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**Literature Overview of Approaches for  
Enterprise-wide Modelling, Simulation and  
Optimisation**

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## **Introduction by Series Editor**

The Kingston Business School Working Papers series enables rapid publication of work by researchers associated with Kingston Business School. This Working Paper adds to a series which showcases the strength and diversity of research activity at Kingston. In addition, the individual Working Papers provide an opportunity for discussion of the research to date, leading to revisions and more formal publications.

Dr Elena Fitkov-Norris, from the Department of Informatics and Operations Management, spent a sabbatical term at Imperial College London. This provided the opportunity to engage in the research culture, and to prepare a potential research programme at Kingston Business School.

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## **Abstract**

This report highlights different quantitative, qualitative and hybrid modelling and simulation techniques that can be used for enterprise-wide modelling and simulation. The report identifies the three main challenges posed by enterprise-wide modelling and simulation, namely: the complexity of the task, the inherent uncertainty of the environment enterprises operate in and the multi-scale nature of enterprises.

This report found that quantitative modelling was least suited to dealing with very complex systems, although its strength lies in its tractability and inherent ability to produce results that are easy to interpret and analyse. Qualitative approaches, on the other hand, provide a convenient tool for modelling uncertainty and generalising complex systems, but generate results that are difficult to interpret. Hybrid approaches counteract some of the limitations of purely quantitative/qualitative modelling techniques and, as this report shows, have been used successfully to create a variety of enterprise-wide models and simulations.

Agent based modelling and systems dynamics are the two hybrid approaches that appear most suited to modelling complex, multi-scale systems such as a chemical plant, operating in an uncertain environment. However, these approaches have some inherent problems that need to be overcome to ensure their successful application to enterprise-wide simulation. The main problem with agent based modelling is that the causal relationships between model variables are not explicitly defined, and this may hinder the analysis of the results. While systems dynamics explicitly specifies the causal relationships between variables and overcomes this particular problem, this modelling approach encounters problem with model validation and transparency as the causal loop modelling framework it adopts is unstructured. Therefore, this approach requires the identification of a suitable enterprise architecture framework, suited for chemical plant modelling. Although it has been recognised that enterprise-wide modelling is challenging, this fascinating subject offers scope for further research and development.

## Terms of Reference

The report was commissioned by Prof. Nina Thornhil and its purpose is to present an overview of the current state of the art in enterprise-wide process modelling, simulation and optimisation techniques. The objectives of the report were to evaluate the effectiveness of existing approaches for enterprise-wide modelling, identify their strengths and weaknesses and suggest possible avenues for future research.

The report was completed as part of the author's sabbatical term and the time constraints on the work mean that although representative of the current state of knowledge, this overview is not necessarily exhaustive.

## Acknowledgements

I would like to thank the Department of Informatics and Operations Management for sponsoring my sabbatical, and offer my deepest gratitude to Professor Nina Thornhill from the Centre for Process Systems Engineering at the Department of Chemical Engineering, Imperial College London for giving me this invaluable opportunity to fall in love with research.

## Methodology

The literature review was completed using the ISI Web of Knowledge web interface (<http://apps.isiknowledge.com>), which provides access to journal articles, conference proceedings, books, reviews and meetings. Due to the significant time limitations, this was the only information management tool used to identify suitable academic outputs. The following search terms and their combinations were used as topics to identify appropriate articles:

strategic, process, optimisation/optimization, plant-wide, enterprise-wide, system, dynamic, modelling/modeling, performance management, performance optimisation, dynamic optimisation, system dynamics, Srinivasan, Singapore, control, decision support system (DSS), operations, enterprise resource planning (ERP), process integration, scheduling, planning, supply chain.

The search results were narrowed down to articles related to modelling and simulation of chemical processes or engineering and other complex systems (e.g. ecological or biological) and relevant articles downloaded when available.

## **Findings**

The following sections give a general introduction to the modelling process, before discussing the different approached approaches for modelling complex systems identified by this research.

