Steady State Simulators for Your Project

By
Donald F. Schneider, P.E.
Chemical Engineer

Stratus Engineering, Inc.
PMB 339
2951 Marina Bay Drive #130
League City, Texas 77573
(281) 335-7138
fax: (281) 335-8116
e-mail: dfsstratus@aol.com

Introduction

Process simulators are an integral part of today's industrial projects. Calculational models provide the basis for equipment design, specification, and purchasing. These powerful tools shorten project time-lines and provide added assurance that project requirements and goals are met. With their growing complexity and capabilities, process simulators are used for a wide array of project functions.

Simulator's Role

Where is a steady state simulator used in a typical industrial project? What can a computer model of a process provide? While the details are specific to each effort, in general mathematical models of systems deliver the raw data on which many project decisions are based. By their nature process models are flexible and accommodating. Finding the answer to the many *What if?* questions of the typical project is eased by steady state simulators.

Economics. Products, yields, and the equipment necessary to produce the required product in the prescribed amount can all be analyzed with a steady state simulator. This information is then directly used to determine the profitability of the proposal. Preliminary project screening may take place in the big picture, back of the envelope world. At some point, however, harder numbers are needed. How much is this thing really going to cost and how much money are we really going to make? A system model and its resulting data firm up less rigorous screening reviews. Iterations between marketing, management, and the project are typically employed to resolve expectations and realities. An easily modified computer model is a powerful tool assisting this optimization. The assessment of constraints and their influence on profitability is simplified using a mathematical model. A number can be assigned to the cost and value of an option allowing rigorous scenario comparisons. All of this can be done without letting a single equipment purchase order. Of course getting it to work on paper is only the first step, but reducing your risk through thorough analysis by itself enhances profitability.

Regulatory. The industrial regulatory climate is complex and varied. Federal, State, and Local entities may all consume project man-hours to meet environmental and safety requirements. Simulators can assist development of much of the information needed for permitting and compliance. The data they provide also supports Process Hazards Analyses (PHA's) and pre-startup safety reviews. What chemicals are present and in what quantity? Where do waste and product streams go, in what amount, and what do they contain? What process alternatives exist for waste management? What air emissions are expected and what effect do process changes and operating incidents have on them? What emergency system loads are expected? What impact do foreseeable debottlenecking options have? The answers to these questions may be altered by various changes as the project progresses. Yet adherence to permit and regulatory limits must be maintained. Managing the large amount of information involved with many regulatory concerns is a job for which computers are suited. Steady state simulators are one of the tools used.

Design. Equipment specification and design evolves directly from heat and material balance data derived from a process model. Getting the nuts and bolts installed and operating properly is the ultimate goal. A foundation of accurate system parameters is an important first step. Process temperatures, pressures, flow rates; compositions and physical properties are all data that steady state simulators produce. This information is used as the basis for equipment sizing, selection, and design.

The power and capabilities of modern steady state simulators allow consideration of a large number of design scenarios to firmly ground the design. Start-up and shut-down operation, start-of-run and end-of-run performance, Summer and Winter conditions, alternative or opportunity feeds, future expansion plans, emergency events: All these situations and more can be reviewed to ensure acceptable equipment operability under all conditions. Or, if operability cannot be secured under all conditions, these constraints can be identified up-front. Knowing a design attribute has been traded-off against cost or project schedule makes its future mitigation easier. Examining a representative cross-section of multiple scenarios also permits the reduction of design conservatism. Often this reduces cost. Steady state simulators provide a thorough, consistent database for equipment design reducing the use and magnitude of approximations and design lagniappe.

After completion. A process model often lives on after project completion. Certainly the equipment design information is used and referenced for the life of the equipment. Computer models also are often used after the project is finished. They can be invaluable tools for operating, troubleshooting, and improving facilities. Additionally, process models are often adapted for operator training/development and control/optimization design and implementation. Although these items may be initiated by the project, they are all life of the facility activities that benefit from and use process models.

Project Benefits

Table 1 summarizes some of the benefits you might expect in using a steady state simulator in your project. Every project provides different opportunities for optimzation, but in reviewing these suggestions you may find areas you can emphasize to get the most out of your process model.

