EQUATION-ORIENTED PROCESS MODELLING TECHNOLOGY: RECENT ADVANCES & CURRENT PERSPECTIVES

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INTRODUCTION

Model-based techniques have been playing an increasingly important role across the entire process lifecycle. Over the last decade, model-based applications have spanned the entire range from fundamental development of the process and its chemistry, to design of key equipment items, design of the plant and its control system, all the way to plant operations, troubleshooting and automation. A key element of technology required for supporting such a model-based approach to engineering and operations is “process flowsheeting” software that allows the correct and efficient construction of mathematical models of plants comprising multiple unit operations, often tightly coupled via multiple recycles of material and energy.

Key Elements of Process Flowsheeting Technology

Most process flowsheeting tools have in common certain technological components and features, including:

1. Libraries of models of standard unit operations
2. Physical property models describing behaviour of material
3. Solution methods for different types of computation based on the underlying plant models, such as steady-state and dynamic simulation and optimisation
4. User interfaces for constructing the flowsheet, specifying degrees of freedom, initial conditions etc., and reviewing and analysing the results.

In general, the precise content of the first two items above depends on the sectors of the process industries being addressed. For example, the oil & gas, refining and chemicals/petrochemicals sectors are dominated by fluid-based processing, while the pharmaceuticals and fine chemicals sectors have a strong element of solids processing. These differences are reflected in both the unit operations and physical property models that are included in the corresponding flowsheeting tools.

The Need for Custom Modelling

Even flowsheeting tools addressing the same process industry sector may differ in the degree of physical detail that is included in the model of a given unit operation. Moreover, no matter how comprehensive a tool’s model library is, it may not cover all unit operations of interest to any particular user to the required degree of detail. Consequently, mechanisms for extending the model libraries with user-defined unit operation models (often known as “custom modelling”) constitute another key element of process flowsheeting technology.

Albeit sometimes seen as a secondary consideration in process flowsheeting, custom modelling is actually central to the ability of user organisations to capture and exploit their proprietary knowledge and intellectual property. Using such models for key reaction and separation equipment instead of relying entirely on “black-box” models provided in standard libraries is often key to gaining competitive advantage from the investment in modelling technology.

Beyond Process Simulation

Traditionally, most of the emphasis in the use of process flowsheeting tools has been on steady-state simulation. A very large proportion of the application of such simulations in industrial practice is in trying to improve some aspect (e.g. economic performance) of the plant’s design or operation by varying the available design and operating decisions ("degrees of freedom") while ensuring that key constraints on safety, operability, environmental impact etc. are satisfied. In practice, this has often translated into the user performing multiple trial-and-error simulations which, especially in cases involving more than a few decision variables, are both time-consuming and error prone, without any guarantee of obtaining an optimal solution or even one that satisfies all important constraints. A more effective approach is to directly apply rigorous mathematical optimisation techniques to the underlying plant model, allowing a sophisticated mathematical algorithm to automatically explore the available decision space.

PROCESS FLOWSHEETING

Starting with academic research in the 1960s and 1970s, two main competing approaches to process flowsheeting tools emerged, namely sequential modular (SM) and equation oriented (EO). We review these briefly below.

The Sequential Modular (SM) Approach

In the SM approach, each unit operation model is represented by a "module", i.e. computer code that, given the input streams to the unit and relevant equipment specifications, solves the underlying model equations to determine the output streams and other Key Performance Indicators (KPIs) relating to the unit's design and operation. Usually manually coded, these modules often incorporate algorithms tailored to the specific equations being solved, thereby achieving a very high degree of robustness and efficiency within each individual module. They can also expose highly customised user interfaces (e.g. dialogs for the specification of the information relevant to this module, or reports for the display of the corresponding results).