### ***1 The modelling process***

Modelling is a powerful technique, which allows researchers from various disciplines to analyse and study complex phenomena. In most general terms a model is ‘a (small) finite description of an infinitely complex reality, constructed for the purpose of answering particular questions’ (Kuipers 1994). Although the nature of each scientific discipline will affect the steps taken in the modelling process, as a general rule modelling follows the following three steps:

- Step 1: Model Identification – this step involves identifying the research objectives and the best approach for modelling a particular event. It also includes the definition of the model boundaries in terms of listing key variables and specification of the scope, time frame and reference mode of the model.
- Step 2: Model Building – this step involves representation of the real world dependencies between the variables of interest in an appropriate format. This could be done using a quantitative approach such defining a system of simultaneous Ordinary Differential Equations (ODEs) or linear programming or a qualitative approach such as a structural dependency representation using causal diagrams. There are also a number of approaches known as hybrid approaches, which combine quantitative and qualitative techniques.
- Step 3: Model Analysis and Interpretation – This step involves the derivation of solution(s) for the mathematical equations and/or simulation of the dependencies between variables, in order to answer the particular research questions set out at the beginning of the process. This step may also involve a number of extra steps such as model/simulation initialisation and validation.

### ***2 Modelling Approaches***

Depending on representation of data modelling approaches can be split up in two main categories:

- quantitative and
- qualitative

Quantitative models use ordinary differential equations or management science techniques, such as linear programming, to build a mathematical model of the system under investigation (Grossmann 2005, Bousson et al. 1998, Hangos, Cameron 2001). Some quantitative models are static – identifying an optimal solution to a given set of inputs, but some work has also incorporated dynamic interactions between the variables of interest (Manenti, Manca 2009, Bezzo et al. 2004).

This is the traditional approach to process modelling (Hangos, Cameron 2001) and it has the advantage that the modelling process is transparent and the mathematical equations can be solved to provide a unique solution to a problem. However, one disadvantage of quantitative models is that their complexity increases as the complexity of the system to be modelled increases, making it difficult to identify causal relationships between different variables and thus hindering the model analysis. In addition, quantitative models cannot cope with representation of uncertainty as in many complex systems complete information is not always available (Guan 2003, Akiyoshi, Nishida 1997, Pantelides, Barton 1993).

Qualitative modelling and reasoning were developed as an alternative to quantitative modelling and have been successfully applied to a wide range of disciplines (Bousson et al. 1998, de Jong, Page 2000, Druzovec, Sostar & Welzer 1998, Kiang, Hinkkanen & Whinston 1995). Qualitative models allow modellers to represent variables as entities with incomplete knowledge and deal with uncertainty. One advantage of this approach is that it enables modellers to concentrate on representing causal relationships between variables, leading to significant simplification of models. This approach also generates explanations about the causes of model behaviour more easily. However, despite the development of a range of qualitative modelling frameworks (Hinkkanen, Lang & Whinston 2003, Rebolledo 2006), qualitative models can present some interpretational issues (de Jong, Page 2000, Say 2002).

Significant research effort has been devoted to overcoming the problems and limitations of both quantitative and qualitative models. This has led to the development of hybrid modelling approaches which combine both qualitative and quantitative variables (Gasca, Ortega & Toro 2002, Nebot, Cellier & Vallverdu 1998, Cellier et al. 1996, Yadegar, Pishvaei 2005, Li, Wang 2001).

### ***3 Enterprise-wide modelling and optimisation.***

Enterprise-wide modelling and optimisation is research area that lies in the ‘interface of chemical engineering and operational research’ (Grossmann 2005, pp1846) and is now becoming of interest to researches in the process industries, as pressure to remain competitive in the global market place grows. In most general terms enterprise-wide optimisation involves optimising the operations of supply, manufacturing and distribution operations in a plant with respect to a particular cost function (Bandyopadhyay, Varghese & Bansal 2010).

From a process engineering point of view (Stephanopoulos, Han 1996) the supply, manufacturing and distribution activities fall in the category of process design and optimisation. These can include, for example, measuring the effects of process parameter changes on performance; optimisation using structural and parameter changes; analysing process interactions and optimal control for multi-product operations (Hangos, Cameron 2001).

