Process Simulation: Matching the Computer's Perception to Reality

By
Donald F. Schneider, P.E.
Process Engineering Consultant

Stratus Engineering, Inc.
PMB 339
2951 Marina Bay Drive #130
League City, Texas 77573
(281) 335-7138

March 1997

.

Introduction

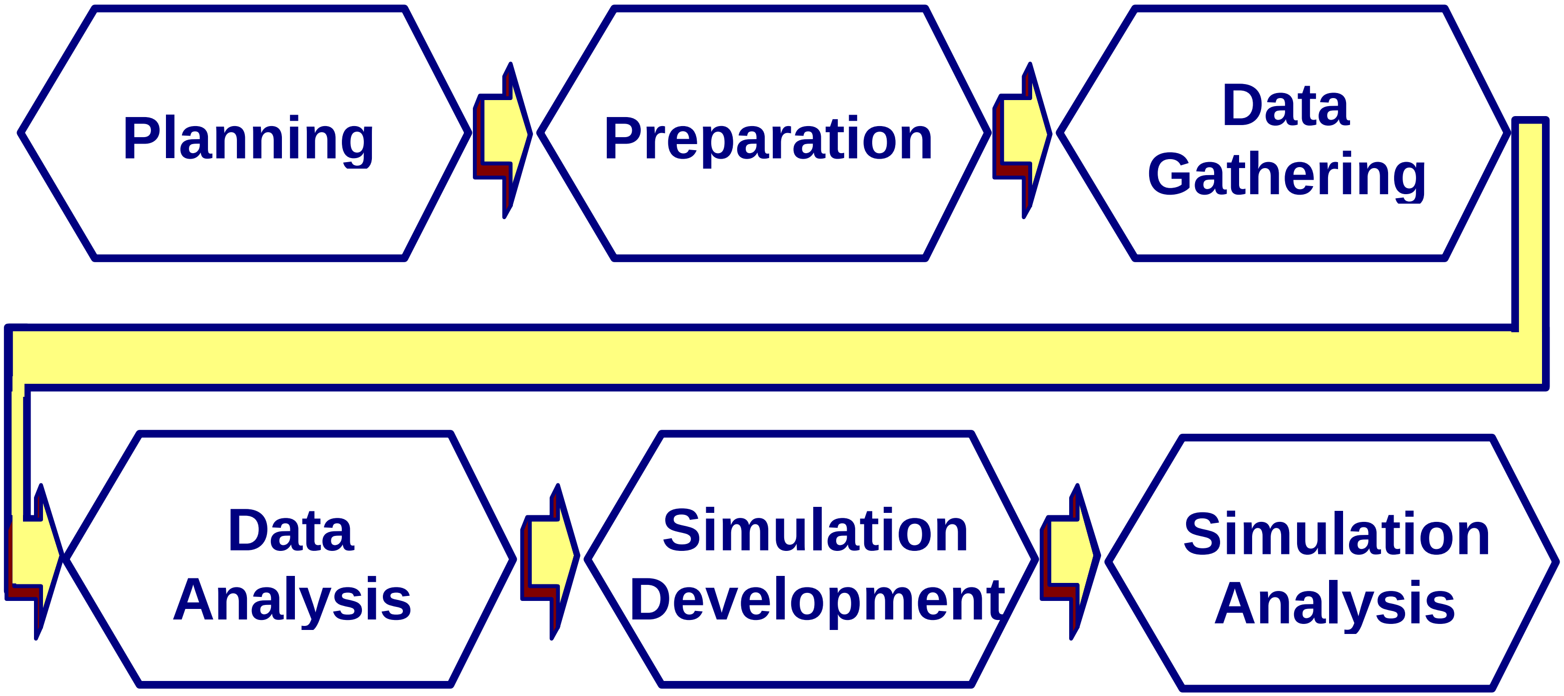
Often one of the first steps taken in unit troubleshooting, optimization, or debottlenecking, a complex system is the development of a computer model of the process. Computer simulation provides a powerful tool for equipment and system analysis. From individual pieces of equipment to groups of several facilities, process models can allow rigorous analysis of current performance, performance prediction under alternative operating conditions, and optimization. Examples of typical process modeling applications include:

1. Acoustical compressor pulsation analysis.
2. Reaction or fractionation simulation.
3. Heat exchanger or heat exchange train modeling.
4. Process unit simulation.
5. Advanced control and optimization.
6. Linear or non-linear models for facility or corporate-wide planning.

Building a robust model is in itself a project that should be approached in an organized fashion. Up-front planning and preparation 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 generalized procedure for developing a process model.

Typically, a model of existing equipment is begun by collecting equipment 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. Computer software is then used to mathematically model the equipment based on the gathered data. This model is evaluated for its consistency with the operating data. If the process simulation under development is not a model of existing equipment, data gathering is replaced by clear definition of a design basis and specifications.

