CAPE SOFTWARE TOOLS FOR MODELLING AND SIMULATION

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Contents

Summary

This chapter presents an overview of dynamic process modelling and simulation techniques and tools with emphasis on their use and application in the Chemical Engineering field. Particular emphasis is placed on the development and validation of detailed process models under time varying conditions in typical Chemical Engineering processes including reaction systems, separation processes, crystallization plants, polymerisation processes, bioprocesses, fuel cells. etc. It is clearly illustrated that the ability to create new process models that can be used in a number of contexts within the Chemical process organisation means that it is possible to recover any investment in developing models many times over. Today, process models are increasingly embedded in customised interfaces and supplied to end users such as operations or purchasing personnel, who benefit from the use of model's power in providing advice for complex

decisions without having to know anything about the underlying technology. To assist this process, there is a growing body of high-fidelity models available commercially, and in equation form from university research and literature, as the fundamentals of complex processes become more and more reliably characterised.

1. Introduction

Process modelling has always been an important component of process design, from the conceptual synthesis of the process flowsheet, to the detailed design of specialised processing equipment such as advanced reaction and separation devices, and the design of their control systems. Recent years have witnessed the model-based approach being extended to the design of complex products, such as batteries, fuel cells and drug delivery systems, which can themselves be viewed as miniature plants produced in very large numbers. Inevitably, the modelling technology needed to fulfil the demands posed by such a diverse range of applications is very different from the standard steady-state flowsheeting packages that served the process industries so well in the past.

Mathematical process models are currently employed, directly or indirectly, for almost all aspects of plant design and operation. Model usage covers the entire process lifecycle, from designing the basic process itself to designing the plant and its control system, training the personnel who are responsible for operating it and detecting and diagnosing faults in its operation. Most early implementations of model-based techniques provided their own mechanisms for describing the underlying process models. Indeed, in some cases, the technique was inextricably intertwined with the model. A typical example is provided by steady-state flowsheeting packages based on the sequential modular approach, in which a model of each unit operation was coupled with mathematical solution methods for calculating the output streams of the unit given its inputs. Several factors have increasingly been providing strong incentives for moving away from this strong coupling between applications on one hand and process models on the other. It is well-known that the cost of developing and validating any non-trivial process model can be quite substantial, and this naturally leads to the desire to make the most of any such model by reusing it in as many applications as possible. Another factor is the difficulty and cost of developing sophisticated model building tools: it is far too wasteful to develop a credible modelling tool simply to use it for supporting a single application.

In recent years there has been an increased interest in the modelling and simulation of processes under time-varying or dynamic conditions. Sometimes this is an inherent part of the process design, as in batch processes or pressure swing adsorption; sometimes it is as a result of external disturbances, for example a change in feedstock or product grade, equipment failure, or regular operational changes such as the diurnal load variation of a power plant or the summer-winter operation of a refinery.

Many processes are intended to run and indeed appear to run at steady-state, and for practical purposes of design they can be modelled as such. However for inherently dynamic processes, or when considering transient aspects of otherwise 'steady-state' processes – for example, start-up, shutdown , depressurisation, and so on – steady-state

or pseudo-steady-state analysis is simply not applicable, or is at best a gross simplification. Such cases require dynamic process models.

By modelling the time-varying aspects of operation we are not simply 'adding another dimension' to steady-state models. There are many factors that, when considered as a whole, represent a step change beyond the philosophy and approach taken in traditional steady-state modelling.

There are of course many different levels of fidelity possible when creating dynamic models, but this chapter uses "dynamic process models" as a shorthand for high-fidelity predictive process models (which generally include dynamics) that typically combine chemical engineering first principles theory with observed, 'real-life' data. It looks at how these can be systematically applied to complex problems within industry to provide value in a whole range of process systems.

