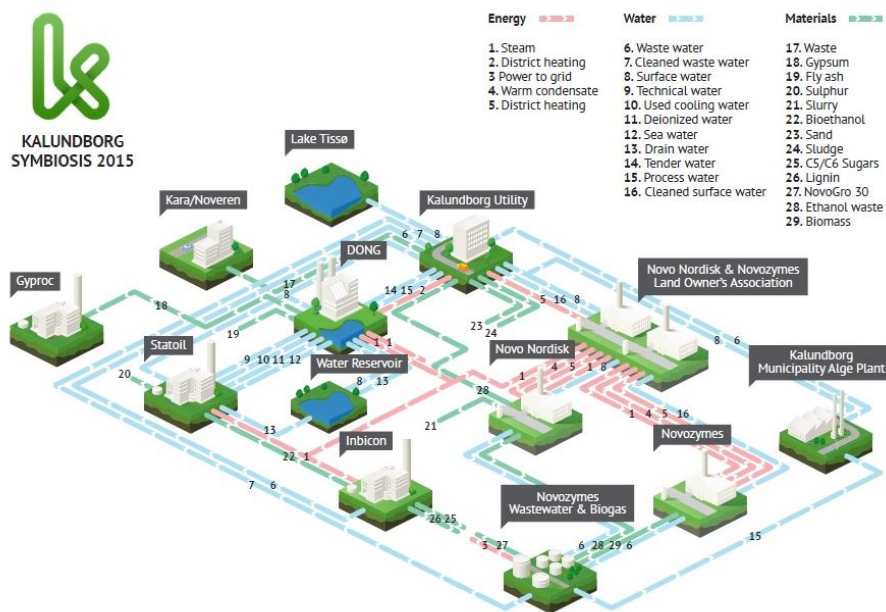


Figure 1: Industrial symbiosis based on exchange of materials, energy, and information at Kalundborg, Denmark, one of the first realisations of an EIP. Source: [16].

While academic studies of EIPs commonly involved the analysis of material, energy, and waste, most of these studies were limited to only one of these aspects without considering

an integrated approach. Far less attention has been placed on the analysis of multiple aspects or coupled networks. The development is held up by the absence of a cross-domain ontology to facilitate machine-enabled communication and interoperability across networks.

The purpose of this paper is to fill this gap by introducing the JPS [5]. Industrial processes of an EIP are modelled combining a cross-domain ontology with the concepts of the Semantic Web, Industry 4.0, and advanced mathematical modelling. Case studies demonstrate the feasibility of M2M communication for enhanced industrial control.

2 Jurong Island EIP

The JPS was inspired by the study of an EIP on Jurong Island, a man-made island amalgamated from seven small islands in the southwest of Singapore. With a total land area of 32 square kilometers it is home to over 100 companies and invested assets of some SGD 50 billion. The companies, that include BASF, BP, Celanese, Chevron Oronite, CIBA, DuPont, Evonik, ExxonMobil, Huntsman, Lanxess, Linde, Lucite, Mitsui Chemicals, Shell, Singapore Petroleum Company, and Sumitomo Chemical form a large chemical cluster covering the oil and gas, petrochemicals, specialty chemicals and pharmaceutical sectors. With 1.3 million barrels of crude oil being processed per day, it is one of the top 10 petrochemical hubs in the world.

It is supported by a shared infrastructure that includes several power stations, several water supply networks, a cooling water network, fire stations, a medical clinic, an extensive road network, numerous tanker jetties, and storage tanks including rock caverns with storage capacity for liquid hydrocarbons of 1.47 million cubic meters at 130 meters below sea level. Singapore's chemicals industry accounted for around 42% of manufacturing output in 2011 [6]. Singapore's chemicals and petroleum refining industries accounted for 33% and 29% of carbon dioxide emissions respectively in 2010 [25].

3 Concepts and Tools

The concepts of the Semantic Web, Industry 4.0, and mathematical modelling using surrogate models are described in this section.

3.1 Semantic Web, Cross-Domain Ontology

The Semantic Web as described by Berners-Lee [4] refers to the concept, challenges and requirements of knowledge representation in machine readable formats to better enable computers and people to work in cooperation. The Semantic Web provides a framework of common standards developed and defined by the World Wide Web consortium (W3C), an international community dedicated to ensuring the long-term growth of the Web.

Knowledge representation applies theories and techniques from three fields: logic, provid-

ing the formal structure and rules of inference; ontology, defining the kinds of things that exist and their relationships; and computation, supporting the applications that distinguish knowledge representation from pure philosophy, see Sowa [30].

A variety of logics systems have been proposed. First-order-logic (FOL) is currently the most widely used. Other systems vary from FOL as regards syntax, subsets, proof theory, model theory, ontology, and metalanguage.

The role of ontologies in supporting knowledge sharing activities gained momentum with the widespread installation of a cyber infrastructure capable of communication between billions of stationary or mobile devices that collectively form the IoT. They include wired or wireless sensors, radio frequency identification (RFID) tags, input-output devices with interactive functions such as displaying, editing, and analysing information, or as control devices sending instructions or commands to sensors or control devices such as pumps, valves, circuit breakers or power supply switches.

Classifications of ontologies and ontology design approaches are found, for example, in Gómez-Pérez [13]. Various ontology modelling techniques have been proposed including those using frames in Minsky [23]. Muñoz [24] described an ontological infrastructure for chemical batch process management; Ge [12] a petroleum related ontology; Yang [34] a multi-agent system to facilitate component-based process modelling and design. For operational process modelling see Hai [15].