From an operational research prospective, these activities come under the umbrella of decision support (in the shape of information management) and supply chain management (involving planning, scheduling, and inventory control). It can be seen that enterprise-wide control ('...the adjustment of available degrees of freedom (manipulated variables) to assist in achieving acceptable operation of the plant' (Larsson, Skogestad 2000, pp 212)) is one aspect of the optimisation procedure and therefore, procedures developed for enterprise-wide control (Ng, Stephanopoulos 1996) and fault detection (Kurtoglu, Tumer 2008) may be applicable when developing enterprise-wide optimisation models. Both process design optimisation and supply chain management analyses rely on the creation of accurate and comprehensive models which integrate information across the various stages that comprise the supply chain of a company (Signorile 2002).

Grossmann, (2005, pp1846), identifies two challenges posed by enterprise-wide optimisation: (the) 'need for development of sophisticated deterministic and stochastic linear/nonlinear optimisation models and algorithms' and 'the integrated and coordinated decision-making across the various functions in a company (purchasing, manufacturing, distribution, sales), across various geographically distributed organisations (vendors, facilities and markets), and across various levels of decision-making (strategic, tactical and operational).'

The challenges outlined above translate into the following modelling requirements:

- Multi-scale – the models developed need to incorporate components that operate of different timescales (from hours to months) and thus have different optimisation horizons (Varma et al. 2007). According to Grossmann, 2005, there is a need for novel decomposition procedures that can work effectively over large spatial (e.g. multi-site plants) and temporal (short, medium and long term optimisation) scales.
- Uncertainty – the models developed have to incorporate the uncertainty associated with market conditions and equipment (level of demand, equipment failure). It is unclear what the best approach for incorporating uncertainty at enterprise-wide level is.
- Complexity – enterprises are complex systems with a large number of integrated components (supply chain, manufacturing, planning) interacting with each other and the need for building and solving/analysis (non-linear) models capturing this complexity is essential to insure that enterprise-wide optimisation can be achieved.

Several papers have overviewed the various approaches taken to enterprise-wide optimisation from the point of view of process modelling and control, and supply chain management (Larsson, Skogestad 2000, Varma et al. 2007, Shah 2005). Other research has concentrated on applying industry-ready decision support tools or benchmark simulation tools to industrial case studies (Bezzo et al. 2004, Jeppsson et al. 2006, Nopens et al. 2009). This report will concentrate on identifying quantitative, qualitative and hybrid approaches to enterprise-wide modelling and optimisation, currently used by chemical, manufacturing and supply chain management and make recommendations for future research.

## **4 Quantitative approaches**

### **4.1 Linear programming**

The quantitative models most widely used in enterprise-wide optimisation are Mixed Integer Linear Programming (MILP) and Mixed Integer Non-Linear Programming (MINLP) formulations.

For example, Manenti & Manca (2009) combine a set point MILP approach for scheduling and planning with the moving horizon methodology typically used in model predictive control (MPC) by sequentially solving the enterprise-wide optimisation problem and successfully apply it to the management of steam supply during the start up of an air separation plant. Zhang & Zhu, 2006 demonstrate the development of MILP for optimising the performance of a chemical plant by using a decomposition method that splits the overall plant model into two levels-site level (master model) and process level (submodel). Savola & Fogelholm (2007) and Savola, Tveit & Fogelholm (2007) present a MINLP approach for modelling a small-scale combined heat and power plant and show that it is possible to find improved power designs that have higher efficiencies and that are profitable for wider ranges of electricity prices and fossil CO<sub>2</sub> emission permit prices.

Linear programming models have been used for cost evaluation of design change in distributed multi-plant collaborative manufacturing environment (Tseng, Kao & Huang 2008, 2009) and a production planning optimisation of a fluidised catalytic cracking unit (Wang et al. 2008).

The main drawback of this approach is that linear programming problems of the complexity to represent plant-wide structures and interactions require numerical, rather than analytical solutions and this can limit the predictive and analytical power of these models (Tseng, Kao & Huang 2008, Wang et al. 2008).