Most SM tools provide extensive libraries of unit operation models. They also support mechanisms allowing these libraries to be extended by the addition of new user-defined unit operations. In most cases, this involves the user providing a corresponding module which incorporates both the model equations and an appropriate solution method. The module is typically coded in procedural computer languages such as FORTRAN, C/C++, or Visual Basic. For the module to be usable within a specific SM flowsheeting tool, it would also need to expose a software interface conforming to that tool's proprietary Applications Programming Interface. A more recent development is the emergence of the CAPE-OPEN standard which defines a standardised interface between Process Modelling Environments (i.e. flowsheeting tools in this case) and Process Modelling Components (such as unit operation modules). Modules exposing a CAPE-OPEN Unit Operation interface can be used directly within any flowsheeting tool that supports the CAPE-OPEN standard; this includes all major commercially-available tools.

In the SM approach, the flowsheeting tool attempts to solve the overall flowsheet model by calling the individual unit operation modules in sequence. This is straightforward for processes without recycles where the process input streams and the equipment parameters are fully specified: in this case, the process model can be solved by tracing a path from raw materials to process products, and calling each unit operation module along this path exactly once.

The simple "once-through calculation" described above is not possible in processes with recycles of material and/or energy. In such cases, the recycle streams need to be guessed ("torn") and the flowsheeting tool calls the unit operations along the recycle to obtain new values of these recycles. This is repeated in an iterative manner until the values of these streams converge. Mathematically, this corresponds to a successive substitution approach that may take many iterations to converge even when starting from a reasonable set of recycle guesses. This problem typically becomes more acute in processes with multiple interacting recycles; and in some cases the iterations may fail because the mathematical conditions for convergence of successive substitution are not satisfied irrespective of the quality of the initial guesses.

Another challenge for SM technology is the handling of non-standard specifications where it is desired to specify some aspect relating to the product streams or the overall process KPIs (e.g. overall raw material conversion), and to compute some aspects of equipment design or operation (e.g. reactor volume). This is problematic as the required information flow is opposite to the fixed input-output structure of the individual modules. The common way of dealing with these specifications is via the introduction of artificial "controllers" that attempt to automatically adjust the values of the computed variables so as to match the user specifications. However, this introduces additional recycles of information that need to be handled in a manner similar to that described above for material and energy recycles.

As mentioned above, the use of rigorous mathematical optimisation techniques in conjunction with process flowsheeting can lead to significant benefits over multiple trial-and-error simulations in terms of both the quality of the solutions obtained and the effort and time required to obtain them. However, the robustness and efficiency of numerical optimisation algorithms depend crucially on the availability of the gradients of the objective function and constraints with respect to the decision variables. In the context of the SM approach, obtaining these gradients would require all unit operation modules to return the partial derivatives of their outputs with respect to their inputs, something which would imply a substantial increase in coding complexity. As a result, the use of SM technology for plant optimisation calculations has been somewhat limited in practice.

The Equation Oriented (EO) Approach

The EO approach is conceptually much simpler than the SM one. Given a mathematical model of each unit operation in the flowsheet in terms of a set of equations and variables, the overall plant model can be formulated simply by assembling the contributions of all unit operations, together with unit-unit connectivity relations, into one large system of equations[1]. Once the user specifies a valid set of degrees of freedom to leave a non-singular square system of nonlinear algebraic equations, the latter is solved simultaneously via an appropriate numerical method, such as those based on Newton's method and its variants, coupled with sparse linear algebra techniques. With modern algorithms and computer hardware, solution of systems of many hundreds of thousands of equations is practically feasible using ordinary desktop computers.

In principle, EO technology can address many of the limitations of the SM approach described in the previous sections. For example, handling multiple interacting recycles is more efficient as all relevant interactions are taken into account within the single system of equations. No special mechanisms are necessary for handling of non-standard specifications provided they also lead to square non-singular systems.

Moreover, extending the model library with a new unit operation model involves only defining the corresponding model equations; the solution of these equations is handled at the level of the flowsheeting tool. This opens the way for the use of "declarative" custom model definition languages which allow new models to be defined in high-level symbolic form rather than in terms of computer code, something which greatly increases the ease and reduces the cost of both model development and model maintenance. The availability of the model equations in symbolic form also facilitates complex operations such as symbolic differentiation for obtaining partial derivative information, which significantly enhances the performance of the solution algorithms, both for simulation and optimisation.

