Software Construction: Building a Process Model

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

Software Construction: Building a Process Model

by

Donald F. Schneider, P.E.
Process Engineering Consultant
Stratus Engineering, Inc.
Houston, Texas

Often one of the first steps taken in unit troubleshooting, optimization, or debottlenecking, a complex system is the development of a computer model of the process. Increasingly, process safety management, operator training, engineering training, and environmental regulatory requirements are also aided by computer simulation. These electronic models provide powerful tools for equipment and system analysis. From individual pieces of equipment to groups of several facilities, process models allow rigorous analysis of current performance, performance prediction under alternative operating conditions, and optimization.

Because of the power of modern computers and simulating software, and the potential payoff in their successful utilization, a system of any size is a candidate for computerized analysis. Examples of typical process modeling applications include:

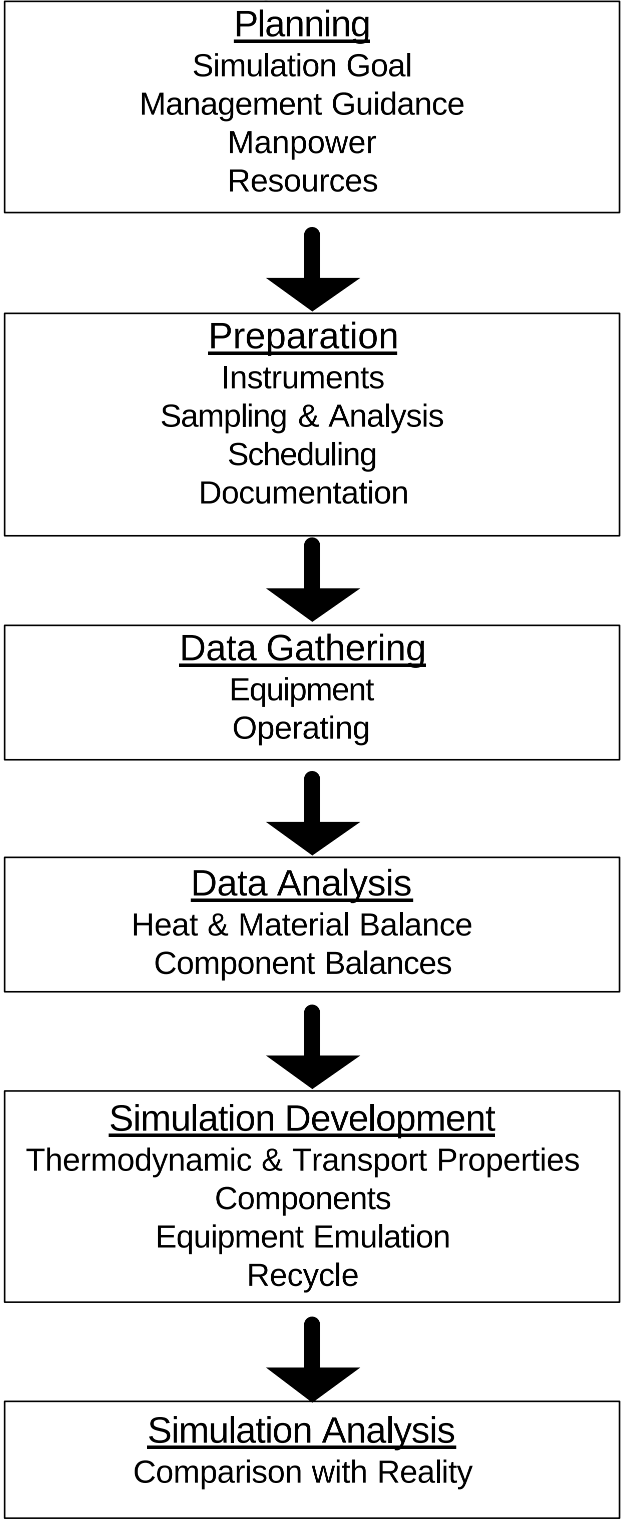
1. <u>Acoustical compressor pulsation analysis.</u> Reciprocating compressors by the cyclic nature in which they add energy to gasses and vapors produce flow fluctuations that must be moderated, or at least understood, to mitigate their mechanical and process effects. Computer analysis can be applied to simulate piping and equipment demands, and simulate system flow and pressure swings.
2. <u>Reaction or fractionation simulation.</u> Thermodynamic analysis of reacting and mass-transfer systems is one of the primary applications of process modeling. These simulations provide a basis for accurate design, troubleshooting, and existing plant revamping or optimization.
3. <u>Heat exchanger or heat exchange train modeling</u>. Energy efficiency and heat integration is typically a central component of hydrocarbon processing. This is increasingly important as environmental regulations require reduced emissions. Reduced heat generation and utility requirements usually lower fuel consumption and associated emissions. Computer modeling can be a powerful ally in optimizing energy transfer.
4. <u>Process unit simulation.</u> A major focus of computer simulation is the modeling of entire units. These tools are utilized in a variety of ways: initial design, operations troubleshooting, production debottlenecking, emissions definition and reduction, safety management, and operations training. Rigorous simulation of equipment and thermodynamic performance is increasingly simple and cost effective. Multiple operating scenario generation for design and

revamp implementation has become derigueur on a scale much greater than previously employed allowing tighter and more flexible design and operation.

5. <u>Advanced control and optimization.</u> Over the last fifteen years, advanced control and optimization have rapidly increased their presence in the hydrocarbon processing industry. Wide-spread installation of distributed control systems, computer power cost decreases, and advances in practical application of theory have catalyzed the growth. Process modeling is an integral part of advanced control and computer process optimization. Simulations provide the tools for understanding and predicting the performance of multivariable control. Models allow object functions to be built which are then optimized.
6. <u>Linear or non-linear models for facility or corporate-wide planning.</u> Yield estimates are often coupled with marketing and sales projections in models which optimize logistics and production targets. Large firms integrate multiple facilities and various functions in these models to maximize profit. At their base, these linear and non-linear simulations provide computer representations of the processes that account for the interaction between manufacturing and sales.