Improved simulator capabilities have decreased the amount of design conservatism necessary in equipment design. In part this is due to more accurate physical property models providing better predictions of operating conditions. But also, the availability of large of amounts of computer power at low cost coupled with sophisticated software allows the designer to examine large numbers of scenarios. By reviewing standard, non-standard, emergency, and future debottlenecked conditions; less insurance in the form of design overage is needed to ensure operation at various conditions. Those conditions are now rigorously analyzed. Not only may equipment sizes be smaller, but additional equipment that may have been installed to account for design uncertainty can be eliminated. Equipment costs may also be lowered by more optimal materials selections. A better understanding of operating conditions and stream compositions at numerous operating conditions could allow the substitution of lower-cost materials, or the original selection of higher cost materials reducing future problems.

Simulation software is easier to use and more powerful than ever. These factors combine to reduce project man-hours and duration. These benefits may not be apparent as initial training and model construction are detailed tasks that should not be short changed without and understanding of the inherent quality risks. However, after the simulation is built, its ease of adjustment and modification accelerate project analysis and the production of information for equipment sizing.

The flexibility and complexity of process simulators allow nearly all design data to be derived from a common source - the model. Detailed heat and material balances support the Process Flow Diagram so that everyone's equipment design basis starts from the same foundation. This reduces the amount of estimation necessary in equipment specification and design.

Equipment that is ancillary to the project can be more highly integrated into the design using a steady state simulator. Utility demands can be examined as a subset of the primary model and optimized. Once again costs can be reduced and operability improved.

The overall benefit of a well-implemented steady state simulation is reduced project risk. The project is more likely to meets its goals through the use of a well thought out accurate process model.

Choosing a Simulator

Many options are available when selecting a simulator for your project. Base your decision on a combination of factors. The availability of an in-house or software package already purchased or licensed by your firm is compelling, but if your project requires capabilities outside the scope of this program, the cost of a simulator that is more applicable might be small compared to an inadequate design.

Table 2 lists a number of available steady state simulator packages and details some of their features. There are a large number of programs available with a broad continuum of capabilities. Some may be purchased, others only leased.

The computer platform on which the software will run is a primary factor in selecting a simulator. Many simulators are available for a wide range of platforms (UNIX, Windows, DOS). However, some are limited to a single platform. Typically a lower cost package is designed for a single platform. Cost also comes into play when choosing the features you need in the simulation software. Greater capabilities usually mean higher cost.

These capabilities and your need for them are also a significant factor in simulator selection. What system are you modeling? The more difficult your system is to model, the fewer the number of simulators that can meet your needs. Special chemical systems, polymers, biochemical or batch systems are all examples of project particulars that shape your simulator decision.

Steady state simulators often have applications beyond the immediate equipment design concerns. Models built using simulation software are often employed in assisting operator training, developing advanced control and optimization, and as a basis for dynamic or real time simulation analysis. If your model is to support these or other down-stream applications, be sure the software selected facilitates these efforts.

One of the final determinants in software selection is personal preference. Despite their core similarity, each steady state simulator vendor’s software appeals to different individual’s tastes. People’s tendency to have strong preferences for one word processor over another doesn’t disappear just because the software cost is orders of magnitude higher as can be the case for modeling software. Preference and past experience does impact the performance of those doing the work and should be considered when choosing the project’s simulation software.

Usage Tips

As with any facet of the project, the steady state simulation's scope and basis are the starting point. Without a firm understanding of the model's purpose and design basis, its output and accuracy may not meet the project's needs. A written description of the simulation's equipment scope, required end product, and design scenarios ensure the ultimate customer of the model's data receives a useful product.

With the scope and design basis defined, simulation techniques and options are selected. Here decisions can be made decreasing the complexity of the simulation. Simplifications reduce the likelihood of errors and diminish the computer time and horsepower needed to run the software. In any complex system one of the easiest ways to simplify is to break the whole into smaller pieces. This allows necessary in-depth analysis to be carried out in sections where possible. Process models are often amenable to this technique.