The main limitation of EO technology has been the robustness of solution process. This is particularly important at the initial stages of modelling, when the values of the model variables are largely unknown and any initial guesses may be far away from the solution. Being only locally convergent, Newton-type methods are particularly prone to failure at this "model initialisation" stage. Attempts to address this problem either by extending the Newton convergence range using stabilisation techniques or by using alternative solution approaches such as those based on homotopy-continuation methods, have been only moderately successful. Moreover, given the size of the system of equations being solved, it is often difficult to locate the causes of a simulation failure, even when these are associated with errors in user specifications or user-provided models.

Commercial Flowsheeting Tools

Partly because of the perceived advantages in terms of robustness and usability, and partly because of the relative ease of its implementation, the SM approach has been the one adopted by most commercial steady-state flowsheeting tools, such as Aspen Plus® (Aspen Technology Inc.), Aspen HYSYS® (Aspen Technology Inc.), Petro-SIM® (KBC Advanced Technologies plc.), PRO/II® (Schneider Electric SimSci) and UniSim® (Honeywell Inc.).

The implementation of "industrial-strength" EO technology is technically much more challenging, mainly because of the underlying complexity of the software architecture and the mathematical solvers. The commercial availability of this approach has been limited to relatively few tools. The latter include Aspen Custom Modeler® (Aspen Technology Inc.), an evolution of SPEEDUP®, a first-generation EO tool originally developed at Imperial College London [Pantelides, 1988]; and gPROMS ModelBuilder®

[1] The latter may also include calls to external code, e.g. for the computation of physical properties using standard packages.

(Process Systems Enterprise Ltd.), based on the gPROMS second-generation EO modelling platform originally also developed at Imperial College London [Barton and Pantelides, 1994; Oh and Pantelides, 1996], and subsequently substantially re-architected and re-written at PSE. A key focus of all these tools has been on supporting custom model development, especially in the area of detailed models of process equipment (e.g. reactors).

Despite its more limited adoption, the potential advantages of EO technology are well understood and have led to the incorporation of some elements of EO technology within SM tools such as Aspen Plus where some of the unit operation models have both SM and EO modes, and also custom models can be built using the Aspen Custom Modeler. Tools used for real-time optimisation, such as ROMeo® (Schneider Electric SimSci) are also based on the EO approach. However, the emergence of a "true" EO flowsheeting tool that can achieve the full potential afforded by the EO approach requires addressing the fundamental problem of model initialisation.

THE gPROMS MODELLING PLATFORM

The gPROMS platform provides a comprehensive environment for the development of process models. The latter's mathematical complexity can vary from simple sets of nonlinear algebraic equations models of lumped steady-state systems, to mixed sets of integral, partial and ordinary differential and algebraic equations (IPDAEs) describing systems distributed over time and 1, 2, 3 or more spatial and other dimensions, all described in a high-level declarative language. The tool also allows the definition of the model's user interface (e.g. specification dialogs, results reports, documentation etc.) in a purely declarative faction, without the need for computer programming.

Models of complex systems (e.g. process plants) can be constructed hierarchically from lower-level ones (e.g. unit operations) via standard drag-and-drop flowsheeting interfaces. gPROMS also supports the formal validation of models against experimental data, and provides state-of-the-art methods combining symbolic, structural and numerical techniques for the solution of large-scale simulation and optimisation problems, both at steady state and in transient (dynamic) regime.

Over the past decade, Process Systems Enterprise (PSE) has undertaken an extensive internal R&D programme aimed at addressing the robustness issues associated with the use of EO technology in the process flowsheeting context. This has resulted in the development of the novel concept of Model Initialisation Procedures (MIPs) operating at both the unit and the flowsheet levels. A unit-level MIP (U-MIP) is simply a sequence of two or more models of a particular unit operation, such that (a) the first model in the sequence is one which is easy to solve even from poor initial guesses, and (b) the last model corresponds to the actual unit operation model. For example, for a complex non-adiabatic non-isothermal reactor model with axial and radial variations of temperature and composition, the U-MIP sequence could comprise 3 models of increasing complexity, e.g. (a) a model with no reaction taking place; (b) a model with reaction taking place at a specified temperature; and (c) the final reactor model with the full energy balance equations. In general terms, initialising the reactor model could be achieved by solving the three models in the order (a) → (b) → (c). A comprehensive mechanism for allowing developers of unit operation model libraries to specify U-MIPs in a straightforward and purely declarative fashion was devised and implemented in the gPROMS platform, together with proprietary algorithms for maximising the robustness of moving along the trajectory defined by the U-MIP.