At the heart of the approaches described here is a family of methodologies that use models to perform many different tasks: not only to simulate and optimise process performance but to estimate the parameters used in the equations on which those simulations and optimisations are based; to analyse experimental data and even to design the experiments themselves. The methodologies also make it possible to move from relatively little experimental data collected in small-scale equipment to a high-fidelity predictive model of a complex and large-scale industrial unit or process.

As these methodologies are underpinned by a mathematical model, or series of mathematical models, they are known as model-based methodologies – in particular *model-based engineering* and *model-based innovation* and their supporting techniques of model-based data analysis, model-targeted experimentation and model-based experiment design. This chapter describes how these techniques can be systematically applied to create models that are capable of predicting behaviour over a wide range of conditions and scales of operation with unprecedented accuracy.

2. CAPE Modelling and Simulation Tools

Custom-modelling tools based on general-purpose, high-level, equation-oriented, declarative modelling languages are becoming the standard tools of the trade for the development and application of high-fidelity predictive models, particularly when full control over the scope and detail of the process model is required [2]. Such tools can support many of the activities essential for the effective dynamic process modelling that is the subject of this volume.

Since the mid-20th century, 50 years process simulation software for research and development. In 1958 the United States AI. W. Kellogg launched the world's first chemical process simulation program-Flexible Flowsheeting. After several decades of development process simulators reached a professional and commercial level including well known products such as ASPEN PLUS®, HYSYS, PRO® / II, gPROMS®, Design II®, ProSim®, DYNSIM®, Aspen Dynamics®, ECSS®, and so on.

Aspen Plus is a large general-purpose process simulation tool from the United States AspenTech company's products. World's leading chemical, petrochemical, oil refining and other process industry manufacturers and well-known engineering companies are Aspen Plus users. In practice, Aspen Plus can help engineers to easily build large-scale flowsheets, implement several operating procedure, perform detailed design studies, optimize the operation of industrial plants and perform a number of model-based engineering applications (:http://www.AspenTech.com/).

HYSYS was originally a product of the Canadian Hyprotech company. In 2002 AspenTech acquired Hyprotech and HYSYS became a product of AspenTech.. HYSYS is well known for its capabilities to perform safety analysis of industrial installations, implement control tools, perform analysis of the operation of an equipment identify production bottlenecks, determine safe start-up procedures, implement batch production safety issues, perform dynamic studies, etc. (website:http://www.AspenTech.com/Orhttp://www.HYSYS.com/.)

PRO / II is originally the United States SimSci-Esscor chemical process simulation tool, and currently under the INVERSYS Company. PRO / II can be widely used in a variety of petrochemical processes to perform rigorous mass and energy balance calculations, from the oil and gas separation to reactive distillation. PRO / II provides a comprehensive, effective and easy to use solution to these problems. It can be also used to perform steady-state simulation, physical properties calculation, equipment design, cost estimation / economic evaluation, environmental impact assessment and other calculations. The tools can can simulate the entire production plant, including pipes, valves to almost all the common unti operations, in oil and gas processing, oil refining, chemical, polymers, fine chemicals and pharmaceuticals, etc.

Processs Systems Enterprise Ltd (www.psenterprise.com) has developed a general process simulation tools, gPROMS (general Process Modelling Systems) which is characterized by the equation-based model building of any complex process. gPROMS features model equation editing, allows users to modify and enhance high fidelity models. It can be used to design any new process research and development as it illustrates unique capabilities of experimental design, parameter estimation, statistical analysis of data and advanced optimization techniques. The tool is particularly applicable to dynamic process modeling as well as to distributed models. gPROMS can facilitate the establishment of simulation training systems for production plants based on operators training, process control, safety analysis, etc. gPROMS has been widely used in the chemical industry, petrochemical, oil and gas processing, pulp and paper, food industry, pharmaceutical and biological processing industries. (http://www.psenterprise.com/ or http://www.gPROMS.com/).