The multidisciplinary shared knowledge base DBpedia is described in Mendes [22]. Meanwhile, the focus in academia has remained on single application domain ontologies. Less attention has been paid to the development of multi-domain ontologies to describe the complexity of models at the intersection of multidisciplinary projects involving a diversity of private and public stakeholders from industry, infrastructure, residential communities, environmental protection agents and urban design.

Turning logic and ontology into executable action requires computable models. Several computer languages have been recommended by the W3C as suitable for the Semantic Web. They vary in their implementation of FOL. The most recent version of the Web Ontology Language (OWL 2) has been adopted as a standard. It is based on Description Logic (DL), a subset of FOL. Its primary exchange syntax is RDF/XML [32].

3.2 Industry 4.0

The term “Industry 4.0” refers to the 4th Industrial Revolution characterised by the ability of industrial components to communicate with each other. It extends the concept of the Semantic Web to include machine-to-machines (M2M communication) in real time in industrial processes. For processes that combine hardware, software and communication infrastructure in such innovative ways the terms smart factories or cyber physical systems (CPS) have also been coined. A CPS monitors physical processes, creates virtual copies of the physical world, and makes decentralised decisions. Embedded computers and networks monitor and control the physical processes, usually with feedback loops where physical processes affect computations and vice versa. Drath [10] describes a CPS using the engineering data format AutomationML and how virtualization, decentralization and network building changes the manufacturing landscape. Industry 4.0 builds on

technological development that is often referred to as the “Internet of Things” (IoT). IoT is characterised by the pervasive presence of a variety of things or objects around us which through unique addressing schemes, are able to interact with each other and cooperated with their neighbours to reach common goals. Atzori [2] suggested that the IoT could be realised using three paradigms: semantic-oriented (knowledge), things-oriented (sensors), and internet-oriented (middleware).

3.3 Advanced mathematical modelling using surrogate models

Mathematical modelling and model development is a fundamental activity in the field of engineering. Gorissen [14] gives a brief literature review. For an outlook on the future of computational modelling in process engineering, see Kraft [18].

A surrogate model (or metamodel) is an approximation of experimental and/or simulation data designed to provide answers when it is too expensive to directly measure the outcome of interest. Two key requirements thereof are reasonable accuracy and significantly faster evaluation than the original method. Surrogate models are used to explore design space of a simulation or an experiment; calibrate predictive codes of limited accuracy and bridging models of varying fidelity; account for noise or missing data; and to gain insights into the nature of the input-output relationship (data mining, sensitivity analysis and parameter estimation).

Producing a surrogate model involves choosing a sampling plan (an experimental design), choosing a type of model and fitting the model to the gathered data. Numerous sampling and fitting techniques are available, see Crary [9].

Developing a virtual system primarily based on surrogate models significantly reduces required computation time and storage space and allows for dynamic modelling and studies otherwise impossible to conduct.

4 JPS Structure and Components

The JPS is a Java-based tool with a graphical user interface (GUI) that serves as information hub and interactive simulation platform for designing, CAPE and managing an EIP. The GUI is available for download as Java applet from the JPS Webpage [5].

The JPS builds on a cross-domain ontology based on the upper level and chemical engineering domain ontology OntoCAPE [20] and extended to include an electrical engineering domain ontology derived from Küçük [19].

The JPS has a modular structure consisting of data storage, data processing, and data editing/visualisation as its three key components. The components are connected with each other and exchange data via the Internet. With this structure the JPS is able to process data from multiple sources, at multiple process levels, and in multiple data formats and provide universal access to the data.

For data storage and retrieval the cloud-based mapping and data storage platforms ArcGIS for Server and ArcGIS Online [11] are used. The Java applet allows visualisation and

editing of a wide range of data. Any changes made during an editing session are saved by the Java applet by connecting to the ArcGIS database servers in real time. The ArcGIS servers process any data record updates in both batch and interactive mode.

Data processing is carried out in real time based on a client-server configuration using Web services. The Java applet client connects to a Java servlet that is hosted by the JPS server running Apache Tomcat Web and application services. The JPS server also hosts third party applications such as chemical engineering simulation software package AspenPlus (AP), and electrical engineering simulation software package PowerWorld (PW). Other software applications can be added.

The JPS contains multiple models representing multiple layers including water, electricity, steam networks, and CO₂ emissions island-wide. Currently there are 76 different types of layers populating the 4 hierarchical levels: equipment unit level; process level; plant level; and industrial network level, see Figure 2.