## **4.2 Dynamic simulation models**

Quantitative simulation models for decision support have mainly been applied in the area of supply chain management applications. Pitty et al. (2008) build a decision support tool, implemented as a simulator, called Integrated Refinery In-Silico (IRIS), in Matlab/Simulink, incorporating a dynamic simulation of a refinery supply chain, which integrates discrete supply chain activities and continuous production and demand management activities. Using a functional approach, the authors specify the relationships between different entities in the supply chain and are able to specify their behaviour over time as either deterministic or stochastic. The analytical power of their model is demonstrated using a variety of different scenarios involving decisions at both tactical and strategic level. Their decision support system has been applied to the problem of optimising supply chain design and operation for a refinery (Koo et al. 2008). Their results indicate that the proposed framework works well for supporting policy and investment decisions.

## **5 Qualitative approaches**

While quantitative approaches have long been considered superior in analysing in social sciences (management science, operations research), they have generally dealt with the problem of incomplete or imprecise knowledge by approximation of the problem under consideration (Kiang, Hinkkanen & Whinston 1995, Trave-Massuyes, Ironi & Dague 2003). Qualitative approaches on the other hand, model the causal relationships between entities as diagrams consisting of a set of nodes and their interconnections and thus fall under the general umbrella of structural modelling techniques (Dolado 1992).

### **5.1 Qualitative Reasoning**

Qualitative reasoning focuses on the use of qualitative representation of knowledge to reason about the everyday physical world (Kuipers 1994) and quantitative reasoning frameworks are normally “based on some sort of qualitative calculus and present a particular way of how to define qualitative operands and qualitative operations” (Hinkkanen, Lang & Whinston 2003, pp 380). In many cases the application of qualitative reasoning is preceded by the definition of a quantitative model of the system under consideration (Guan 2003, Akiyoshi, Nishida 1997, Fouche, Kuipers 1992). The qualitative reasoning modelling approach follows the same steps as a quantitative approach but at the model building phase the output is a set of qualitative differential equations (QDEs) instead of ordinary differential equations (ODEs). These are used to represent the relationships between the variables with incomplete knowledge qualitatively and as input constraints for the qualitative simulation model used for behaviour prediction. In some cases the qualitative simulation results are refined

used quantitative values. Direct comparisons between quantitative and qualitative simulation has shown that qualitative models produce the same range of outputs as quantitative models (Cellier et al. 1996, Zhang et al. 2006) but the mixed approaches behave like sampled-data control systems, exhibiting larger oscillation amplitude and a smaller oscillation frequency, compared to the purely quantitative simulation.

The qualitative reasoning approach has been applied successfully to complex problems in a number of disciplines such as biology (King, Garrett & Coghill 2005) medicine (Druzovec, Sostar & Welzer 1998) and engineering (Gasca, Ortega & Toro 2002, McDonnell 1990, Brandl, Wotawa 2008). Qualitative reasoning has also been used successfully in the supervision, diagnosis and monitoring of continuous chemical and biotechnological processes (Bousson et al. 1998, Tang, Zain & Rahman 2008, Hangos, Csaki & Jorgensen 1992, Lai, Yu 1995, Vianna, McGreavy 1995, Kitamura et al. 1996, Leyval, Montmain & Gentil 1994). The application of qualitative reasoning to industrial processes is well established and (Bourseau et al. 1995) offer an excellent survey of qualitative reasoning techniques and applications.

While integrated qualitative frameworks for modelling both discrete and continuous systems and their optimisation have been suggested (Hinkkanen, Lang & Whinston 2003), there are significantly fewer reported applications of qualitative reasoning to optimisation of business and management problems (Kiang, Hinkkanen & Whinston 1995, Ozutam 2007).

Despite its advantages as a modelling approach in presenting vague and uncertain information (Rebolledo 2006), some disadvantages of qualitative reasoning models have been identified. De Jong & Page (2000) report problems with model scalability for very complex systems, while Say (2002) show examples of problems with the feasibility and scope of the qualitative models. Problems with robustness and interpretability have also been identified and strategies for overcoming these have been suggested (Guglielmann, Ironi 2005) Despite these limitations, qualitative reasoning could provide a good foundation for enterprise-wide process modelling and this has been reflected in the wealth of hybrid approaches that have been developed.

