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Parameterisation of a biodiesel plant process flow sheet model

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ABSTRACT

This paper presents results of parameterisation of typical input–output relations within process flow sheet of a biodiesel plant and assesses parameterisation accuracy. A variety of scenarios were considered: 1, 2, 6 and 11 input variables (such as feed flow rate or a heater's operating temperature) were changed simultaneously, 3 domain sizes of the input variables were considered and 2 different surrogates (polynomial and high dimensional model representation (HDMR) fitting) were used. All considered outputs were heat duties of equipment within the plant. All surrogate models achieved at least a reasonable fit regardless of the domain size and number of dimensions. Global sensitivity analysis with respect to 11 inputs indicated that only 4 or fewer inputs had significant influence on any one output. Interaction terms showed only minor effects in all of the cases.

1. Introduction

Every industrial actor strives towards better understanding and, ultimately, optimisation of any and all of its activities. That applies on each level beginning with workforce schedules and individual pieces of machinery, through specific processes, ending with entire plants. Traditionally the main objectives of such an optimisation are minimising resource use and maximising profit. However, as environmental concerns become ever more pressing ecologically-focused targets such as reducing pollutants, creating cleaner manufacturing processes or reducing carbon footprints rise in prominence.

Those trends prompted significant academic and industrial interest in the concepts of "sustainable development" (Brundtland et al., 1987), "industrial ecology" (Hoffman, 1971; Watanabe, 1972; Allenby, 2004, 2006) and "industrial symbiosis" (Chertow, 2000). The latter concept brings together separate industries in a collective approach to competitive advantage involving physical exchange of materials, energy, water and by-products (Chertow, 2000). Ecological industrial development based thereon is often realised as eco-industrial parks (EIPs).

An EIP is defined as an industrial park where businesses cooperate with each other and, at times, with the local community to reduce waste and pollution, efficiently share resources (such as information, materials, water, energy, infrastructure, and natural resources), and minimise environmental impact while simultaneously increasing business success (Pan et al., 2015). An example of an EIP exists in Kalundborg, Denmark where an exchange network is centred around Asnæs Power Station, a 1500 MW coal-fired power plant, and linked to the local community and several other companies (Chertow, 2000; Desrochers, 2001). Sample exchanges include selling excess steam from the plant to Novo Nordisk, a pharmaceutical and enzyme manufacturer, and to Statoil power plant or using extra heat to heat local homes and a nearby fish farm. Also, one of the plant's by-products, gypsum, is purchased by a wallboard producer, helping to reduce the amount of necessary open-pit mining (Ehrenfeld and Gertler, 1997).

Primary academic interest stems from EIPs' ability to create more sustainable industrial activities through the use of localised symbiotic relationships (Boix et al., 2015). To this date a great number of studies concerning various aspects of EIPs have been conducted. Many of them probe methods suitable for optimal design, focusing primarily on employing mathematical programming to create exchange networks of materials, water and energy connecting members of the EIP in question (Cimren et al., 2012;

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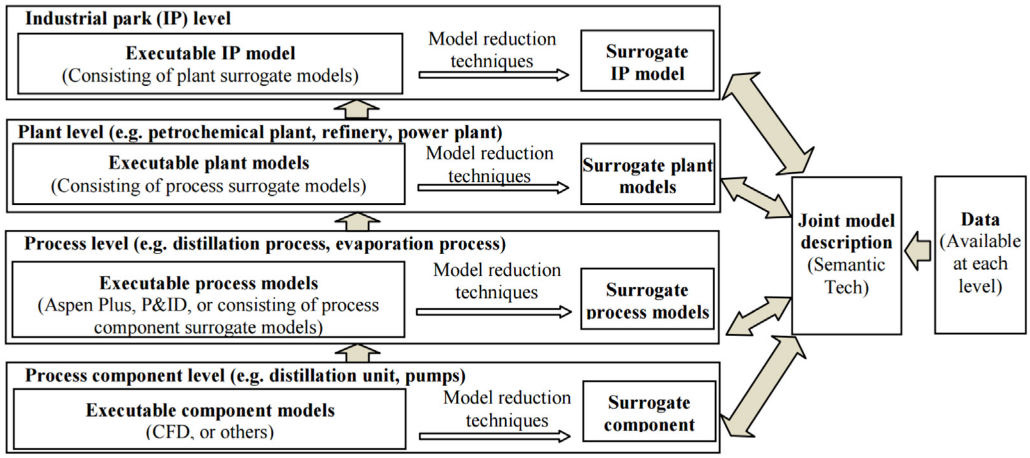

Fig. 1. Framework of EIP modelling based on Industry 4.0.