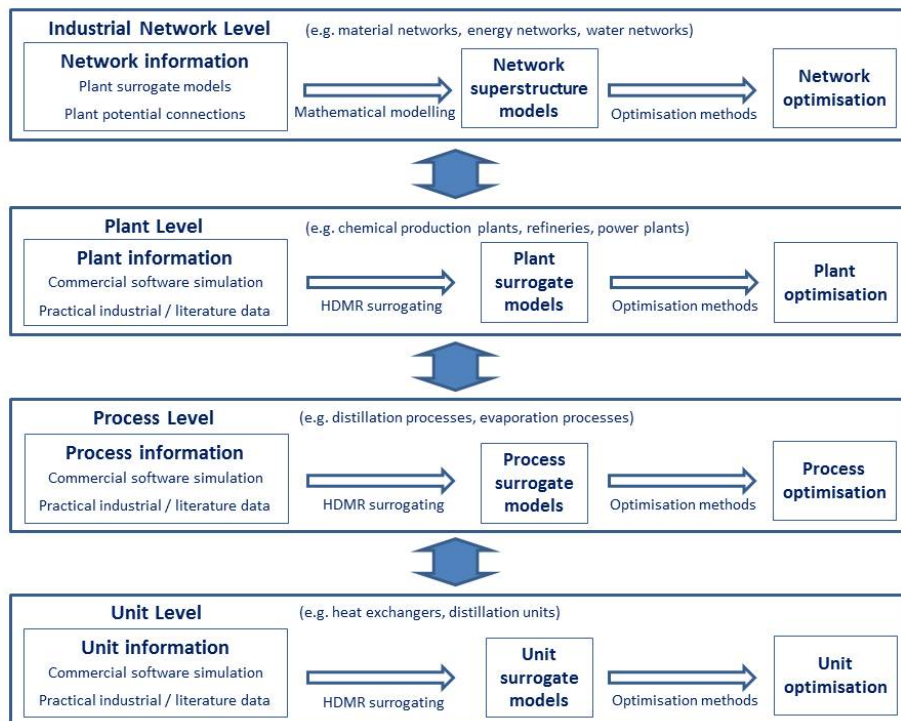


Figure 2: The JPS consists of networks of surrogate models each representing an equipment unit, process, plant, or industrial park superstructure. The networks are interconnected through multiple hierarchical levels. The graph is reproduced from Pan [26], with permission.

In the multiple layers the JPS contains representations of basic geographical features, infrastructure assets and mobile assets, residential and industrial activities, and civil, chemical, mechanical, and electrical engineering related processes. For each of these layers it holds master data and collects, processes, and makes available variable data originating from multiple machine and human sources.

This structure combines characteristics of a flat network of models within one level with a

hierarchical structure of models at multiple levels. Each model consists of one or several layers that are represented by one or several instances, and by their relationships with other layers, both within the same level as well as between levels.

The layer types can be summarised into a few broad categories: collecting data such as sensors; relaying material, energy, or data, such as roads, power lines, gas lines, water lines; processing material, energy, or data, such as chemical processing equipment such as pumps, mixers, reactors, separators, heat exchangers; controlling equipment that makes decisions, and/or sends instructions or commands to other instances.

High-dimensional models representing a multitude of layers and corresponding variables and parameters can be consolidated into superstructures at a higher level with a reduced set of layers, variables and parameters.

The JPS covers the domains of *civil engineering* including infrastructure such as public roads, bridges, tunnels, jetties, and water supply networks above and under ground; *geospatial engineering* where object data include GPS coordinates, digital aerial imagery, and building heights that provide the basis for location-based services or wind flow simulation and analysis; *urban planning* where object data include types of ownership, degree of development of land lots such as those with or without power or water supply; *electrical engineering* including power generation facilities, electricity networks above and under ground, related transformers, inverters, capacitors, substations, and bus-couplers; *chemical engineering* including all chemical process plants, storage tanks, supply lines, waste product disposal lines, oil & gas conversion plants (such as LNG terminals), and collection and transshipment points.

Networks of surrogate models are employed to conduct real time simulations that quantify CO₂ emission reduction using for example WHR, and carry out cross-domain simulations both at steady-state and in transient operation.

The advanced software application Model Development Suite (MoDS) [8] was used to sample data, produce surrogate models and computer global sensitivities. MoDS includes a broad range of tools such as data-driven modelling, multi-objective optimisation, generation of surrogate models, data standardisation and visualisation, global parameter estimation, uncertainty propagation, global and local sensitivity analysis, and intelligent design of experiments. Sobol sequence [29], a quasi-random low discrepancy sampling method, was employed for sampling data and polynomial fitting and HDMR fitting were used to generate surrogate models. The JPS server hosts a portfolio of surrogate models that were derived from the chemical and electrical engineering processes using MoDS.

A separate OPAL-RT OP5600 server hosts eMEGAsim [3]. All software applications AP, PW, eMEGAsim and the surrogate models are executed using Python scripts that make use of local file systems. Output data are sent to the ArcGIS server to update the data records. From there they are sent via the Internet to the Java applet for display.

To process semantic queries the JPS also makes use of the ontology OntoCAPE. To this end the JPS server hosts the ontology editor and framework Protégé [31] and keeps a complete data set in OWL format. Protégé acts as semantic parser, reasoner and data retriever and returns the result to the Java applet frontend for display.

5 Case Studies

The JPS represents a wide range of real world aspects in a virtual world. The following case studies demonstrate the functionality and key characteristics of the JPS.

5.1 Wealth and complexity of data

The wealth and complexity of data at multiple levels and across domains are united in a shared data and information hub with a Java applet as GUI that serves different users and applications. It currently contains 206,000 property values of 6000 objects in 76 types of layers in ArcGIS proprietary and RDF/XML format.

5.1.1 Multiple networks with multiple layers

Electricity, water, steam, and road networks were modelled. The electricity network includes 6 power plants in 4 locations producing approximately 6000 MW(e) of power, a power line connecting Jurong Island to the main island allowing for additional power supply to be imported or exported between the islands. Power consumption at the chemical plants is represented by 179 loadpoints across the island. They are linked to power supply via High Tension (22 kV) buses, Extra-High Tension (66 kV) buses, Ultra-High Tension (230 kV) buses, and related inverters, transformers and sub-stations. Bus-couplers provide redundancy in the event of a power failure.

The steam supply network includes five chemical plants producing biodiesel, butyl rubber, butadiene rubber, industrial gases, and middle distillates using hydro cracking technology. The plants were connected via a network of steam pipelines with a natural gas fired co-generation plant in the area added as a possible source of fresh steam. The plants were selected based on their relative vicinity to each other.

A CO₂ emission map of Jurong Island was modelled, see Figure 3. It quantifies CO₂ emissions based on an economic input-output life cycle assessment(EIO-LCA) model that was built by a team at Carnegie Mellon University [33].

A finance module visualises both aggregate and detailed costs of individual equipment units broken down into the major cost components: material, labour, maintenance, and utilities. Utilities costs are broken down further into water, fuel (as a proxy for steam or CO₂), and electricity. The financial data are extracted from financial property data fields from multiple layers. Visualisation options include common chart types such as bar, line, or pie charts.