## **5.2 Fuzzy Inductive Reasoning (FIR)**

While the basic paradigm for simulating uncertainty is through probabilistic representation (Uesbeck et al. 1998), in cases when insufficient information is available for building the probabilistic model, uncertainty can be represented by fuzzy intervals similar to the probabilistic model. Comparative studies have shown that simulation using fuzzy logic and probability density functions produce reasonably close results (Sevastjanov, Rog 2003). Fuzzy logic has been used, for example, in fuzzy differential inclusions (FDIs), which represent a fuzzy

extension to crisp differential equations. FDIs allow modellers to represent dynamic uncertainty within some specified limit and have been successfully applied to complex fuzzy systems in bio-medic and atmospheric cybernetics (Majumdar, Majumder 2004). Fuzzy interval representation has also been extended to Petri Nets (Loures, Pascal 2004, Sawhney, Mund & Chaitavatputtiporn 2003).

Fuzzy inductive reasoning (FIR) is a tool for general system analysis that has been developed to enable the study of conceptual models of behaviour of dynamical systems (Nebot, Cellier & Vallverdu 1998, Cellier et al. 1996) and is particularly well suited to modelling and simulation systems whose structure is partially or wholly unknown<sup>1</sup>. It is a qualitative methodology that is based on the observation of input/output behaviour of the system rather than on structural knowledge about its internal composition. The approach has two main tasks – to identify qualitative causal relationships between the variables in the model (using fuzzification (Stephanopoulos, Han 1996) and quantitative measurements of these variables) and to predict the future behaviour of the system (in terms of quantitative forecasts) (Nebot, Cellier & Vallverdu 1998).

Although there seem to be no reported applications of FIR models to enterprise-wide modelling, FIR has been successfully applied in modelling the dynamic behaviour of complex system such as the stock market (Tay, Linn 2001), closed ecosystems (Uhrmacher, Cellier & Frye 1997) and in medicine (Nebot, Cellier & Vallverdu 1998, Nebot, Cellier & Linkens 1996).

## **6 Hybrid approaches**

As suggested by the name hybrid approaches combine components of qualitative and quantitative methods in modelling processes. In doing so these methodologies allow the researcher “...to exploit the advantages of simulation models and reasoning techniques within a single system” (Fishwick et al. 1994, pp 1433). There are a number of different hybrid approaches, the most significant ones being systems dynamics and agent based modelling.

### **6.1 System Dynamics**

System dynamics is a structural modelling approach that used diagrammatic representation of the system under consideration in similar manner to qualitative reasoning but simulate them using quantitative rather than qualitative variables. In addition, system dynamics provides explicit facility for depicting feedback in the system and in recognition of the advantages in modelling feedback, attempts

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<sup>1</sup> For an alternative qualitative approach to system structure identification see Stolle & Bradley (1998).

for integrating qualitative simulation and systems dynamics for complex systems such as socio-economic models have been made (Dolado 1992).

System dynamics has been successfully applied to evaluate the effect of changes to enterprise resource planning systems (Tatari, Castro-Lacouture & Skibniewski 2008), integrated manufacturing and service networks (Viswanadham, Desai & Gaonkar 2005) and multi-echelon food supply chains (Georgiadis, Vlachos & Iakovou 2005).

Examples of the use of system dynamics for enterprise-wide modelling and simulation have been briefly summarised below.

Ben-Arieh & Grabill (2008) present a methodology for presenting a concise simulation of a manufacturing enterprise in a competitive market environment. The simulation takes into account the various levels of decision making (long, medium and short term) and process aggregation and presents a methodology for linking various components such as discrete event simulation, system dynamics, input aggregation and analytical simulation into a successful enterprise model. Their results show that the use of analytical and discrete event simulation minimises the computational intensity of the problem while maintaining a high level of realism in the model<sup>2</sup>.

Rabelo et al. (2005) propose a hybrid approach of discrete event simulation (DES) and system dynamics (SD) to a plant-wide simulation model of a semiconductor production enterprise and a sealer process plant. Their results suggest that the integrated hybrid model can be used to evaluate the impact of local decisions on the entire enterprise as well as the interactions of decisions made at various management levels. They conclude that the integration of DES and SD can provide a robust framework for enterprise-wide simulation. A similar conclusion is drawn by Venkateswaran & Son (2005) who apply system dynamics (SD) at the higher decision level and discrete event simulation (DES) at the lower decision level to model a hierarchical production planning architecture. The interface between the two levels is done using the exchange of eXtensible Markup Language (XML) based messages via High Level Architecture's (HLA) RunTime Infrastructure (RTI) and experimental results from a single-product manufacturing enterprise demonstrate the scope and validity of the approach.