Building a robust and authoritative process model is in itself a project that may be executed alone or as a part of a larger effort. An organized approach is required to coordinate the many resources that may be involved in constructing a complex computer simulation. Up-front planning and preparation defines the desired results, reduces the risk of omitting the collection of critical information during data gathering, and provides a firm basis for simulation development. Figure 1 illustrates a procedure, typical of a project, for developing a process model. In order to review these steps in greater detail, this article examines the generalized case of building a process model for a hydrocarbon processing unit such as a Crude Unit, Olefins Plant, Diesel Hydrotreater, or FCCU. The following discussion can be modified and applied to any process model construction - such as those mentioned above.

Figure 1


Planning
Simulation Goal
Management Guidance
Manpower
Resources
Preparation
Instruments
Sampling & Analysis
Scheduling
Documentation
Data Gathering
Equipment
Operating
Data Analysis
Heat & Material Balance
Component Balances
Simulation Development
Thermodynamic & Transport Properties
Components
Equipment Emulation
Recycle
Simulation Analysis
Comparison with Reality

Planning

What is the simulation's purpose? For what will it be used? The answer to these questions greatly impacts the work required. They should be answered during initial planning to provide a guide for subsequent decisions. If the simulation is going to be used in the design of new equipment, a high level of detail is probably warranted. What if there are significant safety or environmental questions? Highly exothermic reactions like hydrocracking, aromatics saturation, or hydrocarbon oxidation are examples of situations where inaccurate modeling may produce unacceptable results. These drivers may demand intricate examination of system parameters. On the other hand, accurate simulation of part or all of a system may not be possible. Perhaps only the fractionation section of an Alkylation plant is restricting production. Reaction section rigorous modeling may not be necessary. Or, the system under review may not be well understood, such as the hydraulics of a utility distribution network. Sacrificing exactness to arrive at results that meet your needs is often wise, and cost effective. However, if you do not plan for this at the outset, you many never realize when you have finished. In one process model of the instrument air distribution system of an integrated refinery and chemical complex, there was always consternation that the obtainable system data revealed that the amount of air produced by the air compressors never matched the amount of air consumed by the users. However, the process simulation matched the system pressures fairly well which suggested the model was "good enough". The complex under study was 50 years old and covered over 1,000 acres. Miles of undocumented and unknown air system pipe existed. Plants had come and gone through the years. Very few system flow meters were in place. Sometimes an accurate process simulation is not worth the cost of developing, while an inaccurate model can be invaluable.

Early involvement by management, maintenance, operations, and engineering helps ensure the purpose and capabilities of the developed simulation are understood and that necessary resources are available. Although the size of the effort varies with the simulation's scope, the amount of work needed to produce a meaningful model can be greater than expected. Planning for process simulation development should follow existing procedures and guidelines for project execution.

Management overview, approval, and guidance are essential in shaping the simulation's goal, and to producing a meaningful product. For large efforts such as process unit modeling or advanced control and optimization implementation, project cost and resource demands require management approval. Additionally, during discussion of the simulation's purpose, future requirements or boundaries can be defined by management to set the project scope. For example, a unit feedstock change may be in the offing for the unit understudy, but this information may not yet be widely known. Incorporating future operating scenarios into planned simulation work increases the value of the model.

Maintenance personnel are often involved in preparation for gathering data from existing equipment and in the data collection itself. Craftsmen may in fact have sparked simulation development through their observations and reports. Maintenance manpower and scheduling are included in the planning phase to ensure their availability. Maintenance forces may be asked to: calibrate instruments, install or modify sample stations, optimize equipment, describe or alter upcoming maintenance plans, describe known equipment specifics or peculiarities, and to gather equipment inspection records.

Operations personnel are integral to the collection of data from operating equipment, and often contribute significant information regarding equipment performance and the potential benefits to be derived from a process simulation. Operations manpower and scheduling are included in the planning phase to ensure their availability. During simulation development, Operations is typically asked to: record instrument data, pull samples, optimize and steady equipment operation, make step changes in equipment operation, and to describe known equipment specifics or peculiarities. Samples for analysis may require special handling; Operations may be the focus for this effort.

Engineering personnel will ultimately build the simulation under development and usually describe the limits and potential of the simulation under discussion. During planning, Engineers detail what minimum data must be gathered, and what data would be nice to have but is not absolutely necessary. Engineers often serve as the interface between Maintenance, Operations, and other support groups such as the Lab. Engineers also gather and review design information and describe known equipment oddities. Safety reviews and risk assessment associated with data gathering may be focused with Engineering personnel.

Table 1 summarizes project planning by providing a list of some of the activities and associated man-hours involved with building a process model for an existing 'typical' 100,000 bpsd Crude and Vacuum unit. Fractionation system performance is examined in Table 1 while rigorous heat exchange train simulation is not included. Adding this analysis could as much as double the man-hour estimates. Keep in mind that the goals and requirements of each simulation are different - your mileage may vary.