The JPS can perform a comparison of operating costs or CO₂ emissions by quick visual inspection of two chemical plant models, one without and one with WHR. The results can be displayed in both chart and table format.

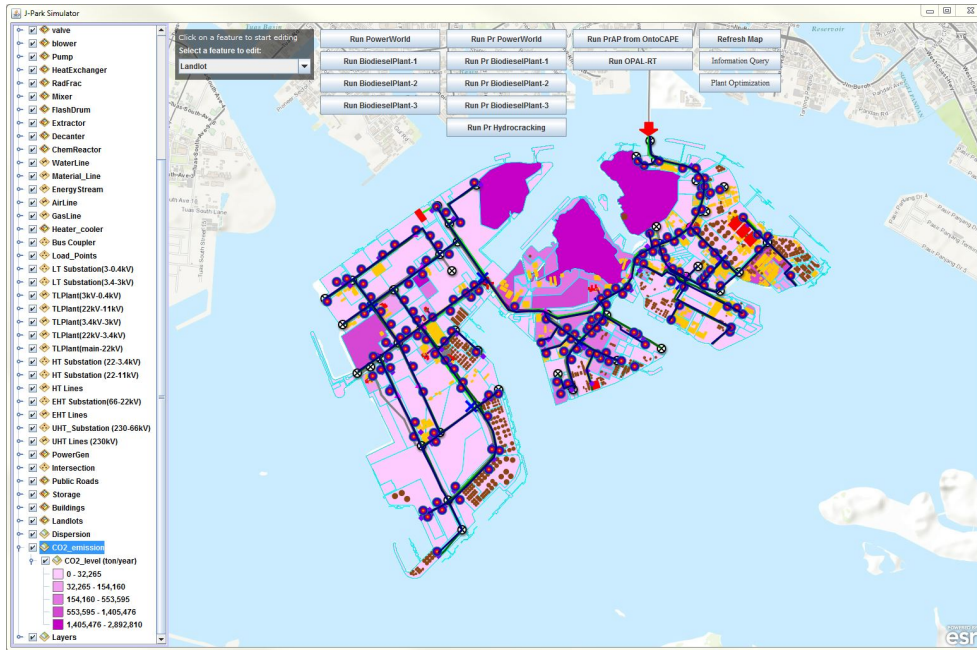


Figure 3: Map of CO₂ emissions as displayed by the JPS. The purple shades indicate emission intensity of each plot on Jurong Island, with the darkest shade corresponding to between 1.4 and 2.9 megatonnes per year.

5.1.2 Toxic gas dispersion model

The dispersion of a toxic gas leak was modelled and a multi-dimensional sensitivity analysis was performed. The results can be displayed in the JPS using simple bar charts. The study was based on a pressurised storage tank of cylindrical shape, 29 meters in diameter and 19 meters high. A containment area surrounding the tank was modelled according to regulatory standards. The tank was filled with liquid ammonia kept at -33°C and 9.7 bar. The outside temperature was $+25^{\circ}\text{C}$. A pressurised tank can only be filled up to 85% of its volume. Therefore a vapour phase formed at the top of the tank above the liquid phase and in the case of a leak the content would have emanated in vapour phase from the tank.

The simulation model assumed that the leakage rate would depend on the following factors (in brackets the range of minimum and maximum boundaries): diameter D of the leaking hole (0.2-10.0 cm); pressure p inside the tank (100-500 kPa); temperature T inside the tank (238-296 K); height h of the tank (0-19 m).

We simulated two scenarios. In the first scenario the toxic gas emanated in vapour phase from the top of the tank. In the second scenario the toxic liquid spilled from the bottom of the tank into the containment area and from there boiled off into the atmosphere. The sensitivity analysis showed that the gas phase leak dispersion largely depended on the diameter of the hole in the tank (Global Sensitivity Index (GSI)=0.76) followed by the pressure inside the tank (GSI=0.14). The temperature of the gas had no influence on the speed of the dispersion (GSI=0.001). The liquid phase leak dispersion largely depended on the temperature of the liquid ammonia in the pool (GSI=0.64), followed by the time that had lapsed after the spill (GSI=0.24). The area of the pool had only a very small

influence (GSI=0.03).

5.2 Simulations in Real Time

The JPS can perform live simulations characterised by interactive modification of data and calculation and display of results in real-time. CO₂ emission reduction can be quantified by comparing two otherwise identical chemical plant models, except that one is without and the other one with a WHR module.

Chemical plants were modelled using piping & instrumentation diagrams (P&ID) that were converted into an application model using the software package AP [1]. The JPS allows the user to display and modify the physical properties, static and variable data, and the behaviour of each of the objects in the chemical process model, visualise various configurations of its components, and calculate operating conditions. Objects in this context can be both equipment units and chemical materials. In the first instance, the objects assume fixed GPS coordinates and the corresponding model is therefore more intuitive to use and to evaluate. Defining a chemical processing plant using chemical materials as primary objects allows the user to set up, modify and evaluate the model from a different perspective.

The application model was visualised in a Java applet using the ArcGIS Online and ArcGIS for Server software applications. All data were stored in ArcGIS Online and were displayed via interactive windows that contained all physical properties of the selected feature.

The JPS calculated a new equilibrium solution in the event one or several of the process parameters were changed. As an example, as the input material quantity changed from 30 to 33 kmol per hour the JPS calculated and displayed a change of output product from 86.6 to 94.3 kmol per hour at the rectification column.

