Applied Energy xxx (2017) xxx–xxx

Contents lists available at ScienceDirect

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy

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

Li Zhou [a,1], Ming Pan [b,1], Janusz J. Sikorski [b], Sushant Garud [a], Leonardus K. Aditya [c], Martin J. Kleinelanghorst [c], Iftekhar A. Karimi [a], Markus Kraft [b,c,*]

[a] *Department of Chemical and Biomolecular Engineering, National University of Singapore, 4 Engineering Drive 4, Singapore 117585, Singapore*
[b] *Department of Chemical Engineering and Biotechnology, University of Cambridge, New Museums Site, Pembroke Street, Cambridge CB2 3RA, United Kingdom*
[c] *School of Chemical and Biological Engineering, Nanyang Technological University, 62 Nanyang Drive, Singapore 637459, Singapore*

HIGHLIGHTS

- The concept of constructing an expert system called JPS for EIPs is introduced.
- A biodiesel plant is implemented into the system as a first step.
- OntoCAPE is adapted to establish a knowledge base for the biodiesel plant.
- Plant-wide process simulation and optimization can be carried out via JPS.
- Simple information query can be carried out based on the developed knowledge base.

ARTICLE INFO

Article history:
Received 16 January 2017
Received in revised form 27 April 2017
Accepted 1 May 2017
Available online xxxx

Keywords:
Eco-industrial park
Knowledge base
Ontology
Process simulation
Process optimization
Query

ABSTRACT

In this paper, we introduce the concept of constructing an ontology-based decision support system called J-Park Simulator for the design and operation of eco-industrial parks. 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 J-Park Simulator. Firstly, information query can be performed. Information of the biodiesel plant can be extracted through natural language query. Secondly, J-Park Simulator 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 J-Park Simulator. 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.

1. Introduction

The study of Eco-Industrial Parks (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 [1,2]. 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. [3], 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. [4] presented two interplant water integration schemas, direct integration via

---

[*] Corresponding author at: Department of Chemical Engineering, University of Cambridge, West Cambridge Site, Philippa Fawcett Drive, Cambridge CB3 0AS, United Kingdom.

E-mail address: mk306@cam.ac.uk (M. Kraft).

[1] These authors contributed equally.

http://dx.doi.org/10.1016/j.apenergy.2017.05.002
0306-2619/© 2017 Published by Elsevier Ltd.

Please cite this article in press as: Zhou L et al. Towards an ontological infrastructure for chemical process simulation and optimization in the context of eco-industrial parks. Appl Energy (2017), http://dx.doi.org/10.1016/j.apenergy.2017.05.002

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. [5] 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. [6], 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. [7].

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 [9] and applied to several case studies [10,11]. Most recently, Nair et al. [12] 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. [13] to analyze by-product synergistic networks that involve material processing and transport among companies. Haslenda and Jamalusin [14] 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 [15] to optimize the waste exchange between power plants, palm oil mills and bio-refineries.

The aforementioned studies decouple and optimize 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 by 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-control [16,17]. Furthermore, information will need to be shared and exchanged among the relevant entities autonomously. 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 [18–20], electrical engineering [21,22], pharmaceutical engineering [23,24], building [25], transportation networks [26], etc. These ontologies can be utilized as base work to describe the engineering activities take place in an EIP (Fig. 1).

Among the reported ontologies for chemical process engineering domain, OntoCAPE [20] 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 [27], which is a multi-agent framework that supports the retrieval of desirable process modeling components from model libraries. Brandt et al. [28] 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

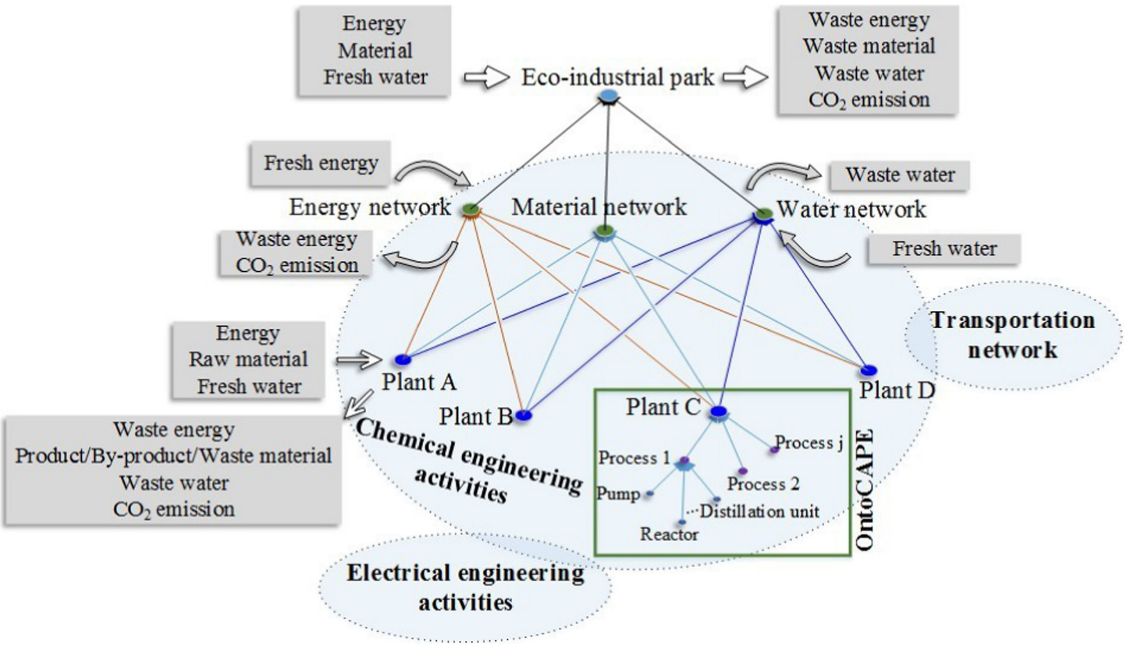

Fig. 1. Engineering activities conducted in an EIP.

Please cite this article in press as: Zhou L et al. Towards an ontological infrastructure for chemical process simulation and optimization in the context of eco-industrial parks. Appl Energy (2017), http://dx.doi.org/10.1016/j.apenergy.2017.05.002