Table 1 - Existing 100,000 bpsd Crude Unit Process Simulation Man-hour Estimate Rigorous Heat Exchange Train Simulation is Not Included

All values are man-hours

Task	Management	Engineering	Maintenance	Operations	Other (Lab etc.)	Total
Planning						
Kickoff/Basis/Scope/Deliverables	8	10	2	2	2	24
Documentation		4				4
Preparation						
Instrumentation			24	4		28
Sample Stations			16	4		20
Coordination		4	2	2	2	10
Computer or DCS	2	4	3	1	3	13
Documentation	1	12				13
Data Gathering						
Equipment Files	4	24	4	4		36
Unit Operating Data & Stream Samples		8		12		20
Lab Analyses	1	2			24	27
Data Analysis						
Heat & Material Balance - Component Balances		16				16
Value Verification & Cross-Check		16	2	2	2	22
Spreadsheet or Database Construction		12				12
Simulation Development						
Crude Breakdown & Light HC Definition - Yield Estimates		20				20
Thermodynamic & Transport Properties		4				4
Pseudocomponent & Component Selection/Analysis		4				4
Equipment Emulation (Tray counts etc.)		8				8
Simulation Construction & Convergence		60				60
Simulation Analysis						
Comparison w/Unit Data & Simulation Modification		32				32
Final Report	4	40	4	4		52
Total	20	280	57	35	33	425

Preparation

Typically, a model of existing equipment is based on operating and design data. Thorough data gathering is the best investment that can be made to help your simulation avoid the onerous 'garbage in - garbage out' moniker. Equipment and personnel preparation before gathering data from operating equipment increases the likelihood of collecting meaningful data.

With the simulation goal in mind, a list of required and desired operating data is developed. This list should be in the form of a log sheet so that it can be easily communicated and understood. Those gathering the data can use the log sheet to record information. If possible, provide an electronic version of the log sheet on a spreadsheet or database so that data can be directly entered. Each specified operating reading to be recorded should have a description, and an instrument number (or location if a local instrument) to ensure precise data gathering. Additional information such as P&ID references may also be helpful. In fact, providing a set of PFD's or P&ID's marked with data gathering points is a good idea. Operations may find it easier, especially for local instrument readings, to record required data on these drawings. Whatever the mechanism, data entry should provide sections for date, time, and the responsible person's initials entries so that future checking and reconstruction of events are facilitated. Once the appropriate instruments for data gathering have been identified, ensuring their proper operation is the next step.

Because day-to-day operations often depend on relative changes rather than absolute values, the condition of the instrumentation in an existing unit may not be optimal for gathering data to construct a process model. For example, the exact reflux rate to a distillation column may not be critical to unit operation so long as production is not constrained by the column and the products are on specification. However, the goal of the simulation under consideration may be to evaluate the unit for increased capacity. An accurate measure of reflux is important to understand column internal hydraulics and condenser/reboiler capacity. Likewise, accurate temperature measurement may not be critical to a process operation as long as control is steady and process objectives are met. However, accurate temperature data are important in assessing the degree of exchanger fouling and its impact on energy efficiency. A check and calibration of instruments critical to process model development should be performed. This can often substitute or supplement routine or planned maintenance thereby reducing its cost and intrusion into operations.

Besides instrument calibration, functionality may also be a concern. Some instruments that are not routinely used for operation may have fallen into disrepair. Local instruments such as pressure gauges and dial thermometers may be broken or painted over. Some repair and replacement may be required. Have a pocket knife handy to scrape away paint from gauges, instrument tags, and name plates.

Even though existing pressure gauge and pressure transmitter readings are recorded for later use and verification, a detailed system pressure survey is best performed using a single, calibrated pressure gauge moved from tap to tap. This 'single gauge survey' eliminates the discrepancies between gauges and ensures accurate readings with a calibrated instrument.

Existing temperature instrumentation may also require supplement. There may not be temperature indication where desired to support model development. Though unreliable and inaccurate, pipe and vessel surface temperature measurements may provide useful information where none exists. Additionally, hand-held thermocouple readout instruments can be used to field verify control room thermocouple temperature indications or to check duplicate thermocouples in the field. Many unit thermowells are often installed without a temperature sensing element. These wells can be probed with a hand-held device to multiply available temperature data.

Differential pressure flow meters may also benefit from direct field measurement. By recording the inches of water differential across an orifice, the flow rates can be calculated for orifices without transmitters; those with transmitters can be verified.

On-line analyzers are good sources of information that are often used in building a process simulation. These devices are no different than other instruments in that they require maintenance and calibration to produce accurate results.

Modern distributed control (DCS) and computerized historical information systems greatly facilitate unit data gathering. Review the existing available reports - they may be all you need. Include a request for these reports in your data gathering log sheets. If useful summaries do not exist, specialized output may be easily developed if requested ahead of data gathering.

A list of required and desired stream samples is also produced during preparation. This log sheet contains the same type of information as provided for the instruments: description and location in addition to time the sample was caught and any special handling or disposition instructions. Existing sample stations may require revision, or new sample stations may need to be constructed for non-routine sample points. Reacting and vaporizing samples require special handling to ensure accurate analysis. Coordination between sample collector and analyzer makes this possible. Often non-routine tests or the use of outside labs is associated with process model development. Special attention is due in these circumstances. Additionally, an understanding of the purpose of the test increases the likelihood meaningful results will be obtained.

A general overview of planned and potential unit activities is useful during data gathering preparation to stabilize operation. Check for planned unit maintenance work or unusual feed conditions. If the unit is fed from tankage, monitoring the tank for days or weeks in advance of data gathering may pay off by avoiding unexpected charge composition variations. Alert up and down stream facilities to the planned work so they can help smooth operation.

In addition to log sheets, other documentation should be considered. Putting together a communications package commensurate with the proposed size and scope spreads understanding of the project goals, helps others provide input and effort to meet desired results, and provides a summary for future review of the data basis. Include a summary of the project and its purpose/scope, a responsibility and contact list, schedule, special instructions or procedures, drawings, and log sheets.

Requirements for each simulation effort will vary. Address each model development effort individually to match the necessary preparation items and their extent to the work at hand. Additionally, resource limitations may not allow all the up-front work desired. Be sure to identify key instruments, samples, etc. that are critical to simulation development. Other items may have to be done without.

Data Gathering

It is much easier to ignore collected data that is not needed than to generate needed data that was not collected. Gather all the data you can from operating equipment to support the modeling of an existing unit. Seemingly unimportant information may prove informative later while you are mulling over an irregularity in the data. Distributed control systems and computer information systems have greatly increased our ability to collect and analyze data. Use them to their fullest when constructing a simulation.