U-MIPs are designed to ensure robust solution of any individual unit operation model. Flowsheet-level MIPs (F-MIPs) are essentially a set of mathematical algorithms for combining U-MIPs to allow the reliable and efficient convergence of entire flowsheets. F-MIPs are implemented entirely within the gPROMS platform and operate transparently to both the developers of unit operation models and the end-users of the flowsheeting tool.

By allowing robust solution of steady-state simulation calculations with little or no user intervention, MIPs represent a fundamental breakthrough in EO flowsheeting, addressing its main disadvantage in comparison with SM technology while retaining all its inherent advantages, including handling of flowsheets with multiple interacting recycles of material and energy, handling of non-standard specifications, and straightforward extendibility via fully integrated custom modelling. The latter is particularly important for developing and delivering enhanced model libraries comprising a wider range of unit operation models. Moreover, once an initial converged steady-state solution for a flowsheet is available, it can form the starting point for more complex calculations, such as dynamic simulation or optimisation.

THE gPROMS PROCESSBUILDER

The deployment of MIPs within the most recent versions of the gPROMS platform has allowed the development of the gPROMS ProcessBuilder, the first truly-EO general-purpose tool for steady-state and dynamic flowsheeting.

The ProcessBuilder includes a set of model libraries of commonly occurring unit operations, encompassing those available in commercial SM flowsheeting tools but extended both in scope (e.g. via the inclusion of less common operations such as periodic adsorption and membrane processes, and a comprehensive library of process control elements) and in degree of modelling detail (e.g. tubular reactor models ranging from simple homogeneous models to heterogeneous models with axial, radial and intraparticle variations; and distillation and absorption models ranging from tray-by-tray models based on standard phase equilibrium assumptions to packed bed models for reactive distillation/absorption, with properties varying both axially and within the films at the liquid/vapour interface).

In addition to its own model libraries, ProcessBuilder provides the full power of custom modelling afforded by the gPROMS platform. This allows users and third-party specialist model suppliers to develop and maintain proprietary models and model libraries that can be deployed and used in conjunction with the standard libraries. One particularly important aspect in this context is the protection of the proprietary intellectual property that is embedded within such models.

In addition to plant equipment modelling, ProcessBuilder also aims to cover a wide range of material behaviour, including mixtures with highly polar compounds, molecules exhibiting strong association interactions via hydrogen bonding, and polymers. Therefore, in addition to the standard thermodynamic models (e.g. based on cubic equations of state and activity coefficient models), ProcessBuilder incorporates two state-of-the-art models based on the Statistical Associating Fluid Theory (SAFT), namely the SAFT-VR SW model [Gil-Villegas et al.,1997] based on molecular interactions, and the group contribution-based SAFT-γ Mie model [Papaioannou et al., 2014]. Because of their foundation on fundamental intermolecular interactions, such models offer superior predictive accuracy over wider ranges of operating conditions compared to more conventional approaches. However, until recently, the associated computational cost made their application to process flowsheeting problematic in all but the simplest cases. The gSAFT implementation deployed in ProcessBuilder incorporates several advanced developments in applied mathematics and numerical methods to overcome this issue.

The models in ProcessBuilder are designed to support the entire workflow, from basic mass and energy balances, to steady-state sizing calculations to dynamic simulation. In contrast to earlier EO technologies (see, for example, [Pantelides, 1988]) which always attempted to solve essentially the full set of equations and variables under all circumstances, ProcessBuilder automatically determines and solves the minimal subset of the model that is necessary to address the problem being posed by the user at any particular point in the workflow, thus resulting in significantly enhanced efficiency and robustness.