5.2.1 Representation Accuracy of Surrogate Models

We investigated the performance of surrogate models compared to equilibrium solutions obtained from application calls of the original software applications AP and PW. Our studies showed that the time to completion was reduced from 101 seconds for the AP call with WHR (97 seconds without WHR) to less than 1 second for the corresponding surrogate model. The accuracy of the surrogate models varied from zero to a maximum value of 0.51%, see Table 1.

5.2.2 CO₂ Emission Reduction Using WHR

The JPS can quantify CO₂ emission reduction by running a simulation of two otherwise identical chemical plant models, except that one is without and the other one is with a WHR module. In the model in Figure 4 the circle with the dotted line highlights the additional heat exchanger.

Table 1: Comparison of Accuracy of Application Call vs Surrogate Model.

Model	Output Variable	Unit	App Call	Surrogate Model	Rel Error
w/o WHR	Flowrate	kmol/h	86.6	86.62	0.02%
w/ WHR	Flowrate	kmol/h	86.6	86.61	0.02%
Ch+El	Heat Duty	kW	1078.48	1075.54	0.27%
Ch+El	PU Voltage	kV	0.995	0.995	-
Ch+El	Bus Angle	deg	-0.198	-0.197	0.51%
Ch+El	Bus Voltage	kV	3.383	3.383	-

Table 2: Change in Resource Utilisation Using WHR.

Observed Output	Unit	WHR Before	WHR After
Heat Load	kW	561.8 (w/o)	602.2 (w/o)
	kW	436.2 (w/)	476.6 (w/)
Fuel Flowrate	kmol/h	6.2 (w/o)	6.6 (w/o)
	kmol/h	4.8 (w/)	5.2 (w/)
Fuel Price	USD/h	11.60 (w/o)	12.50 (w/o)
	USD/h	9.00 (w/)	9.90 (w/)
CO ₂ Emission	kmol/h	25.5 (w/o)	25.9 (w/o)
	kmol/h	24.1 (w/)	24.5 (w/)

Changing the temperature of the feedstock going into the heater from 30°C to 27°C in the two chemical plant models resulted in outputs presented in Table 2.

The additional heat exchanger led to a reduction of steam, water and fuel consumption and of CO₂ emission as shown in Table 3.

Assuming a capital expenditure of USD 52,400 for the additional heat exchanger, annual cost savings of USD 52,029, and a Weighted Average Cost of Capital of 8% we obtained a payback period of 1.1 years. The Net Present Value was USD 299,000 after 10 years excl. terminal value.

Table 3: Change in Resource Utilisation Using WHR.

Con-sumption	Unit	Without WHR	With WHR	Diff-erence
Steam	kmol/h	259	231	-11%
Water	kg/h	4,670	4,150	-11%
Fuel	kg/h	589	500	-15%
CO ₂	kg/h	1,626	1,380	-15%

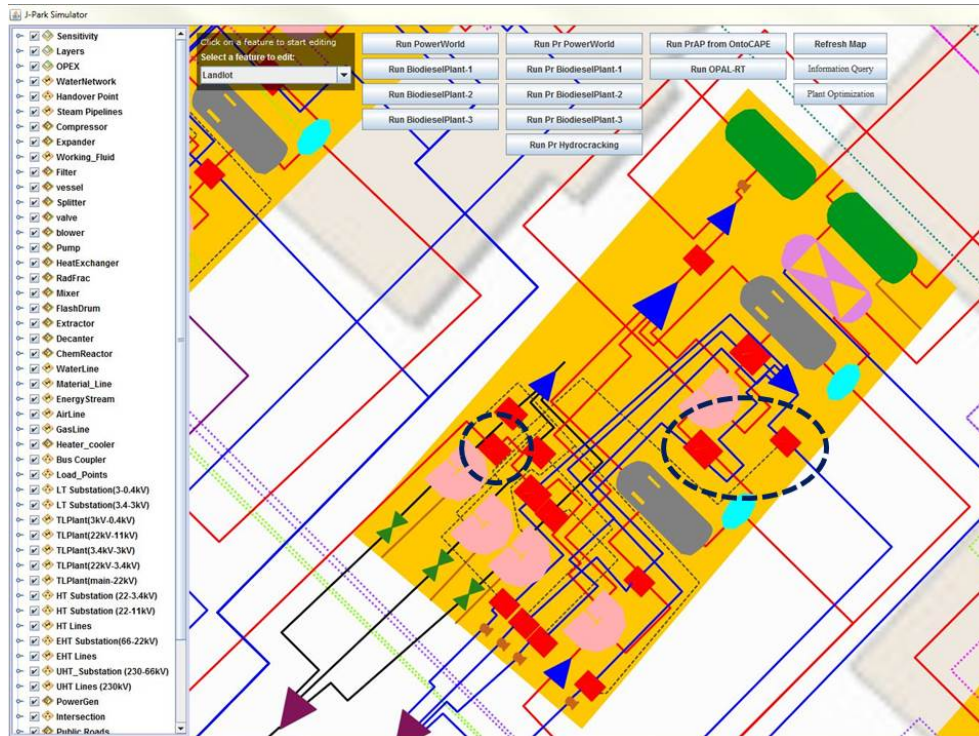


Figure 4: Heat exchangers were added to the chemical plant model to capture waste heat for reduced fuel consumption and cost savings. The heat exchangers are highlighted by blue circles in the chemical process diagram.

5.2.3 Cross-domain Simulation in Steady State

The JPS allows a chemical process model to interact directly with an electrical engineering model using a cross-domain ontology. The electrical engineering modelling tool PW [27] was used to model the electricity network of a chemical plant. PW is an interactive tool that visualises the topology of an electricity network, and calculates operating conditions of its components. Figure 5 illustrates the change to the process condition of the chemical process and the direct impact it had on the electricity consumption in the chemical plant. The top right hand side of the figure shows the chemical process model while the bottom left hand side shows the electrical circuitry model.