However, there is a great deal of information computers typically do not have access to that is also important for successful simulation development. Equipment design datasheets, maintenance logs, and inspection records are needed to accurately model performance. Operator and Maintenance personnel comments and observations can provide necessary insight into equipment capabilities.

A great deal of time will probably be invested reviewing the design and maintenance files for the equipment under study. Much can be learned about potential and existing constraints from this information. Files covering new equipment may be highly detailed and contain physical property and mechanical configuration amplification that will ease simulation construction. Older equipment files may provide a history of modifications that could suggest known problems or describe previous upgrade attempts that were fruitful, or errant. Table 2 suggests items to look for by equipment type while reviewing the files. It is useful to develop tables of some of this information for later use developing the simulation. Some of this information, such as equipment design pressures and pump driver and impeller size data, may already be maintained by crafts personnel.

Gathering of the unit operating data and stream samples for analysis should take place during as small a time window as possible. This produces a snap-shot of running data and analyses. Time averaged readings or those gathered over a long time period may also be a useful reference. However, averages can hide important swings and counteracting conditions while data gathering over a long period (certainly greater than one shift) may mean the initial data bear little correlation to the final recordings. Pull unit stream samples for analysis as close as possible to the time during which data are gathered.

In addition to the numbers themselves, conditions surrounding the data should be recorded. Record the date and time the information was gathered. Was is raining during or shortly before the data pull? What was the ambient temperature? For sample analyses, the date and time the sample was caught and the date and time the sample was analyzed should be recorded so that the treatment of samples that react or weather off can be scrutinized.

Table 2 - Equipment File Information

Equipment Type	Information to Look For
All	Design pressure & temperature Nozzle sizes Materials of construction Corrosion allowance
Columns	Tray/packing types, sizes, spacings, passes Internals modifications & replacements Distributor designs & sizes Reboiler feed configuration Demister pad size & placement Sidedraw configurations Flash zone configuration Diameter & length
Drums	Inlet configuration Demister pad size & placement Diameter & length Boot configuration & distance Two-phase settling provisions
Pumps	Performance curve Driver horsepower Serial number Impeller size and modifications Maximum impeller size
Shell & Tube Exchangers	TEMA type Diameter & length Number of shell & tube passes Depassing opportunities or implementations Two-phase service Design pressure drop and duty
Air-Cooled Exchangers	Length & width Number of fans per bay Forced or induced draft Number of tube rows & passes Two-phase service Design pressure drop and duty

Besides typical process data like flows, temperatures, and pressures, other less obvious information should be collected during a thorough data-pull:

- Feel piping checking for vibrations that may be caused by water or hydraulic hammer, unexpected two-phase flow, a poor two-phase flow regime, or cavitation.
- Visually confirm column feed and draw points, especially if there are multiple valved locations.
- Along with flow data, pump suction and discharge pressures can be used to verify a pump's on curve operation.
- Note how many pumps are operating in each service.
- Record control valve position and pressure drop. These can be used later to confirm flow indications or to provide approximate flow rates for streams without measurements.
- Note the disposition of control valve and exchanger bypasses. Open bypasses may signal hydraulic or thermal limitations and certainly change the meaning of raw temperature and pressure data.

Table 3 summarizes data that might be included in data gathering efforts.

Because simulation development often entails detailed examination of equipment with dedicated manpower, it also may be an opportune time for other activities. Much of the information gathered in these ancillary assignments may be useful in simulation development. Consider including the following tasks in the data gathering phase:

1. Recording pump make, model, and serial numbers. Analysis of unit flow data may suggest a pump is performing substantially at odds with its design data. The serial number can be checked versus the equipment files to confirm the use of the correct performance curve.
2. Recording rotating equipment vibration readings.
3. Fugitive emissions surveys.
4. Recording relief device numbers, set pressures, and last inspected date.
5. Checking rupture disk integrity.
6. Field verifying P&ID's.

Table 3 - Data to be Collected for Simulation Development

Temperatures (Skin, read values @ field wires)
Pressures (Single gauge survey, calibrated if possible)
Flows (At what T&P? Corrected to std. conditions?)
Orifice plate differentials.
What is limiting the unit?
Number of fans operating on air-coolers.
Utility flows & conditions: steam T&P, cooling water T&P, others.
Lab analyses.
On-line analyzer data.
How many pumps are running in each service?
Control valve positions.
Control valve bypass positions.
Exchanger bypass positions.
When were exchangers last cleaned?
Motor amperage or horsepower.
Unit condition: SOR, EOR.
Are fractionator trays known to be missing or damaged?
Catalyst fouled or poisoned?
Tank gauges.
Ambient conditions (Temp, rain, barometric pressure)
Column nozzle draw & return locations.
Original equipment datasheets & post manufacturer modifications.
Inspection records.
Take photographs.
Operator comments.
Maintenance comments.

Data Analysis

Review of the collected information is critical to ensuring accurate simulation development. An initial examination of the data should be made to eliminate obviously questionable values. Often typos or misplaced entries can be corrected by talking with those involved in the data pull. An overall first impression of the collected information can be a harbinger of its acceptability.

A systematic check of the data is performed. This is often accomplished by starting at the feed inlet and moving through the process. Where it is possible, use different information to confirm the same value. A good example of this is comparing tank gauging outages with unit feed flow meters. Additionally:

- Check temperature and pressure profiles to ensure they increase/decrease properly.
- Calculate the duty of each side of an exchanger and compare.
- Compare operating temperatures and pressures to relief set-points and equipment design conditions.
- Compare lab and on-line analyzer information with typical analyses.
- Compare pump flow and ΔP data to pump performance curves.
- Use control valve information to confirm or question flow rates.
- Confirm that BPD data are at standard conditions and that gpm data are at operating T & P.
- Confirm that vapor volumetric flow rates are at standard conditions or at operating T & P.
- Double check orifice flow meter readings with orifice pressure drop data if necessary.