Even with today's *intelligent* software, the garbage-in/garbage-out phenomenon is still alive and well. In fact, the risk of generating and using flawed information may be rising. Increases in desktop computing power have made complex simulating software more accessible - perhaps available to those without sufficient training. Additionally, simulating software sophistication has risen shielding the user from technical complexity, but also reducing the amount of technical input and evaluation required. Finally, modern graphical interfaces present both accurate and faulty answers in a handsome format - the numbers sure *look* good. "That's what the computer said" should not be used as an engineering justification. Sound engineering principles must be applied when using process-modeling software.

A general knowledge of how steady state simulators work and what they can be expected to do can be gained through experience using any modern simulator. All of their fundamental underpinnings are similar. Selection and use of the proper system physical properties is still the most crucial decision in simulator use. Despite the extensive, continuously improving physical property prediction methods available, nearly every project will have to contend with some mathematical model short-coming that results in important simulator result deviations from reality. Understanding this allows mitigation so that the impact is minimal.

Training specific to a particular software package is also needed in addition to a general expertise in using modeling programs. Each vendor's simulator has its own peculiarities often touted as features. Frequently, you select a simulator for use because of its features, which differentiate it from a competitor. If you are unfamiliar with a simulator package selected for the project, many vendors offer application specific training to get you up to speed.

Good engineering practice requires that someone other than the person who did the work check calculations. This axiom certainly holds true for steady state models, which are, at their base, a collection of engineering calculations. A thorough check of even a small simulation is difficult. Some software packages by design provide a better means than others for a detailed review of the model basis. Simulator result output reports may facilitate or frustrate attempts at review. Checking a simulator involves an understanding of the basis (selected physical property and equipment models), a review of the system nodes and layout (are stream connections correct?), and a detailed examination of the numbers (feed and product compositions, physical properties).

Simulator output data are often used *as is* in equipment specification and design. However, simulator reports are typically not the best formats for those not familiar with the software to use in equipment specification and design. Even those familiar with simulator reports are better served with a sanitized report usually presented as Process Flow Diagrams, heat and material balances, or other standard reports. There are simply too many extraneous numbers in simulator software printouts. Even a small model generates thousands of numbers most of which are not directly used in the project. It is too easy to select the wrong value from traditional computer output. Additionally, simulator output typically does not precisely match design conditions. Physical properties, temperature, pressures or other data might need adjustment to reflect the desired design basis. Some simulator calculations are just plain wrong in that there is no available means to accurately estimate reality or because some simplifying compromise has been made in the calculation. Finally, simulators often produce data that, while correct, could be misleading to the project.

A good example is heat exchangers. Design calculations require the duty and requisite stream properties and conditions for any heat exchangers. However, the heat transfer coefficient and surface area of the exchanger required to affect the necessary duty is dependent on many factors undefined before mechanical design. Cost estimates based on preliminary data are fine. But design specifications wrought from unscrutinized simulator results can become expensive errors. As an example, if the simulator you are using is asked to rate a heat exchanger design, which heat transfer coefficient does it report and where? At least three heat transfer coefficients are typically calculated: assuming a clean bundle, the required coefficient for specified conditions, and the coefficient as rigorously calculated per the mechanical design. Each of these coefficients has an associated required surface area. Even if you know which value you are looking for, extracting it from the report takes care to prevent errors. Someone unfamiliar with the software and its output is unlikely to *guess* correctly.

Conclusion

Like any tool, the ultimate utility of a steady state simulator is determined by its suitability to the task and by the manner in which it is used. The right software package in the right hands lowers project costs and risks. Create an environment in your project to benefit from these computer applications to better meet your customer's needs.

Author Biography

Donald F. Schneider
Donald F. Schneider is President of Stratus Engineering, Inc., Houston, TX (281-335-7138; Fax: 281-335-8116; e-mail: dfsstratus@aol.com). Previously he worked as a senior engineer for Stone & Webster Engineering, and as an operating and project engineer for Shell Oil Co. He holds a B.S. from the University of Missouri-Rolla, and an M.S. from Texas A&M University, both in chemical engineering. Don is a registered professional engineer in Texas.

Previous publications:

"*How to Calculate Purge Gas Volumes,*" D. Schneider, Hydrocarbon Processing, November, 1993.

