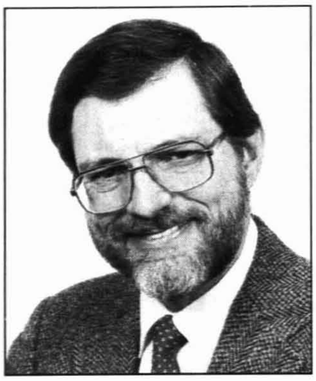
Process Simulation - A Valuable and Essential Tool for the Chemical Process Industries



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An expert on modeling and simulation of distillation systems, Boston has more than 10 years experience in the development and marketing of engineering software in the process industry. Among the organisations he has workedfor in this field are Union Carbide, Monsanto and Bechtel.

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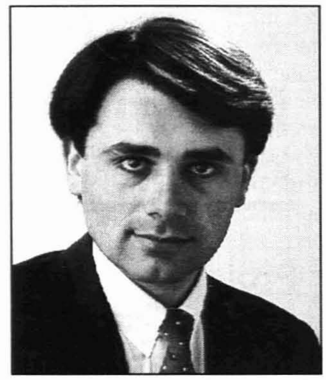

Process modeling and simulation has already proven to be an engineering tool which can help companies achieve improved business results. Advances in the technology behind such systems have made them more accurate and more applicable for a wider array of processes. At the same time, improvements in user interfaces have made simulators easier to use, making them accessible to a broader community of engineers.

Today, the process industries are facing two major challenges: increased competition and the need for greater innovation. Competitive pressures have intensified as the industry has become completely global in scope. Competitors will seek to exploit every advantage, whether it is from a better raw materials position, better technology, or better access to markets. Also, as the commodity products segment of the business has faced severe price competition, companies are racing to bring out new products with a high value in use. This leads to a need for greater innovation.

Process modeling plays an important role in responding to both of these challenges. By enabling engineers to systematically study a wider range of viable options quickly, simulation is helping companies to achieve improved economic results. Examples of how companies are using process modeling include:

- **Saving Time in the Redesign of Processes**

A fine chemicals company producing large quantities of dye applied single-stage reverse osmosis to purify effluents. In order to meet new environmental regulations, additional osmosis modules were required. Engineering needed to reconfigure the production process so that the module investment was minimized while the effluent purification standards were attained under various conditions.

To avoid the time and expense needed to test in a pilot plant, a process model was used to simulate the candidate configurations and to compare performance and economics.

The optimum configuration was decided on in two weeks, saving five and a half months of engineering resources valued at $ 50.000,— and avoiding a loss in production and customer shipment delays. And no governmental fines were levied, as the environmental regulations were met on schedule.

- **Reverse Engineering a Competitor's Process**

A competitor of a fine chemicals company filed a patent which claimed a 20 % improvement in product efficiency, thereby reducing both production costs and waste water pollution. The general manager wanted to know if the claim was justified, and if so, how his company could match it without violating the patent. The obstacle was the difficulty in translating patent data into a detailed understanding of a competitor's process.

Research and development built a model of the competitor's process using simulation, and confirmed, in theory, that the claim could be achieved. Using the model, the company succeeded in identifying the changes to their own process which achieved close to a 20 % improvement without violating the patent.

The chemical company was able to match their competitor's action. Modeling enabled them to react months sooner, saving significant market share.

- **Improving the Efficiency of Distillation Column Operations to Increase Production**

A flavor and fragrance chemicals plant of a major fine chemicals company needed to increase the volume of one of the company's flavorants. The higher volumes were displacing the batch column capacity of other products, and created added incentive to improve operations. The plant manager wanted to increase the flavorants' profit margin through more efficient operation of the distillation column.

The manager was uncertain how changes in the operating conditions would affect costs and quality.

By simulating the actual operating steps involved in purifying the product using simulation, the manager was able to evaluate alternative operating strategies. An improvement in the profit margin worth $ 600.000,— was achieved in the first year.

Process Simulation is in use in many of the leading process industry companies worldwide. Companies in the business of chemicals and petrochemicals, pharmaceuticals, petroleum refining, synthetic fuels, power generation, metals and minerals, pulp and paper, and food are prime users of simulation. More and more practicing chemical engineers in these companies have studied and done research related to modeling and simulation in their undergraduate, graduate and doctorate programs. These engineers belong to professional organizations, such as the CAST division of the American Institute of Chemical Engineers and the European Federation of Chemical Engineers, where advances in process modeling and simulation technology are discussed and new applications are introduced.

The latest developments in the area of process simulation have been recently discussed during the ComChem '90, the European Symposium on Computer Applications in Chemical Engineering held in May this year in The Hague.