After initial data verification is complete, heat and material balances are made. The old rule that the sum of the *GOES-INTOS* must equal the sum of the *GOES-OUT-OFS* must be obeyed. For simulations of limited scope, one heat and material balance covering all equipment may be sufficient. For complex simulations, several balances covering groups of equipment, and one balance enclosing all equipment might be necessary.

Spreadsheets are excellent tools for use in heat and material balance development. Software packages are also available that provide gross error checking of data and perform heat and material balances. This might be a favored option if the same equipment is to be evaluated many times.

The nature and extent of the heat and material balance differs with each simulation. For equipment without reaction, gross mass and energy balances supplemented with component balances will probably be sufficient. If reactions are included in the simulation, atom balances should be made around the reactor where possible. This is especially true if reactor yields are based on empirical or vendor predictions. This type of prediction may not accurately conserve composition on the atomic level. For example, in simulating a diesel hydrotreater unit ensure that the total reactor inlet and the total reactor outlet have the same hydrogen content. For boiling point components hydrogen content must often be inferred from UOP or Watson K values. Tracking sulfur and nitrogen species is also probably justified for this type of unit.

It is rare that heat and material balances will be at or very near zero upon first review. Typically some correction needs to be made. Often one reading or another stands out as in error. Secondary means can be used to confirm flows. Tank readings, estimated pump rates based on performance curves, and other data may be used to infer flowrates and confirm direct measurements.

Simulation Development

Modern graphical interfaces ease the chore of stringing unit operations together to build a simulation. Keyword entries have been replaced with drag-and-drop icons. Lengthy output can be summarized by graphical output and statistical analysis packages. However, the underlying basics of simulation development have not changed. Robust and representative physical property definition, accurate equipment configuration, and wise execution layout and scope are all fundamental to a successful simulation. Even today's sophisticated modeling programs cannot wrest these decisions from the developer.

Physical properties form the foundation of simulation analysis. Proper selection of thermodynamic properties can make the difference between a simulation that is well behaved and one that is not; between one that accurately describes the system under study, and one that does not. Most simulation packages today provide several thermodynamic method options and recommend specific methods for common problems. Many simulators have special property packages for non-ideal systems or particular applications such as amine treating or hydrofluoric acid Alkylation. Even with the breadth of thermodynamic system capabilities available to the developer, many pitfalls remain. Some to watch for are:

1. Liquid - Liquid equilibrium or extraction systems typically require binary pair interaction data.
2. Superfractionators (Ethane - Ethylene distillation) often require binary pair interaction data.
3. Systems with solids should be closely scrutinized.
4. Highly non-ideal systems or conditions push methods to their limits.
5. The presence of water can cause problems. Water's physical properties differ markedly from typical hydrocarbons making modeling of systems with both, a common situation, difficult.
6. The presence of hydrogen can cause problems. Hydrogen solubility estimations are very unreliable. Hydrogen physical properties are difficult to model and unexpected results occur due to its negative Joule-Thomson coefficient.
7. Viscosity modeling typically assumes Newtonian behavior which is often not the case.
8. Molecular weight correlations yield varying values when heavy hydrocarbons are modeled. These differences can be significant and impact equilibrium temperatures.

The number of components included in the simulation should be enough to accurately characterize the performance of the system, but not so many that calculation time and the risk of the simulation not converging are increased. How many components or pseudo components do you need to predict the most important characteristics of the simulation? For example, if you have C4's in your stream, do you need all 12 of them or will 3 be sufficient? This decision should be based on the purpose of the simulation, which component details do you want to examine, and the required accuracy.

Systems with boiling range petroleum pseudo-components require special attention. Figure 2 illustrates feed stream boiling point curve and its division into pseudo-components. Flat regions of the curve require fewer pseudo-components to accurately describe the stream while steep regions require more. Be sure to include enough pseudo-components near boiling points where cuts are made even if these cut-points are on relatively flat portions of the boiling point curve. If you have pseudo components in a reactor feed and product stream, two different sets of pseudo-components may be required: one set for the reactor inlet, and one set for the outlet. Too few pseudo-components will decrease your simulations ability to represent reality, too many will slow down execution and could increase calculational instability.

Accurately constructing the equipment in your simulator is as crucial as physical property estimation to realistic simulator results. Equipment design documentation is the primary source for simulator equipment configuration input. However additional information may be gleaned from maintenance and inspection records, P&ID's, and operator and maintenance personnel comments (e.g. "We damaged trays 5 through 10 during the last power failure", "exchanger E-823 was depassed last turnaround"). Separation and reaction processes must be evaluated for their approach to equilibrium. Common methods can be used to approximate the number of equilibrium stages involved, but this estimate must be fine tuned using operating data. Equipment internal design must be reviewed to assess its impact on the simulation.

Accurate simulation modeling involves more than understanding equipment configuration. Simulators take liberties with physical representations of equipment that ease modeling but may unacceptably skew results. The best example of this is distillation column reboilers. Most simulator's default assumption is that the reboiler performs like a kettle reboiler. Sometimes this is the only option. If the primary process concern is reboiler duty, this assumption may not be important. However, when sizing column internals, trays and reboiler piping and exchangers, liquid and vapor flow and condition information is critical. A thorough understanding of the simulator's calculational technique is necessary to ensure results, such as reboiler performance, are appropriately accurate.

Extraneous factors may greatly impact existing equipment data gathering and simulation scenario selection and should be considered during model construction. Many units have significant performance variations between their start-of-run (SOR) and end-of-run conditions. This is especially true of hydroprocessing units such as hydrotreaters, hydrocrackers, and reformers. Fouling heat exchanger systems such as Crude preheat trains or olefin and polymer systems may exhibit significant performance degredation. Supplement gathered data with SOR or EOR information if available and account for equipment operation deviations from ideal. Units with expected large differences between SOR and EOR operation probably require a simulation scenario for each case. A middle-of-run (MOR) scenario may also be appropriate if the SOR conditions are short-lived start-up transients. The MOR and EOR cases then predominate and better represent operations. Weather might be another factor which alters operation. If extreme weather conditions are experienced at the site under study, make accommodations for their impact. Separate summer and winter simulations may be required.