Design II is a product of the United States WinSim Inc.'s. After nearly 30 years of development and improvement, Design II process simulation has become a pioneer of specific applications. Many Design II innovations, such as online Fortran and strict tower calculations have established a process simulation standards. (http://www.WinSim.com/).

ProSim company is headquartered in France, to provide simulation and optimization software to enhance industrial productivity and return on investment; for different sectors, such as chemical, oil refining, gas processing and specialty chemical industries, as well as the pharmaceutical, food, energy, etc. (:http://www.prosim.net/).

Aspen Dynamics is a product of AspenTech. It is built on a mature technologies, including complete set of unit operations and control model library. Batch process, semi-batch process and continuous process can be easily modelled using open and user-oriented modelling capabilities. The tool is integrated with Properties Plus to make accurate and reliable calculation of thermophycial properties, and steady-state simulation based on exactly the same basis. Aspen Dynamics can be easily used in the engineering design and operation of the entire process flowsheet, simulation of the dynamic characteristics of individual equipment thereby enhancing operating flexibility in the plant, ensuring production security, and investigate ways to increase capacity.

Among the above commercial general-purpose process simulation tool the most widely used by industrial and academic users are PRO / II, ASPEN PLUS, HYSYS, and gPROMS.

Therefore, this chapter presents a short overview of the above modelling tools

The historical background of these tools, the unit operations model library, Physical property systems, and other characteristics are summarised in Table 1.

Software Name	gPROMS	Aspen Plus	Hysys	PRO / II
Historical background	1997 as a spin-off product from Imperial College London	Originally developed at MIT, USA in 1981	Developed in 80s by the Canadian HyproTech	Developed by Simulation Science
Version of the product	PSE's V. 3.0	ASPENTECH Company V.2004	HONEYWELL / AspenTech Inc. V. 3.2	Invensys Company V.8.0
Unit Operation Model Library				
Three-phase flash	Available	Available	Available Free portfolio	Available
Multi-stage separation tower model	Available	Available		Available
Reactor model	Available	Available	Available	Available
Solid handling	Available	Available		Available
Physical Property calculations	Available gPROMS, g-SAFT, OLI, DIPPR,			

Number of pure compounds	Aspen Properties Plus and other	5941	More than 2000	More than 2000
VLE binary interaction coefficient	CAPE-OPEN properties database, user's own physical property data	40,000 Group	18,000	Group of more than 3000
Electrolyte system	Available	Available		Available

Table1 Basic capabilities of world know process simulation tools

2.1 Mathematical Formulation of Dynamic Process Models

Process systems under dynamic conditions are often most readily specified in terms of a mixed set of integral, partial differential and algebraic equations, or IPDAEs, and this is the chosen representation of most established software designed specifically for process systems engineering.

Traditionally, IPDAE systems are reduced into a mixed set of ordinary differential and algebraic equations, or DAEs. While ordinary differential equations (ODEs) typically arise from the conservation of fundamental quantities of nature, algebraic equations (AEs) result from processes where accumulation is not important or transients are considered to occur instantaneously, as well as by introduction of auxiliary relationships among variables.

Discontinuities in the governing phenomena of physical, chemical and biological systems frequently arise from thermodynamic, transport and flow transitions as well as structural changes in the control configuration.

While some of these transitions are intrinsically reversible and symmetric discontinuities, others are reversible and asymmetric or irreversible discontinuities. State-of-the-art languages incorporate powerful mechanisms to declare any type of transitions (for example, if-then-else and case constructs) which can be nested to an arbitrary depth.

A second class of discontinuities arises from external actions imposed by the surroundings on the system at a particular point in time, typically discrete manipulations and disturbances such as operating procedure or imposed failures.

The ability to incorporate complex sets of discontinuities describing a series of states in the formulation of a DAE system leads to the concept of state-task networks (STNs) [1]. Many, though not all, modern custom modelling tools are capable of solving complex problems involving arbitrarily complex combinations of DAE and STN systems.

