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Opportunities for Agent-Based Models in Computer Aided Process Engineering

Koen van Dam[a], Zofia Lukszo[a], Rajagopalan Srinivasan[b] and Iftekhar Karimi[b]

[a] *Department of Energy & Industry, Delft University of Technology, P.O.Box 5015, 2600 GA Delft, the Netherlands, K.H.vanDam@tudelft.nl*
[b] *Department of Chemical & Biomolecular Eng., National University of Singapore, 10 Kent Ridge Crescent, Singapore 119260*

Abstract

When considering process systems as socio-technical systems there is a need for computer models that can describe their full complexity. The Agent Based Model (ABM) paradigm promises to offer new modelling methods and tools that can complement the well established Computer Aided Process Engineering (CAPE) approaches. In this paper guidelines for the application of ABM are discussed and the suitability is demonstrated with a number of applications, ranging from chemical supply chains and oil refineries to the control of combined heat and power units. When ABM are used in combination with traditional CAPE techniques, it can be a very powerful and flexible way to model complex systems and optimise their behaviour, especially when dealing with social aspects in the system that are more difficult to catch in mathematical formulas.

Keywords

Agent based modelling, socio-technical systems, literature review, methodology

1. Introduction

Process Systems Engineering (PSE) is concerned with the improvement of decision making processes for the creation and operation of the chemical supply chain [1]. Computer models are an important instrument in the PSE research. Over the years, algorithms have become smarter and computers more powerful. As the size and complexity of process systems have increased over the years, the need for more complex models has also become apparent. A new paradigm from distributed artificial intelligence, called Agent Based Models (ABM) promises to offer new modelling methods and tools that can complement the well established *Computer Aided Process Engineering* (CAPE) and *Operations Research* (OR) approaches.

Agent Based Modelling involves developing a model of a system (including the decision makers) by describing it in terms of constituent agents and relations between agents. Agents are defined as software entities that are autonomous, reactive, pro-active and capable of social interaction [2]. Key advantages of ABM include flexible and modular description of the system, bottom-up descriptions of problems and the ability to include social relations on top of technical systems. This allows a variety of computational experiments including changes in system structure (e.g., a part of a network is acquired by another agent), sensitivity (the technology does not work properly anymore), or policies (the introduction of financial incentives) to find answers to 'what happens if' questions.

Technical systems, such as reactors, distillation columns or other process units, and the pipes and wires that connect these nodes can form a network. Next to that, social relations, such as trade contracts or governmental policies, are important. Together they form a *socio-technical system,* consisting of organisations, scientific components and legislative artefacts in addition to the physical artefacts. The addition of the social layer to a technical system makes a system complex.

A *complex system* has many components that are heterogeneous (i.e., many different types of components), have non-stationary, non-linear dynamics, contains feedback loops (i.e., the output of components is input to another components), is organised and nested (i.e., contains hierarchies and subsystems which themselves can again be seen as complex systems) and shows emergence (i.e., the behaviour of the system cannot be predicted by looking at the behaviour of the lower level components) [3]. The socio-technical systems that are the topic of this paper all have these characteristics.

In this paper we look at applications of ABM to model complex socio-technical systems. First, in Section 2, an overview of the suitability of ABM for a system is discussed. Two case studies that demonstrate the power of ABM in combination with mathematical optimisation are presented in Section 3. Finally, Section 4 summarises the paper and gives directions for future research.

2. Agent Based Modelling in Chemical Engineering

Agent-Based Modelling is specifically suited to model socio-technical systems with multi-actor, multi-level, multi-objective and dynamic complexity. Such models can contribute considerably to more effective and efficient utilisation of industrial plants. In this Section a brief overview of Agent Based Modelling, guidelines for application and links with traditional CAPE methods is given.

2.1. Agent Based Modelling and Ontologies

As mentioned above, ABM are modular. The models are defined at the level of entities (the agents). The main advantage of building models in a bottom-up approach is that it provides a flexible environment in which different experiments can be done. By modelling components rather than the entire system the structure of the system is not pre-defined. Because agents can communicate with other agents without having to program the relations between them, different networks can be created by changing the behavioural rules. This social ability of agents is brought about using ontologies – formalised specifications of the concepts used in a certain domain [4] – which serve as the cornerstone of ABM. When an ontology is shared between two agents, it serves as a language for their communication and when shared between modellers it ensures interoperability.

2.2. Guidelines for the application of ABM

An ABM is appropriate for modelling a socio-technical system characterised by multiple decision makers, each with their own goals and objectives that are both proactive and reactive. Such systems have a distributed character, and communication plays a role in the decision making process. Subsystems (consisting of one or more agents) can operate in a highly dynamic environment. ABM offer a valuable formalism to help solve problems in complex domains [5]. Of course ABM should not be used when other modelling techniques are more applicable, for example in a system that is very well understood and does not contain aspects such as human behaviour that are "softer" than the technical parts. Also, sometimes it is desirable to model the behaviour directly at a system level rather than modelling all components of the system. This depends on the goals that are behind the model and the type of questions one wants to ask from the model.