Taken together, the above technological advances result in substantial gains in robustness and efficiency. As an example, Figure 1 shows an integrated air separation unit, a process involving three tightly integrated distillation columns. The initial solution of this model in ProcessBuilder starting with no user-provided initial guesses is accomplished within 35 CPUs on a standard desktop workstation; subsequent sensitivity calculations take 0.5 CPUs each. These execution times are 1-2 orders of magnitude smaller than those typically observed when SM technology is applied to the same flowsheet.

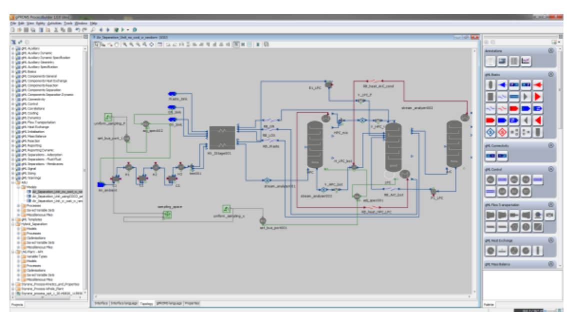

Figure 1: Integrated Air Separation Unit model in the gPROMS ProcessBuilder

The much faster solution times afforded by EO technology are welcome in their own right, but more importantly, they open the door to a wide range of advanced applications that have not been feasible in the past. For example, ProcessBuilder takes full advantage of the optimisation capabilities in the gPROMS platform, which makes it possible to apply rigorous optimisation to the design and operation of individual unit operations (e.g. reactors or distillation columns), plant sections (e.g. multiple distillation column sequences) or entire plants integrating reaction, separation and utility sections. For example, the model of the olefins plant shown in Figure 2 incorporates a detailed model of the cracking furnace, tray-by-tray models of the various distillation columns and a model of the various refrigeration cycles.

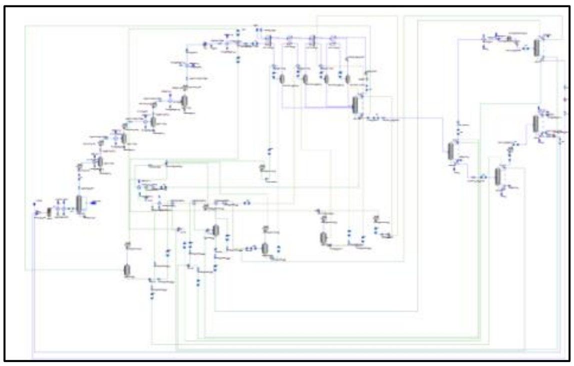

Figure 2: gPROMS ProcessBuilder model of olefin plant integrating hot and cold sections, including refrigeration cycles

One notable feature in this context is the ability to handle both continuous and discrete decisions; the latter may include aspects such as the numbers of trays and the feed locations in distillation columns, the heat integration between different units (e.g. column reboilers and condensers), or indeed the existence of some units in the flowsheet. A good demonstration of the potential benefits of applying this type of new technology to whole-plant optimisation was provided by a case study relating to the design of a new process for propylene oxide production by REPSOL [Martín-Rodríguez et al., 2010]. The cost savings between the initial design and the fully optimised solution were reported to be of the order of tens of millions of euros per annum.

CONCLUSIONS

Process flowsheeting plays a central tool in model-based process design and operations throughout the major sectors of the process industries. The relative advantages and disadvantages of the SM and EO approaches to process flowsheeting have been widely understood and accepted for the best part of three decades. The general consensus during this period has been that, whilst the EO approach is potentially much more powerful in terms of the scope of problems that could be addressed, only the SM approach was capable of providing the degree of robustness that is necessary to support wide deployment of these tools.

However, recent technological developments in EO technology, especially in the area of model initialisation procedures but also in the enhanced usability of the software tools, are leading to significant changes in the relative balance between the two approaches. This opens the way for the power of EO flowsheeting to be made available to a much wider range of process industry users than has hitherto been possible.

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