After the physical equipment characteristics are defined, process specifications must be set for process operations with remaining degrees of freedom. Fractionation towers almost always require process specifications. Heat exchangers, compressors, pumps, and control valves might also require them. If there is a device in the system capable of altering the performance of a piece of equipment (e.g. a controller), the simulation should be reviewed for the placement of a process specification. For example, a simple distillation tower typically requires two process specifications (e.g. bottoms draw rate and reflux ratio). Note that even if two sets of specifications should produce the same simulation results, they may be different enough in the effect on the mathematical solution that one set of specifications fails to converge while the other solves easily. It is often best to choose very firm specifications like molar flow rates and temperatures during the early phases of simulation development. After stable initial estimates are generated in this manner, more complex specifications that accurately reflect the desired result may be implemented.

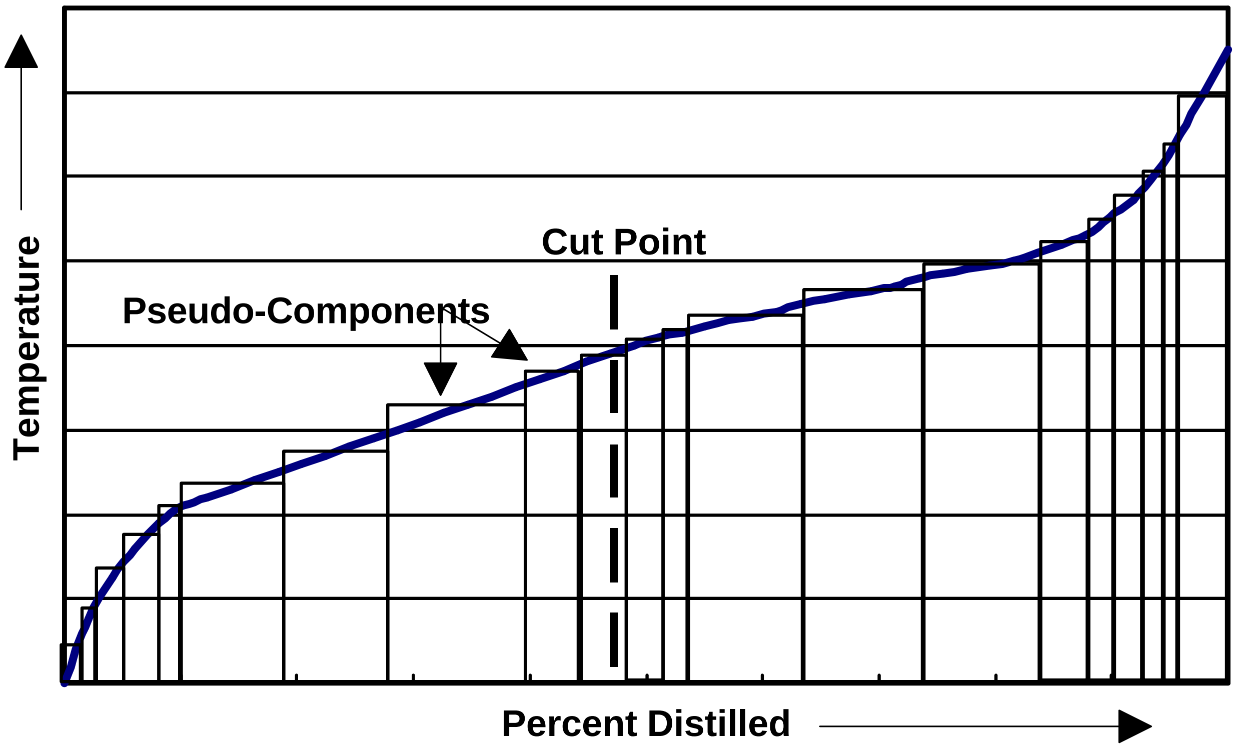
During simulation development, the execution sequence and extent of the final product must be kept in mind. Each calculation in the model that alters results ahead of its own execution creates a recycle of information that greatly increases solution time and model complexity. Recycles should be minimized. Simulators iterate calculations until the previous solution and the final solution differ by only a small amount. Often these convergence tolerances can be loosened, especially during simulation development. This reduces calculation time at the cost of reduced accuracy. Once a simulation is built and operating well, the tolerances can be tightened to yield a final result. Starting the simulation with good initial estimates also reduces calculation time and may be the only way to achieve simulation convergence. Update the estimates as the model grows or conditions change.

Don't be trapped by the desire to have the simulator do everything. With calculation blocks and OLE links to software outside the model, modern simulators are capable of most calculations imaginable. However, does it make you money? If you are doing the same thing over and over, investing in the needed programming and computer horsepower to have the simulator make the calculations will pay off. Even if this makes sense be cognizant of hidden costs: once a simulation is built, it has to be maintained. Additionally, even our ever more powerful computers take a significant amount of time to:

- Get answers that are good enough for the task at hand,
- Perform rigorous equipment analysis (e.g. rigorous exchanger calcs or hydrodynamic evaluations)
- Solve recycle loops.

Complex simulations not only take a great deal of computer horsepower and are more difficult to converge, they are also more difficult to debug. How do you find a problem in a large simulation? It can be like the needle in the haystack problem. Often you don't find the problem in a simulation until you sit on the needle. The larger and more complex a simulation becomes the more likely an important parameter will be missed or updated improperly. Building a simulation in sections and checking each as you go is the normal, sound approach to breaking a complex problem into pieces to arrive at a solution. This certainly applies to simulation development.