A change in the steady state of the process conditions was triggered by changing the flow rate of the input material entering the chemical plant. This change is indicated by dark blue dotted lines highlighting the mixing chambers in the centre at the top of the figure. To the right of the mixing chambers, the reactors linking these two topologies are highlighted with red dotted lines. They are highlighted in both models and in the table in the bottom right hand side of the figure where all the equipment is listed that impacts the power consumption, either in the form of steam or electricity.

In a test simulation the feedstock flow rate was changed from 30 to 33 kmol per hour. The model used surrogate models derived from AP and PW using MoDS. The heat duty in reactor 1 increased from 1075.5 kW to 1161.3 kW and the phase shift angle decreased from $\theta = -0.197^\circ$ to $\theta = -0.215^\circ$.

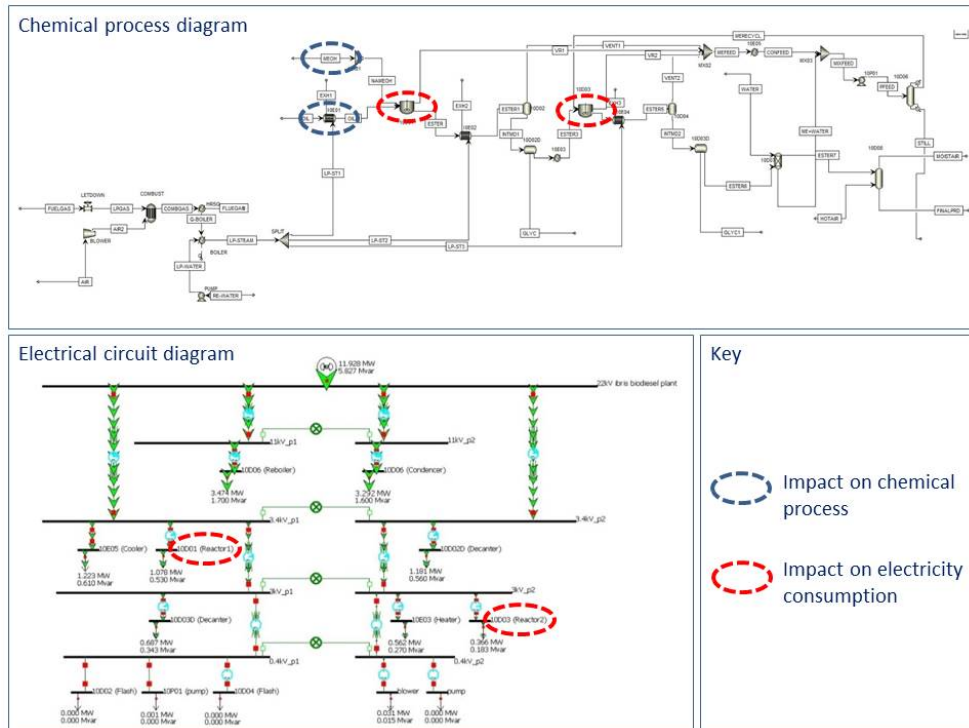


Figure 5: *Cross-domain simulation involving interaction between surrogate models of chemical and electrical engineering domains. A change of the input quantities highlighted by the blue circles leads to a direct change of the heat duty in the reactors highlighted by the red circles.*

The change of the angle theta is significant. It has been estimated that a lagging power factor, mostly caused by induction motors, is responsible for as much as 20% of all grid losses in the USA, equivalent to about 1.5% of total national power generation and costs on the order of USD 2 billion per year [21].

Another reason for concern about power factors are the transformers. They are rated in kVA, not Watts, since it is heating caused by current flow that causes them to fail. By correcting the power factor, a transformer can deliver more real power to the loads. This can be especially important if loads have increased to the point where the existing transformers can no longer handle the load without overheating and potentially burning out. Power factor correction can avoid the need for capital expenditure spent on additional transformer capacity.

5.2.4 Cross-domain Simulation of Transients

PW can only perform steady-state simulations. Using RT-LAB and eMEGAsim the JPS can also simulate transient operations. For this purpose the electricity component of the chemical plant was modeled in RT-LAB and a cross-domain simulation was carried out to obtain the transient states. The response function shown in Figure 6 provided valuable information because the transient could overshoot and reach values that may be large

enough to damage connected equipment units.