2.3. Link between ABM and traditional CAPE

An agent-based model does not preclude traditional modelling and optimisation techniques based on strong mathematical formalisations. These can also be applied to describe the behaviour of the constituent agents. The overall system model can be used to gain insight about the relation between the behaviour of an agent and the total system performance (e.g., efficiency, security of supply, reliability). Taking this into account, local behaviour (by one or more agents)

Table 1: Agents in the oil refinery model

Agent	Role
Procurement department	Coordinates the crude procurement process. It retrieves the list of crude available for spot purchase and decides which crude to purchase and in what quantity. To do this, it needs information about crude availability, refinery targets, and logistics.
Sales dept.	Provides product prices and demands, both current and forecasted.
Operations dept.	Decides which crude and how much to process every day.
Storage dept.	Manages the crude inventory and releases crude to operations.
Logistics dept.	Arranges transport of crude from the oil supplier terminal to the refinery.

can be steered in such a way that the overall system performance criteria are met.

3. Illustrative applications of ABM in PSE

This section presents two examples of agent-based models applied to process systems engineering, namely in an oil refinery and for the control of combined heat and power installations, and a review of applications by other authors.

3.1. Oil refinery

The daily operation of a crude oil refinery is buffeted by numerous exogenous and endogenous factors which makes modelling and analysis complex. Many activities span across multiple departments, adequate performance by each is critical to the overall success of the activity. One such is crude procurement, possibly the most important supply chain activity in the refinery, and one which has a significant direct impact on the refinery's economic performance. Large buffers of crude degrade the economics of the refinery due to the high inventory cost; insufficient crude would lead to crude stock-out situations that necessitate unit shutdowns – both should therefore be avoided. The complexity of crude procurement stems from the numerous interactions between several departments in the refinery as well as third parties. It therefore serves as a suitable illustration to explore the benefits of agent-based modelling in supply chain management. The key agents for this activity are shown in Table 1.

In addition, the actions of oil suppliers and third party logistics providers are important determinants in the dynamics of the refinery supply chain. An agent-based dynamic model of the refinery supply chain was developed and used for decision support [6]. This ABM model incorporates traditional optimisation methodologies such as Linear Programming used by the refinery departments. Since abnormal events in crude supply can lead to huge economic impacts, the monitoring of this activity is also critical.

Table 2: Agents in the combined heat and power model

Agent	Role
Energy supplier	Sells gas for fuelling the μCHP and additional electricity for households. Furthermore, the supplier buys any electricity that is produced by the household but not consumed by them.
Household	Chooses best way to meet its electricity and heat demand by controlling the operation of the μCHP unit (Incl. Stirling engine and an auxiliary burner).
Energy market	Provides gas and electricity to the supplier.

3.2. Combined Heat and Power

Residential Combined Heat and Power units based on Stirling engine technology (micro-CHP, from now on referred to as μCHP) are expected to pervade the electricity infrastructure on a large-scale in the future. This will have an effect on the generation methods, transportation and supply of electricity. A μCHP unit produces heat from gas (like a traditional central heating unit common in most households), but in addition it also produces electricity. Here we focus on groups of households interacting with their energy supplier in electricity sales. This is a *virtual power plant* control concept in which households cannot trade electricity amongst themselves. For the distributed control of μCHP units a MAS approach is used.

Table 2 shows the key agents in this system. The choices the household agent has to make (power levels of the Stirling engine and auxiliary burner, amount of gas and electricity to buy, etc) are modelled with a mathematical optimisation method. See [7] for more details. The power of the use of an ABM is that various households can be included in the model, each with different characteristics, while the main model of the household remains the same. Also the interaction between supplier and household is flexible and can easily be adjusted, for example to include other control concepts such as a *microgrid*. The bottom-up modelling approach makes this possible.

3.3. Other applications in Process Systems Engineering

The MAS formalism has started to receive much attention in PSE with applications towards process design, modelling, control, optimisation and supervision. In [8] agent-based learning is used to model the dynamics of microbial growth. [9] and [10] illustrate the suitability of MAS for process monitoring and control. The use of MAS for three different problems in chemical process engineering (intelligent search, process design and configuration of team members) is explored and a number of other PSE areas where the MAS formalism is beneficial are highlighted in [11]. One such was further investigated in [12], using multiple optimisation agents to derive the Pareto front for a multi-objective optimisation problem.

4. Final remarks

ABM can be valuable in various PSE applications, ranging from chemical supply chains and oil refineries to the control of combined heat and power units. Especially when used in combination with traditional CAPE techniques, it can be a very powerful way to model complex systems and optimise their behaviour. Agent-based techniques complement traditional CAPE techniques especially when dealing with social aspects in the system that are more difficult to catch in mathematical formulas. Work is still ongoing and ABM of complex process systems are increasingly being developed. Validating them with real life cases is an important next step. Currently, reuse of agents developed for one application for another remains a challenge. Developing a generic CAPE ontology that can be used for various applications in process systems can be one way to address this and enable the exchange of models.

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