Figure 2 - Stream Boiling Point Composition



Simulation Analysis

After the simulation's operation is stable, it must be tuned to match operating plant data thus ensuring representative modeling. Simulation modifications are then made assuming a close approximation to real-world responses. Which simulation results do you match to reality and to what tolerance? The depth of the analysis depends on the model's purpose, and on how much conservatism you require. Often a model will accurately reflect the magnitude and direction of operational changes even though its absolute accuracy is poor. If this level of accuracy is sufficient, development time and cost can be reduced.

Table 4 and Figures 3 and 4 detail some comparisons that might be made between simulation results and operating data. Tabulating important data and comparing them to simulation results on a rigorous basis using absolute and percentage differences provides an important picture of simulation accuracy. Trends can also be spotted in this manner. For example, all product gravities may be found to be one number low.

Simulation generated physical properties should be examined closely. In particular, transport properties which can be difficult to predict may be important to your model. For example, viscosities of non-Newtonian fluids typically must be modeled using non-standard methods to garner accurate results. Figure 3 illustrates a comparison between lab viscosity data and simulation estimates for a crude column bottoms stream. Figure 4 details a comparison between lab data and simulation results for a product distillation curve. Graphing results where possible often adds value to the analysis. Due to sampling and testing limits, it is not unusual for lab data and simulation results to diverge at the front and back ends of distillation curves. However, the middle portions of the curves and the liquid volume 50% point temperatures should be in sync.

Process simulation results are meaningful only within the context of their basis. Step away a little bit from the basis to predict behavior, and you should have an accurate tool. Step a large distance from the basis to predict behavior and you may only have a crystal ball.

Once built, a model is compared to its base data to confirm accuracy. The degree of precision required depends on the simulation's intended application, and on available resources. Often a model will accurately reflect the magnitude and direction of operational changes even though its absolute accuracy is poor

Table 4 - Comparison of Simulation Results to Plant Data

Item	Units	Plant Data	Simulation	Absolute Difference	Percent Difference
Crude Charge	BPSD	54,611	55,411	800.0	1.5
Crude Charge	F	95.0	95	0.0	0.0
Crude Charge	API	31.1	31.1	0.0	0.0
Desalter	F	227	227	0.0	0.0
Desalter	psig	248	248	0.0	0.0
Flash Drum	F	412	412	0.0	0.0
Flash Drum	psig	66.0	67	1.0	1.5
Flash Drum Bottoms	BPSD	48,792	48,322	-470.0	-1.0
Flash Drum Bottoms	API	26.4	26.0	-0.4	-1.5
Flash Rectifier Ovhd	F	338	338	0.0	0.0
Flash Rectifier Ovhd	psig	65.0	66	1.0	1.5
Flash Rectifier Btms	F	396	400	4.0	1.0
Flash Rectifier Reflux	BPSD	1,325	1,325	0.0	0.0
Furnace Outlet	F	638	636	-2.0	-0.3
Resid Str. Flash Zone	F	632	631	-1.0	-0.2
Hvy AGO Overflash	BPSD	928	928	0.0	0.0
Hvy AGO Overflash	F	593	602	9.0	1.5
Hvy AGO Overflash	API	29.1	28.1	-1.0	-3.4
Resid Str. Btms.	F	611	623	12.0	2.0
Resid Str. Btms.	psig	34.0	34.0	0.0	0.0
Steam to Resid Str.	lb/hr	2,603	2,603	0.0	0.0
Resid Str. Ovhd	F	608	625	17.0	2.8
Resid Str. Ovhd	psig	31.0	31.0	0.0	0.0
Resid	BPSD	29,890	28,515	-1375.0	-4.6
Resid to Sto.	F	133	133	0.0	0.0
Resid	API	17	15.9	-1.1	-6.5
Crude Col Btms	psig	32.0	30.9	-1.1	-3.4
Hvy AGO Str. Feed	F	593	602	9.0	1.5
Hvy AGO Str. Feed	API	29.1	28.2	-0.9	-3.1
Hvy AGO Str. Btms.	psig	31.0	30.8	-0.2	-0.6
Hvy AGO Str. Ovhd	F	518	602	84.0	16.2
Hvy AGO to Sto	BPSD	2,881	2,882	1.0	0.0
Hvy AGO to Sto	API	28.6	28.1	-0.5	-1.7
Hvy AGO to Sto	Flash, F	178.0	164	-14.0	-7.9
Hvy AGO to Sto	F	152.0	152	0.0	0.0