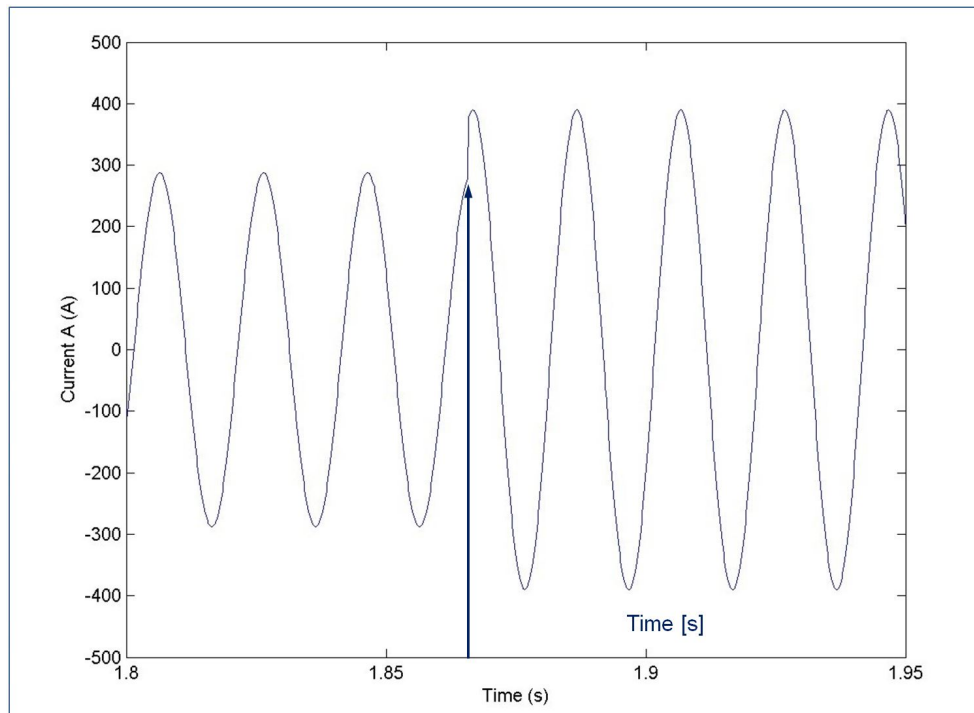


Figure 6: Response function produced by the eMEGAsim simulation tool showing a step change in the delivered current as a consequence of a sudden change in material flow rate within the chemical plant.

5.3 Semantic Query

The cross-domain ontology of the JPS provided a knowledge base for machine-to-human (M2H) communication. It was used to implement semantic query capabilities. The Java applet provides the user access to this ontology through its semantic search module. A search term entered in the applet user interface is sent to Protégé hosted on the JPS server. Protégé acts as semantic parser, reasoner and data retriever and returns the result to the Java frontend for display, see Figure 7. This graph quantifies CO₂ emissions in real time including accurate GPS coordinates of the CO₂ emissions source. The database returns a list of instances matching the search word and its associated attributes including the GPS location of all entities matching the search term. The GPS locations are passed to the Java Applet for visual representations on the screen.

6 Conclusion

A modelling platform, called JPS, for designing, computer-aided process engineering (CAPE) and managing an EIP was described. It combines the concepts Industry 4.0,

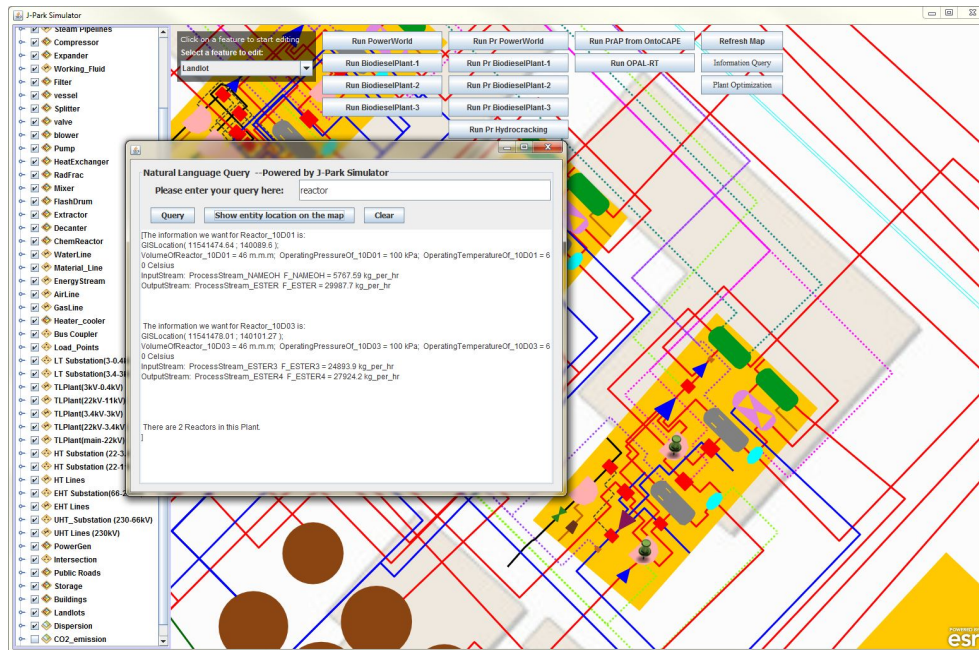


Figure 7: Semantic query result with its corresponding GPS coordinates shown on the map. This graph shows the location of all CO₂ emission sources within the chemical plant selected. When hovering over the icon with the cursor a separate popup window lists all properties associated with this object in the database.

the Semantic Web, and advanced mathematical modelling to provide a central information hub that serves different users and applications to make informed decisions for the reduced use of finite resources, reduced operating cost, or reduced carbon footprint. Its system architecture was described. Case studies demonstrated the viability of the system architecture, quantified CO₂ emissions of a model chemical plant, and cost savings associated with WHR. A cross-domain simulation linking chemical and electrical engineering domains highlighted the versatility of the modular system architecture. A transient simulation demonstrated its real time capabilities. A W3C compliant OWL format database provided the JPS with semantic query capabilities.

Acknowledgements

The authors gratefully acknowledge the support from the National Research Foundation, Prime Minister's Office, Singapore under its CREATE programme.