Why Has Computer Simulation Become Standard Practice

In all phases of a typical process life cycle, simulation reduces engineering resource requirements and enables engineers to find better solutions in shorter times. For instance, in research and development, simulation is used to study alternate processing schemes, to scale-up the process, and to interpret pilot plant data. For the design of a new plant, models are used to optimize the design and reduce capital and operating costs. For an existing plant, simulation is used to improve the operation, to reduce raw materials and energy requirements and to debottleneck the process.

In design, once the decision has been made to build a new plant or to modernize an existing plant, a simulator can be used to study trade-offs, to investigate off-design operation, and to investigate the flexibility of the plant to handle a range of feedstocks. Simulation studies during process design can help engineers identify ways to avoid costly mistakes before committing to plant hardware. Process engineers can use a simulation model to optimize the design of the process by performing a series of case studies to ensure that the plant will work properly under a wide range of operating conditions.

For an existing plant, a simulation model can serve as a powerful tool for plant engineers to improve plant operations, to improve yield and throughput, and to reduce energy use. The model can be used to determine changes in operating conditions needed to accommodate changes in feedstocks, changes in product requirements, and changes in productivity. Finally, the model can be used to study possible plant modifications for »debottlenecking« or for revamping the plant to incorporate technology advances such as an improved catalyst, a new solvent, or a new process unit.

These all translate into big economic savings from bringing new products to market faster, from designing plants that require less capital investment and cost less to operate, and from reducing manufacturing costs in existing facilities.

What is Process Simulation?

Process simulation is based upon a »model« which is a mathematical representation of a production process. Input to the model consists of information normally contained in the process flowsheet: The chemical components, the feed stream compositions and flows, unit operations and operating conditions, and how the unit operations connect to each other. The simulation then predicts the performance of the plant by computing the flows and properties of all intermediate and product streams, the performance of every unit in the process, and the capital and operating costs of the plant.

The key to building a reliable model of a process is to mathematically describe the chemical and physical processes occurring in each step and to calculate the material and energy balances. These mathematical descriptions involve systems of nonlinear algebraic equations and, in some cases, such as a packed bed reactor, nonlinear ordinary differential equations. Nonlinear algebraic equations are also derived from the mass and energy balances around unit operation models. Each component in each unit is considered. In some cases momentum balance equations may be included to model pressure drops. Large simulations can contain many thousand equations altogether, though the system of equations is usually rather sparse in form because the flow usually goes from one unit to another, or because stages inside a unit usually affect only their adjacent stages.

The degree of rigor, and hence accuracy, of a simulation model is strongly affected by the representation of the thermophysical properties, such as heat capacities, fugacities, densities, and viscosities. Mathematical models which express the dependence of these properties on temperature, pressure

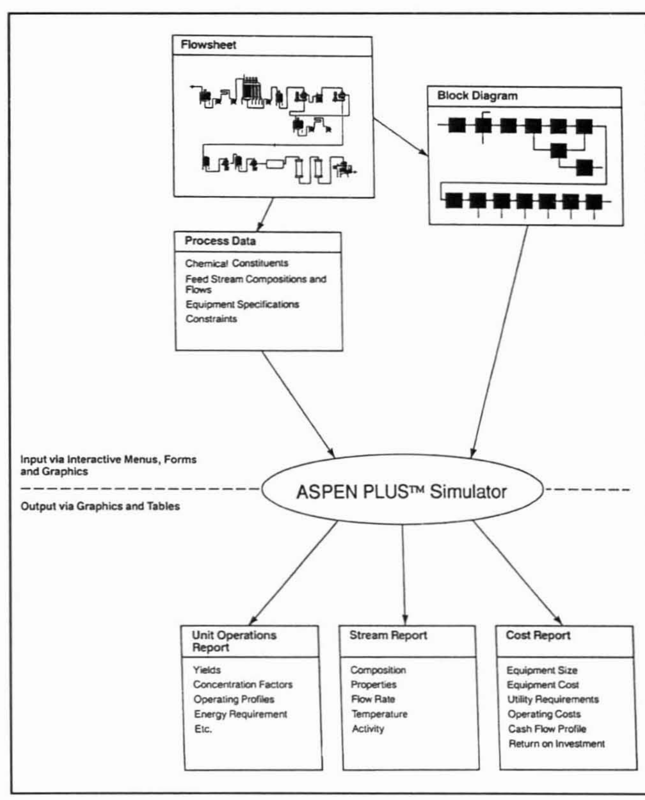

Figure 1: Flow of information in a simulation run

and composition usually contain highly nonlinear terms, and may also occupy the largest share of computing time for simulation, as much as 75 - 90 %.