In this chapter we are not concerned with the mathematics of dynamic modelling; this is well covered in the literature. The focus is rather on the practical and systematic application of the high-fidelity process models, using now well-established principles of model-based engineering, to add value to industrial operations.

3. Dynamic Process Modelling – Background & Basics

The state-of-the-art in process modelling has moved well beyond the 'material and energy accounting' exercises of steady-state flowsheeting applications (which nevertheless still represent a large proportion of process modelling activity) to become a central platform for capture and deployment of companies' Intellectual Property (IP).

A systematic modelling activity using high-fidelity predictive models provides a set of tools that enables companies to adapt – rapidly if necessary – to changing market drivers and gain competitive advantage. Models, if properly constructed, embody valuable corporate knowledge in such a way that it can be rapidly accessed and deployed to generate immediate commercial value. For example, during an economic downturn the models originally used to optimise equipment design can be rapidly redeployed with a different objective: reducing operating cost.

For example a model may be used to capture the definitive set of reaction kinetic relationships that may represent many years' worth of experimentation. This reaction network model can then be used as part of a reactor model to redesign the reaction process, or to adapt an operating process to improve its economics under new market conditions. The knowledge developed during the redesign or adaptation – for example, regarding the performance of alternative reactor internal configurations or catalyst formulations – is often valuable information in itself. This new information can be captured in the model for use in future analysis, or to form the basis of patent applications in support of licensed process development, and so on. It is possible in this way to enter a virtuous cycle where each use of the model generates information that increases its usefulness in the future; every subsequent activity increases the return on initial modelling investment.

3.1 Predictive Process Models

In order to describe modelling approach and practice, it is worth first defining what we mean by a 'process model'. For the purposes of this chapter a process model is considered to be *a set of mathematical relationships and data that describe the behaviour of a process system, capable of being implemented within a process modelling environment in such a way that they can be used to generate further knowledge about that system through simulation, optimisation and other related activities*.

To be more specific, a chemical engineering model – whether written in a programming language such as Fortran or C or a modern modelling language such as gPROMS language or Modellica – is typically a collection of physics, chemistry, engineering, operating and economic knowledge in equation form, coupled in some way with empirically-determined data.

To be useful in design and operational analysis, a model should have a *predictive capability* so that given, for example, a new set of feed or operating conditions or design parameters, it calculates accurate revised rates for the output values of interest.

At its best, a model is capable of predicting actual behaviour with accuracy over a wide range of conditions without refitting the model parameters, making it possible to explore the design or operational space comprehensively and be confident in the results.

In order to be predictive, a model needs to take into account all the phenomena that significantly affect the output values of interest, to the required degree of accuracy. For example, a model that includes very detailed reaction kinetic representation but ignores diffusion effects for a reaction that is severely diffusion-limited will not provide very useful results. Conversely there is little point in including detailed intra-pore diffusion effects in a catalytic reaction model when it is known that reactions are fast and occur largely on the catalyst surface; the unnecessary detail may increase calculation times and reduce model robustness for very little gain in accuracy. Generally, current practice is to construct 'fit-for-purpose' models wherever the modelling software environment allows this; in many cases these can be 'parameterised' in order easily to include or exclude phenomena.

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Biography Sketch

Michael C. Georgiadis is an Associate Professor in the Department of Chemical Engineering at Aristotle University of Thessaloniki, Greece and Honorary Senior Research Fellow, in the Centre for Process Systems Engineering at Imperial College London. He holds a first degree in Chemical Engineering from Aristotle University of Thessaloniki and a M.Sc. and PhD from Imperial College London. His research interests lie in the areas of computer-aided techniques for process modelling, simulation, design, optimisation and control. He has authored/co-authored over 60 journal publications and several books including a seven-volume book series on Process Systems Engineering published by WILEY-VCH. He has long experience in the management and participation of more than 20 collaborative research projects.