References

- [1] Aspen Technology Inc. AspenPlus Webpage. <http://www.aspentech.com/products/aspen-plus/>, 2016 (accessed 2016-Oct-04).
- [2] L. Atzori, A. Iera, and G. Morabito. The internet of things: A survey. *Computer Networks*, 54(15):2787–2805, 2010.
- [3] J. Bélanger, V. Lapointe, C. Dufour, and L. Schoen. eMEGAsim: an open high-performance distributed real-time power grid simulator. architecture and specification. In *Proceedings of the International Conference on Power Systems (ICPS 2007)*, pages 12–24, 2007.
- [4] T. Berners-Lee, J. Hendler, O. Lassila, et al. The Semantic Web. *Scientific American*, 284(5):28–37, 2001.
- [5] CAM.CREATE C4T. J-Park Simulator Webpage. <http://www.jparksimulator.com/>, 2016 (accessed 2016-Oct-04).
- [6] K. Carpenter, W. K. Ng, et al. Singapore’s chemicals industry: Engineering an island. *Chemical Engineering Progress*, 109(4):56–60, 2013.
- [7] M. R. Chertow. “uncovering” industrial symbiosis. *Journal of Industrial Ecology*, 11(1):11–30, 2007.
- [8] CMCL Innovations Ltd. MoDS Webpage. <http://www.cmclinnovations.com/mods/>, 2016 (accessed 2016-Oct-04).
- [9] S. B. Crary. Design of computer experiments for metamodel generation. *Analog Integrated Circuits and Signal Processing*, 32(1):7–16, 2002.
- [10] R. Drath. *Datenaustausch in der Anlagenplanung mit AutomationML: Integration von CAEX, PLCopen XML und COLLADA*. Springer, 2009.
- [11] Esri Inc. ArcGIS Online Webpage. <http://www.arcgis.com/features/index.html/>, 2016 (accessed 2016-Oct-04).
- [12] J. Ge, Z. Li, T. Li, and B. Qiang. Petroleum exploration domain ontology-based knowledge integration and sharing system construction. In *Network Computing and Information Security (NCIS), 2011 International Conference on*, volume 1, pages 84–88. IEEE, 2011.
- [13] A. Gómez-Pérez, M. Fernández-López, and O. Corcho. *Ontological Engineering: with examples from the areas of Knowledge Management, e-Commerce and the Semantic Web*. Springer, 2006.
- [14] D. Gorissen, I. Couckuyt, P. Demeester, T. Dhaene, and K. Crombecq. A surrogate modeling and adaptive sampling toolbox for computer based design. *Journal of Machine Learning Research*, 11(Jul):2051–2055, 2010.

- [15] R. Hai, M. Theißen, and W. Marquardt. An ontology based approach for operational process modeling. *Advanced Engineering Informatics*, 25(4):748–759, 2011.
- [16] Kalundborg Symbiosis. Symbiosis diagram. <http://www.symbiosis.dk/diagram/>, 2016 (accessed 2016-Oct-11).
- [17] C. A. Kastner, R. Lau, and M. Kraft. Quantitative tools for cultivating symbiosis in industrial parks; a literature review. *Applied Energy*, 155:599–612, 2015.
- [18] M. Kraft and S. Mosbach. The future of computational modelling in reaction engineering. *Philosophical Transactions of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 368(1924):3633–3644, 2010.
- [19] D. Küçük. A high-level electrical energy ontology with weighted attributes. *Advanced Engineering Informatics*, 29(3):513–522, 2015.
- [20] W. Marquardt, J. Morbach, A. Wiesner, and A. Yang. *OntoCAPE: A Re-usable Ontology for Chemical Process Engineering*. Springer, 2009.
- [21] G. M. Masters. *Renewable and Efficient Electric Power Systems*. John Wiley & Sons, 2013.
- [22] P. N. Mendes, M. Jakob, and C. Bizer. DBpedia: A multilingual cross-domain knowledge base. In *LREC*, pages 1813–1817. Citeseer, 2012.
- [23] M. Minsky. A framework for representing knowledge. *The Psychology of Computer Vision*, 1975.
- [24] E. Muñoz, A. Espuña, and L. Puigjaner. Towards an ontological infrastructure for chemical batch process management. *Computers & Chemical Engineering*, 34(5):668–682, 2010.
- [25] National Climate Change Secretariat (NCCS) Singapore. Technology Roadmaps. <https://www.nccs.gov.sg/resources/technology-roadmaps/>, 2016 (accessed 2016-Oct-08).
- [26] M. Pan, J. Sikorski, J. Akroyd, S. Mosbach, R. Lau, and M. Kraft. Design technologies for eco-industrial parks: From unit operations to processes, plants and industrial networks. *Applied Energy*, 175:305–323, 2016.
- [27] PowerWorld Corporation. PowerWorld Webpage. <http://www.powerworld.com/>, 2016 (accessed 2016-Oct-04).
- [28] D. Sakr, L. Baas, S. El-Haggar, and D. Huisingh. Critical success and limiting factors for eco-industrial parks: global trends and egyptian context. *Journal of Cleaner Production*, 19(11):1158–1169, 2011.
- [29] I. M. Sobol’. On the distribution of points in a cube and the approximate evaluation of integrals. *Zhurnal Vychislitel’noi Matematiki i Matematicheskoi Fiziki*, 7(4):784–802, 1967.

- [30] J. F. Sowa. *Knowledge Representation: Logical, Philosophical, and Computational Foundations*. Brooks/Cole, 1999.
- [31] Stanford University. Protégé Webpage. <http://protege.stanford.edu/>, 2016 (accessed 2016-Oct-04).
- [32] W3C Consortium. OWL 2 Overview. <https://www.w3.org/TR/owl2-overview/>, 2016 (accessed 2016-Oct-04).
- [33] C. Weber, D. Matthews, A. Venkatesh, C. Costello, and H. Matthews. The 2002 US benchmark version of the economic input-output life cycle assessment (EIO-LCA) model. *Green Design Institute, Carnegie Mellon University*, 2009.
- [34] A. Yang, B. Braunschweig, E. S. Fraga, Z. Guessoum, W. Marquardt, O. Nadjemi, D. Paen, D. Pinol, P. Roux, S. Sama, et al. A multi-agent system to facilitate component-based process modeling and design. *Computers & Chemical Engineering*, 32(10):2290–2305, 2008.