Adopted from Pan et al. (2015).

Kantor et al., 2012; Keckler and Allen, 1999; Liao et al., 2007; Karlsson, 2011). Utility of such designs is evaluated by monitoring environmental, social and economical impacts.

Holistic modelling of complex, highly interconnected networks is a non-trivial and expensive task, especially for EIPs which include numerous physical models of disparate processes. That is why many studies apply mathematical optimisation to simplified models of individual aspects of the parks.

The limitations of this approach may be overcome by exploiting key features of the concept of Industry 4.0 (Pan et al., 2015): creation of virtual copies of the physical world and the ability of industrial components to communicate with each other. Those virtual copies could be surrogate models of physical models produced for a predefined range of inputs. Developing a virtual system primarily based on surrogate models would significantly reduce required computation time and storage space and allow for dynamic modelling and studies otherwise impossible to conduct. Fig. 1 presents a framework of EIP modelling based on Industry 4.0.

A surrogate model (or a 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 (Forrester et al., 2008). Two key requirements thereof are reasonable accuracy and significantly faster evaluation than the original method. The 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,
- gain insight into 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 as documented in a number of reviews. Simpson et al. (2001) provides detailed reviews of data sampling and metamodel generation techniques, including response surfaces, kriging, Taguchi approach, artificial neural networks and inductive learning. It also discusses metrics for absolute and relative model assessment, including R^2, residual plots and root mean square error. An introduction to and analysis of linear regression with a focus on generalised linear mixed models with many examples and case studies is provided by Ruppert et al. (2003).

A book by Forrester et al. (2008) puts the process of data sampling and generating surrogate models into engineering perspective providing numerous case studies and MATLAB code to perform associated calculations. It discusses response surfaces, kriging, support vectors machines and radial basis functions. An in-depth review of kriging, its application and new extensions are provided by Kleijnen (2009). A review and assessment of various sampling techniques is provided by Crary (2002). Reich and Barai (1999) focuses on assessment of machine learning techniques, artificial neural networks in particular, with case studies of modelling marine propeller behaviour and corrosion data analysis. An example of surrogate models bridging models of varying fidelity is provided by Bakr et al. (2000) where a surrogate maps data produced by fine and coarse physical models in order to accelerate optimisation of the fine model. Jin et al. (2003) assesses applicability and accuracy of metamodels for optimisation under uncertainty and reports promising results noting that only a small-size analytical problem was considered. Surrogate models are widely employed in engineering and science for space exploration (Gough and Welch, 1994; Geyera and Schlueter, 2014), modelling (Knill et al., 1999; Crary et al., 2000; Chen et al., 2014), sensitivity analysis (Azadi et al., 2014b; Chapman et al., 1994; Gough and Welch, 1994; Menz et al., 2014; Jouhauda et al., 2007), parameter estimation (Kastner et al., 2013; Bailleul et al., 2010; Braumann et al., 2010a), optimisation in areas ranging from circuit design through nanoparticle synthesis to flood monitoring (Bernardo et al., 1992; Aslett et al., 1998; Roux and Bouchard, 2013). A number of studies addressed application of surrogates to process flow sheet models. Caballero and Grossmann (2008) replace the computationally expensive subsystems of a flow sheet with Kriging surrogates to speed up optimisation. Hasan et al. (2012, 2013), First et al. (2014), Nuchitprasittichai and Cremaschi (2013), and Boukouvala and Ierapetritou (2013) guide sampling of an expensive rigorous model using Kriging surrogates to reduce computational time required for optimisation. Fahmi and Cremaschi (2012) optimise a design of a biodiesel production plant by replacing all subsystems in a process flow sheet model with surrogate models based around artificial neural networks (ANNs) and solving thus defined mixed-integer non-linear problem. Henao and Maravelias (2011) propose a systematic method for creating surrogate models of chemical engineering systems and arranging them into a solvable network (superstructure). The study focuses on ANNs as a base for their surrogate models and describes how a superstructure can be optimised. Kong et al. (2016) employ some of the concepts developed in Henao and Maravelias (2011) for design optimisation of a chemical