The flow of information during the modeling of a process is illustraded in Figure 1. The starting point for developing a process model is the process flowsheet. From this, the engineer prepares a block diagram of all unit operations, feed streams, and waste streams. For each unit block, the engineer chooses the type of model required to represent the corresponding unit operation, e.g. out of the library of unit operation models included in AspenTech's commercial simulator ASPEN PLUS™. The next step is to specify the process's chemical components, the feed streams, and the method for calculating physical properties, and the data to be used in the simulation. The last step is to specify specific design requirements and operating conditions for each unit-operation block.

As input tool an engineer-oriented input language can then be written to provide the problem description as input to the computer, and specify the values of the operating parameters. The most advanced process simulators have a built-in user-friendly expert system which guides engineers step-by-step through the creation and use of such process models supported by graphics, pull down menus and a mouse (e.g. Model-Manager™).

After the problem is defined for the simulator, it then produces a report predicting process performance, including the composition and properties of all streams and the size and performance of the individual process units. Once a base has been prepared, the simulator can then help perform »what if« studies, sensibility analyses, and automatic optimization.

The example in Figure 2 shows how simulation can be used to model the performance of a single piece of equipment and to analyse and interpret this unit operation, e.g. interpret fermentation pilot plant data to make a new antibiotic. In this example, the engineer uses the model to estimate values of kinetic parameters for cell growth and product formation that best match the data. Then the model is used to study the effect of alternative glucose feeding schedules on productivity.

Process simulation can also provide a fast, cost-effective method for estimating capital and operating costs and evaluating process economics, from design and development through plant construction and economics. A comprehensive simulation costing and economic evaluation capability needs two kinds of data to build the total capital cost estimate - the purchased cost of major equipment items and factors that are applied to the equipment costs. One set of factors is used to develop the installed equipment cost estimates and then another set is used to develop the total capital cost estimate. Capital costs are then combined with operating costs, product prices, and raw material costs to estimate the profitability of the project.

Purchased equipment costs, which depend primarily on simulation results and materials of construction, can be estimated from in-house correlations, literature correlations, or, more accurately, determined from actual vendor catalog prices or fabrication schedules. The latter method is incorporated in the Price and Delivery Quoting Service (from PDQ $ of Gatesville, OH) which is used in ASPEN PLUS™. PDQ $ costs are updated on a regular basis to reflect price and labor and material cost changes. Between updates, costs are adjusted using standard indexes such as the Chemical Engineering Equipment Index.

The Roots of Process Simulation

About thirty years ago, the first process simulator was developed. In 1958, the MW Kellogg Company announced the introduction in its company of a program called the Flexible Flowsheet. The date marks the beginning of the era of computer modeling of integrated processes. Actually, the concept had sprung up independently in many different companies and in different countries at about the same time.

Since these first programs were introduced, the industry has seen three levels of simulators, in what is sometimes referred to as first, second, and third generation, determined by the capabilities available.

The second generation followed in the late 1960s. In-house data banks were usually employed to provide an extensive collection of physical properties, and better numerical methods were used for convergence of recycle streams. Still, the systems were usually limited to vapor and liquid phases, fixed-array data structures, and fixed list input data methods.

Second generation simulators are well used in the petrochemical, the chemical or the petroleum industry.

The most advanced simulators are considered to be third generation. These simulators can characterize the more difficult materials such as coal, bauxite ore, corn starch, woodpulp and others that have variable properties depending upon certain characteristic analyses. They have the ability to carry, in a stream, information about different attributes of solids or other components that can be used to determine thermophysical properties and for calculation of unit operations. The information may be variable in length and of arbitrary structure. In addition,

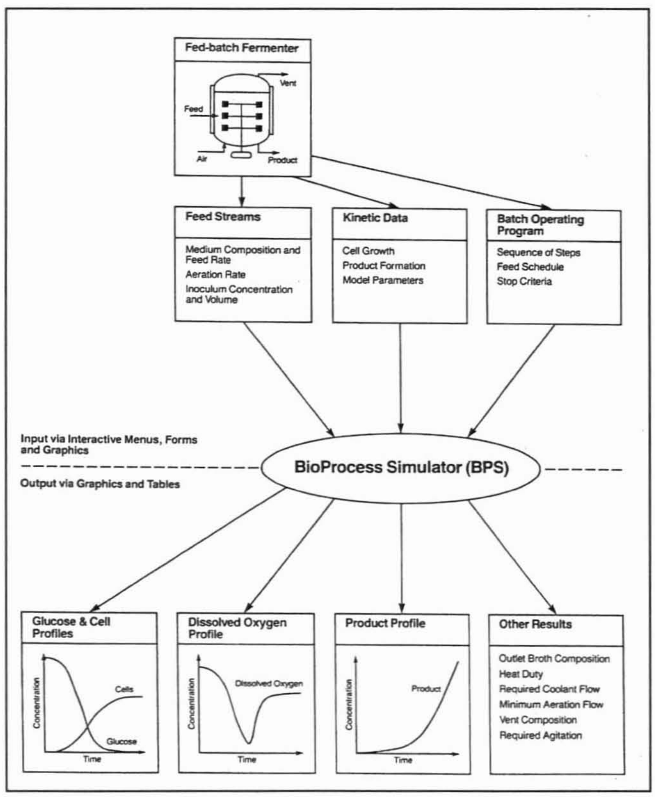

Figure 2: Use of simulation to study a single unit operation

the attributes of the stream can consist of information such as particle size distribution. In order to accommodate the variable nature of certain solids, the user is able to specify the structure of all stream information. Unit operation models for solids are also provided, such as cyclone separators, crushers and grinders, screens, hydroclones, filters, and electrostatic precipitators.