"*Analysis of Alky Unit DIB Exposes Design, Operating Considerations*," D. Schneider, J. Musumeci, R. Chavez, Oil & Gas Journal, September 30, 1996.

"*Deep Cut Vacuum Tower Incentives for Various Crudes*," D. Schneider, J. Musumeci, L. Suarez, Presented @ the AIChE 1997 Spring Nat'l Mtg.

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"*Programming It's not Just for Programmers Anymore*," D. Schneider, Chemical Engineering, May, 1997.

"*Debottlenecking Options and Optimization*," D. Schneider, Petroleum Technology Quarterly, Autumn 1997.

"*Deep Cut Vacuum Tower Processing Provides Major Incentives,*" D. Schneider, J. Musumeci, Hydrocarbon Processing, November, 1997.

"*Build a Better Process Model*," D. Schneider, Chemical Engineering Progress, April, 1998.

Table 1 - Steady State Simulator Project Benefits

Lower equipment cost	Rigorous analyses and case studies diminish the required design overage, permit optimal materials selection, and reduce the likelihood of *unnecessary* equipment installation
Reduced design man-hours	Software packages are easier to use and more powerful than ever
Thorough, consistent design basis	Detailed heat and material balances reduce the need for flow rate and physical properties estimates - everyone uses the same number
Improved ancillary systems estimation	Electricity, steam, water, flare, storage
Facilitated regulatory compliance	Projected operating and equipment data fill the need for regulator information. Define & ensure compliance.
Future planning	Designs are more likely to adequately accommodate planned future expansion or other known future need
Lower overall project risk	Firm economic analyses

Table 3 - Keys to Simulator Usage

Scope of work & basis of design	Simulator work needs a mission and premise just like other project functions
Simplify	Break the model into pieces and eliminate extraneous calculations
Experience & training	In the process under review/design and in the simulator package
Check your work	Review the simulator layout software engineering selections - then review the numbers. Thousands are generated even in a small model. Check all those that will be used. Enlist someone who did not do the calculation to check it.
Massage the data	Simply passing simulator reports to equipment designers may cause problems. Cull needed data and present it in standard formats.

Table 2 - Steady State Process Simulators & Their Features

Simulator	Hysys	Pro/II-ProVision	Aspen	WinCim	PD-Plus	BatchPro EnviroPro	TSWEET SIMPRO
Company	Hyprotech	Simulation Sciences	AspenTech		Deerhaven Technical	Intelligen	BR&E
Phone	800-475-0011	800-231-2754	617-577-0100		617-229-2541	201-622-1212	409-776-5220
Purchase or Lease	Purchase/Lease	Lease	Lease	Purchase	Purchase		Lease
Cost					$1,995		
Platforms Supported	Win 95/NT (Native) (Hysim - DOS)	Win 95/NT(Native) Win 3.x (PRO/II - DOS)	Win 95/NT VAX UNIX	Win 3.x	DOS	Win 3.x	DOS
Minimum Hard Disk							
Minimum RAM							
Maximum # of Nodes							
Physical Properties							
# of Thermodynamic Systems	20+	20+	20+				
# of Pure Components	1400+	1400+					
Petroleum Pseudo Components	X	X	X	X	X		X
Electrolyte Chemistry			X				
Polymers		X	X				
Powders/Solids		X	X				
Amines	X	X	X				X
Sour Water	X	X	X				
Heat Mediums							X
# of Reactor Models		6					
Reaction Data Bank			X				
Unit Operations	X	X	X				
Pump	X	X	X				
Compressor	X	X	X				
Flash	X	X	X				
Fractionation	X	X	X				
Simple Exchangers	X	X	X				
Rigorous Shell & Tube Exchangers		X					
Rigorous Air Coolers							
Rigorous Brazed Al Exchanger							X
Pipe Hydraulics (single/multi-phase)		X					
Batch							
Reactor/Fermentor							
Valve							
Mixer/Splitter							
Cyclone							
Crystallizer							
Decanter							
Filter							
Controller	X	X	X				
Optimizer	X	X	X				
User Defined Routines	X	X	X				
Dynamic Simulation Available	X		X				

Notes:
1. Not all options may be available with the standard or base license.
2. There are other sophisticated steady state simulators that only do hydraulic systems.