An interesting approach for modelling manufacturing enterprises processes is suggested by Agyapong-Kodua, Ajaefobi & Weston (2009). They identify a number of public domain enterprise modelling architectures (e.g. CIMOSA (Computer Integrated Manufacturing Open System Architecture), PERA (Purdue Enterprise Reference Architecture)), methodologies and techniques and tools (such as the Architecture for Integrated Information Systems, the Generic

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<sup>2</sup> The system is currently under implementation and interested parties are invited to contact the corresponding author.

Enterprise Reference Architecture and GRAI-GIM framework and modelling tool developed by the University of Bordeaux). Their article demonstrates the use of CIMOSA for process decomposition in the case of a SME furniture manufacturer, in order to generate multi-perspective models of value streams. The modelling approach is enriched by the use of Causal Loop Diagrams (CLD) to analyse the dynamics of the manufacturing enterprise, although the intermediate steps taken are very unclear. There is significant scope for improvement in the process of integration between enterprise architecture modelling approaches used in enterprise engineering and causal simulation approaches.

Although system dynamics seems a good candidate for enterprise-wide process modelling and analysis at an empirical level, its effectiveness as a tool for evaluating the dynamic consistency of theoretical models needs to be developed (Wittenberg 1992).

## **6.2 Agent Based Modelling**

Agent-based modelling and simulation (ABMS) is an approach to modelling complex systems comprised of interacting autonomous agents (Behdani et al. 2009). In this approach a system is described by defining its actors (agents) and possible interactions between them. The system behaviour then emerges from the behaviour of the model components and their interactions. This allows for a bottom up approach distributed and decentralised systems.

Behdani et al. (2009) list the main agent characteristics as follows:

- Agents have a certain level of autonomy so they can take decisions without a central controller or commander.
- Agents are driven by a set of rules that determine their behaviour.
- Agents are capable of perceiving changes in their environment and acting in response to these changes
- Agents have proactive ability, which means having their own goals and acting to achieve them.
- Agents have social ability to communicate with each other.

A multi-plant enterprise is a modular, decentralized, changeable and complex system. It is heterogeneous and dynamics and its overall behaviour emerge from interactions from its components (departments) and therefore, agent based modelling can be used for enterprise-wide modelling and simulation. For example, Lim & Goh (1997) present a methodology for the development of evolutionary intelligent agents as tools for modelling a self-organising environment within a manufacturing firm and Behdani et al. (2009) demonstrate the use of agent based modelling using the Repast simulation platform to depict the interactions between a system comprising of a customer, a sales department, a multi-site production plant and a supplier. They identify coordination of local

optimisation goals and global optimisation goals and enhancing agent communication as one of the main challenges.

However, the majority of agent based simulations concentrate on the modelling and performance evaluation and optimisation of supply chains (see Signorile (2002) for several definitions of supply chains and a list of the pitfalls that can occur in supply chain management, such as inadequate or incomplete information, uncertainty, organisational barriers). Julka, Srinivasan & Karimi (2002, 2002) develop a flexible framework for agent based modelling of supply chains and demonstrate its application to the development of a decision support system for a refinery. Fox, Barbuceanu & Teigen (2000) discuss two issues associated with the design and application of agent based modelling to a supply chain – the choice of decomposition method and the coordination between components. They recommend an approach for building agents using re-usable components and give examples of the programming language that can be used and applications to a hypothetical and a real supply chain problems with complex structures. De Santa-Eulalia, Frayret & D'Amours (2008) address the difficulties associated with integration of simulation with distributed supply planning tools. Their paper proposes a conceptual framework for modelling “distributed agent-based Advanced Planning and Scheduling” (d-APS), while Signorile (2002) designs and implements a supply chain modelling tool using the ZUES simulation platform and analyse the impact of information sharing and coordination on supply chain performance.