Figure 3 - Comparison of Simulation Viscosity and Lab Data - Resid

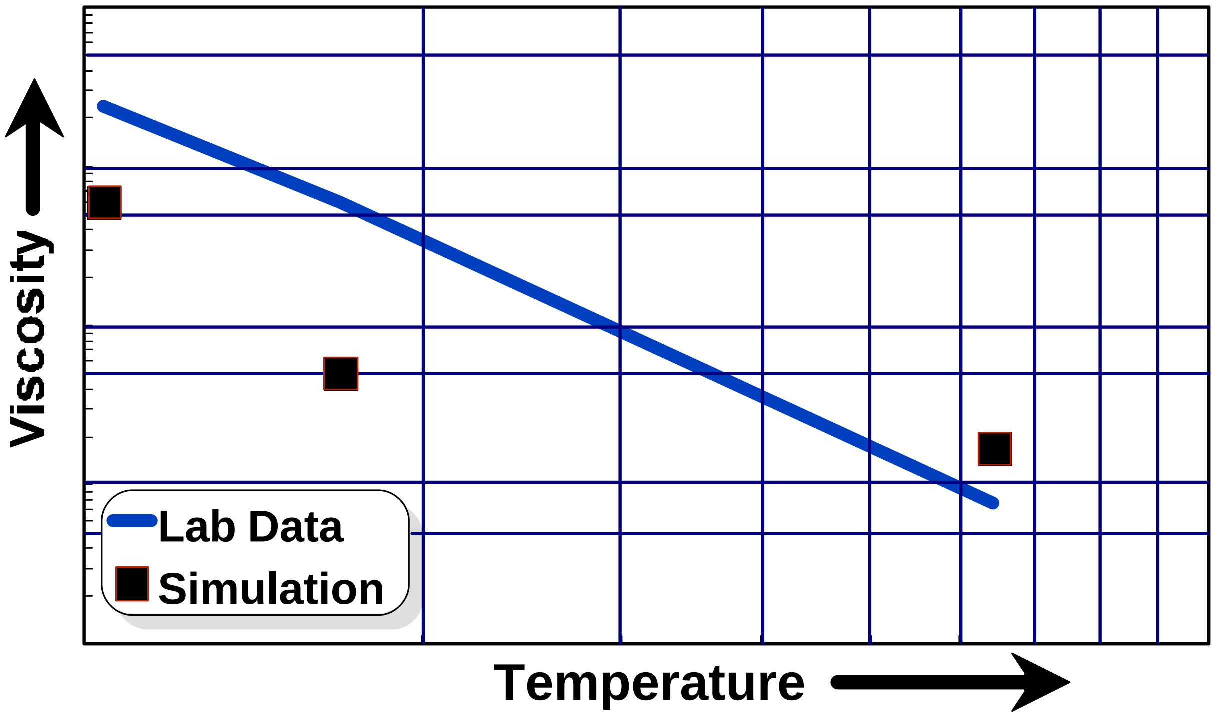
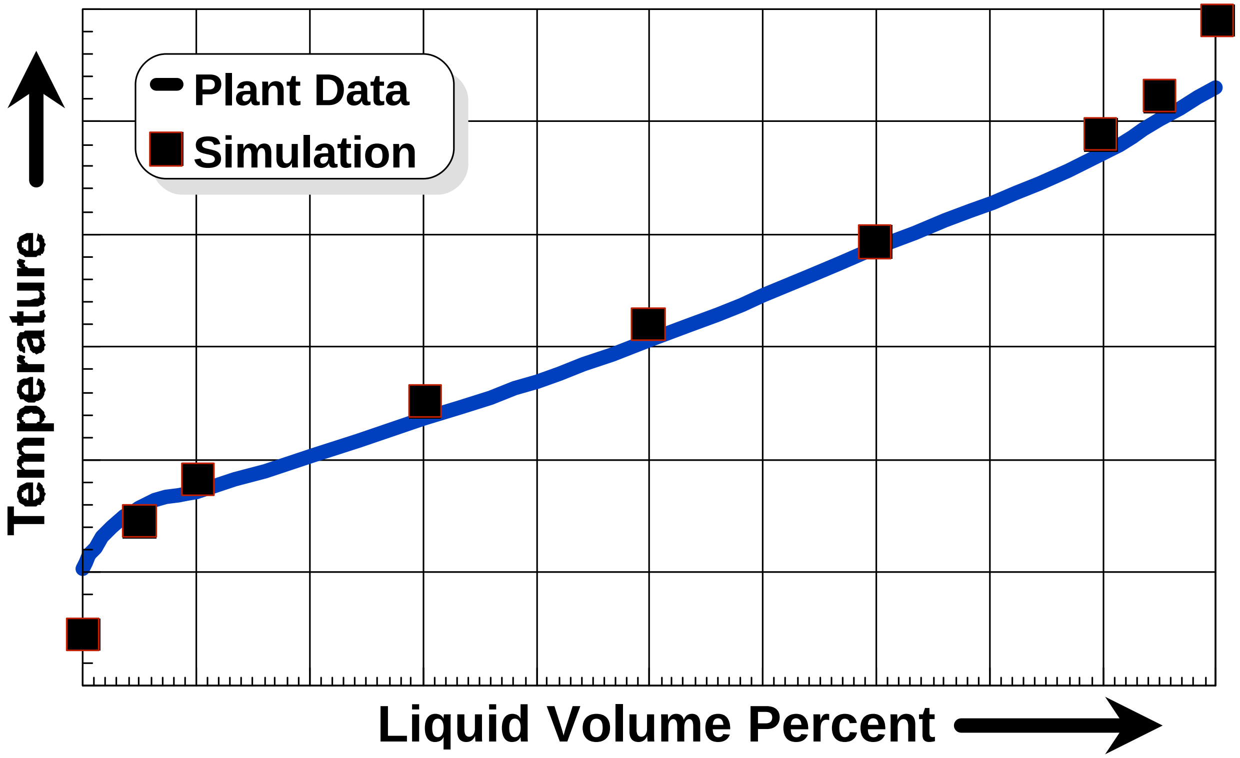


Figure 4 - Comparison of Simulation and Lab Data Product Distillations



Summary

An accurate existing facilities model is a powerful tool allowing rigorous unit operations analysis, 'What if?' investigation, multiple scenario generation, advanced control/optimization, and linear/non-linear programming planning. These analyses greatly enhance decision making confidence when equipment or operating condition alterations are considered. But in the end, the simulation benefits must out-weight its development and maintenance cost.

Ever improving software packages and increasing computer power continue ease model development cost and time requirements. However, building an accurate simulation still requires the involvement of many parts of the organization and an understanding of the fundamentals behind the model such as physical property prediction and equipment characteristics. Additionally, even today's technology cannot do everything... yet. A simulation can typically accomplish a small number of goals very well, and becomes less productive and manageable as demands increase. Knowing and observing limitations increases the likelihood that results will meet expectations.

References

"PRO/II Reference Manual," Simulation Sciences Inc., 1994.

"HYSIM User's Guide," Hyprotech Ltd., 1994.

Author Biography:

Donald F. Schneider is President of Stratus Engineering, Inc., Houston, Texas (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 Univeristy, both in chemical engineering. Don is a registered professional engineer in Texas and a member of GPA and AIChE.