Other important characteristics of third generation simulators are listed below:

- The ability to handle electrolytes as readily as non-electrolyte liquids throughout the flowsheet.
- Preliminary sizing, costing and economic evaluation calculations, integrated with the heat and material balance calculations, so that the engineer can perform analyses in terms of economic results as well as process results. This greatly facilitates trade-off studies and optimization.
- A library of chemical reactor models to enable a wide range of reactor types to be modeled rigorously.
- The ability to handle multiphase equilibrium simultaneously with chemical reactions.
- The ability to perform multistage, multicomponent separation calculations (distillation, absorption, extraction, etc.) for all types of mixtures and all types of columns, including columns with two liquid phases or with equilibrium- or kinetics-controlled chemical reactions.
- Large thermophysical property model libraries, including both state-of-the-art equations of state and activity coefficient models.
- Large thermophysical property data banks containing basic data for upwards of 1500 compounds.
- In-line FORTRAN and user-model interfaces, to enable a user to accomplish simulation tasks that are unusual or unique to the user's company.
- Sophisticated mathematical methods to promoteconvergence of iterative calculations, both within individual models and for the overall flowsheet.
- A generalized optimization capability that enables a process to be optimized as easily - or nearly as easily - as it can be simulated.

How to Choose a Process Simulation System

Most companies find it most cost-effective to purchase a generalized commercial simulator and customize it to their individual production processes through a high level input language. Simulation software is currently available in a variety of hardware platforms - from mainframe computers to PCs.

Before choosing a simulator, one will need to decide which processes need to be simulated and what special capabilities they will require. Many programs available can solve the easy problems. But the real test of a simulator is whether it has the capabilities to handle those cases that may be uncommon - yet very important - or that may have the more difficult-to-handle characteristics of importance to the company, such as electrolytes, solids or distillation with two liquid phases or with chemical reaction. These cases should play a big role in your selection.

The computational power of the simulator will determine what types of problems can be modeled. One should ascertain that the simulator can handle specialized needs such as complex chemical reactors, nonideal physical properties, multiphase equilibrium, solids, nonideal azeotropic systems, systems with electrolytes, preliminary equipment design, costing and economic analysis.

Once one has decided the types of problems to be solved, other factors will come into play such as ease of use, adaptability, expandability, ongoing system development and performance. As mentioned previously, higher level simulators offer easy-to-use expert-system user interfaces. With such an interface, process engineers can create error-free process models at a fraction of the time that was once needed to become proficient in using a simulator. This plays an important role in increasing the usage of a simulator within the company, ultimately increasing the benefits.

Also important to increasing benefits is the adaptability of the program. Some simulators have the ability to interface to other software programs such as engineering databases, computer-aided design packages, and costing packages. It has become possible to integrate the entire engineering process - from conceptual design through construction - by linking process design and plant design tools, and calling on specialized databases.

As the user's experience in simulation grows, the simulator chosen must be able to grow with the user. For example, one should be able to add new unit operation and thermophysical property models as needed.

As one evaluates the simulator, also the supplier should be evaluated. An idea of the level of ongoing system development can be determined by the number and qualifications of the engineers committed to development within the organization. It should be evaluate what training and support programs are available. The range of problems that have been solved by the supplier should be analyzed. References should be asked to find out the experience of other, preferably similar, companies with the simulator and the supplier.

While analyzing the capabilities of the simulator, also the cost-effectiveness of the package should be looked at. More is involved than just the cost of the simulator: The cost of engineers' time, computing and training. The supplier should be able to estimate the total cost of using the system and demonstrate that the economic payback for typical applications will justify it.

ASPEN Technology, Inc.

AspenTech was formed in 1981 as a spin-off of research at the Massachusetts Institute of Technology (MIT). The company has grown in staff from eight initial founders to around 100 employees today. For the past six years, sales have grown by more than 35 percent annualy.

AspenTech is headquartered in Cambridge, Massachusetts, with branch offices in Tokyo, The Hague, and Hong Kong.

AspenTech products and services are used by over 150 companies and 100 universities in more than 25 countries.

For more information please contact the European office - Tel: 0031-70-3541051.