Agent based modelling is a promising approach for dynamic simulation and behaviour analysis. A study by Van Dam et al. (2009) comparing the ease of specification, re-use, extendibility and interpretation of agent based (using the Repast agent platform) and equation based (using Matlab/Simulink) dynamic modelling of a refinery’s oil supply chain, highlights the strengths and weaknesses of each approach. The main problem with agent based modelling approach is that the causal relationships between model variables are not explicitly defined and thus may not be easy to analyse. This can possibly limit the usefulness of these models.

### **6.3 Other Hybrid Approaches**

Various other hybrid approaches, combining quantitative and qualitative components, have been proposed for modelling various complex systems (see Hsieh (2002) for a good overview).

A few examples of hybrid approaches include Chen & Sun (2000) who propose an integrated macroeconomic model (IMEM) with a combined quantitative-qualitative reasoning method to model the economy, Stylios & Groumpos (1998) who demonstrate the application of fuzzy cognitive maps (a combination of fuzzy logic and neural networks) to model a two tier manufacturing control system, and

Yadegar & Pishvaie (2005) who demonstrate the application of mixed qualitative/quantitative modelling techniques combining principal component analysis, along with clustered fuzzy diagraphs and reasoning to the modelling of a continuous stirred tank reactor and a distillation column. Gentil, Montmain & Combastel (2004) combine control theory (specifically the framework for fault detection and isolation), and causal modelling to identify a model based diagnostic approach for on-line process supervision involving human operators, while Hsieh (2002) suggests a new class of a hybrid model able to deal with significant uncertainty within a dynamical system and demonstrate its use in a hybrid approach for designing a multi-stage multi-buffer electronic devise assembly line. A utility cost function, which can be used to evaluate the appropriateness of alternative modelling approaches is also suggested.

## **Conclusions**

This report highlighted different quantitative, qualitative and hybrid modelling and simulation techniques that can be used for enterprise-wide modelling and simulation. The report identified the three main challenges posed by enterprise-wide modelling and simulation as: the complexity of the task, the inherent uncertainty of the environment enterprises operate in and the multi-scale nature of enterprises. This report found that quantitative modelling was least suited to dealing with very complex systems, although strengths of quantitative models lie in their tractability and inherent ability to produce results that are easy to interpret and analyse. Qualitative approaches, on the other hand, provide a convenient tool for modelling uncertainty and generalising complex systems, but generate results that are difficult to interpret. Hybrid approaches, counteracting some of the limitations of purely quantitative/qualitative modelling techniques, have been used for creating a variety of enterprise-wide models and simulations. Agent based modelling and systems dynamics are the two approaches that appear most suited to modelling complex, multi-scale systems such as a chemical plant, operating in an uncertain environment.

## **Recommendations for Future Work**

Despite their potential, agent based modelling and systems dynamics modelling approaches pose their own challenges. The main problem with the agent based modelling approach is that the causal relationships between model variables are not explicitly defined, and this may hinder the analysis of the results. While systems dynamics explicitly specifies the causal relationships between variables and overcomes this particular problem, this modelling approach encounters problem with model validation and transparency as the causal loop modelling framework is adopts is unstructured (Sterman 2000). One approach for dealing with this problem is to identify a suitable process decomposition framework that could be incorporated into the systems dynamics

methodology. For example, Ng & Stephanopoulos (1996) use a hierarchical framework for the development of a integrated multi-horizon, plant-wide control system of a chemical plant, which involves vertical decomposition of the control objectives at each aggregation level until the level with the shortest time-horizon of operation in the plant is reached. This methodology allows one to systemically identify the control objectives in the plant at the level at which they are most significant. Zhang & Zhu (2006) suggest alternative decomposition methods which splits the overall plant model is spit into two levels-site level (master model) and process level (submodel). The master model determines common issues such as raw material allocation and utilities, while the submodels optimise their performance on the basis of these determinations. The results of the submodel optimisations are fed back to the master model for further optimisation. Alternatively, some of the enterprise architecture frameworks suggested by Agyapong-Kodua, Ajaefobi & Weston (2009) may be better suited for chemical plant modelling. Although it has been recognised that interpreting the output from enterprise architecture modelling and using it in decision making is sometimes difficult (Johnson et al. 2007), this challenging and fascinating subject provides scope for further research and development.

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