Figure 1 - Simulation Development



Planning

Early involvement by management, maintenance, operations, and engineering helps ensure the purpose and capabilities of the 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 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.

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.

Preparation

Equipment and personnel preparation before gathering data from operating equipment increases the likelihood of collecting meaningful data. Consider taking the following actions before information is recorded:

1. Ensure no major unit maintenance is scheduled.
2. Steady unit operation, feed composition.
3. Coordinate with upstream, downstream, and offsite facilities.
4. Alert support groups such as the Lab.
5. Calibrate instruments.
6. Gather ancillary instruments such as a calibrated pressure gauge or temperature indicator.
7. Build special DCS or computer data collection systems.
8. Arrange for non-standard sample collection and analysis.
9. Provide documentation:
   a) Goals and summary.
   b) Responsibilities list.
   c) Schedule.
   d) Checklists.
   e) Special operator logsheets.
   f) Lists of data to be collected.

Requirements for each simulation effort will vary. Address each simulation development project individually to match the necessary preparation items and their extent to the work at hand.

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. 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 model 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.

Table 1 details data that might be included in simulation development information gathering efforts.

Table 1 - 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.

Gather operating data within as small a time window as possible so that an accurate snap-shot is taken. Pull 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. 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.

Because simulation development data gathering 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.
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.

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. Heat and material balances can then be 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. Software packages are available which 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 derived from boiling ranges.

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.

Gathered data can also be compared to historical values to classify operation at the time of the data pull as 'normal', 'End of Run', or some other state.

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 separators) 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.

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.

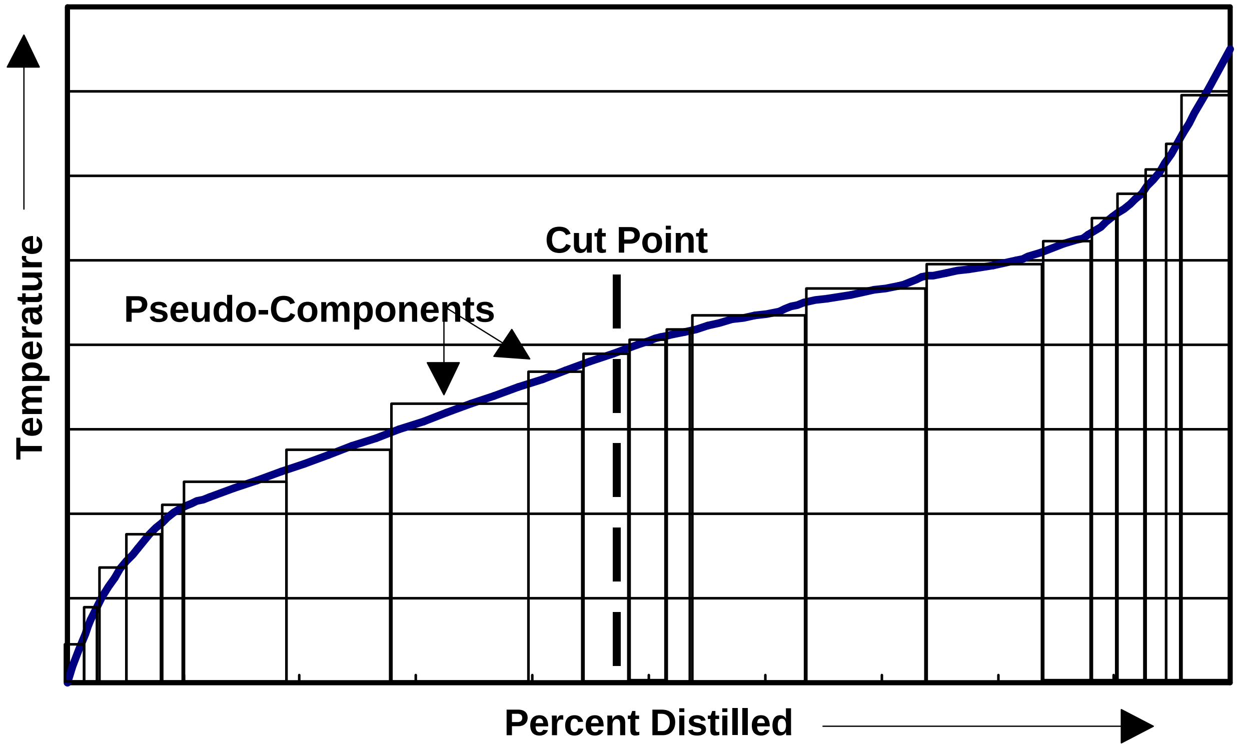
During simulation development, the execution sequence and extent of the final product must be kept in mind. Each calculation in the model that alters results ahead of its own execution creates a recycle of information that greatly increases solution time and model complexity. Recycles should be minimized. 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 2 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 2 illustrates a comparison between lab data and simulation estimates for a crude column bottoms stream. Figure 3 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 2 - 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

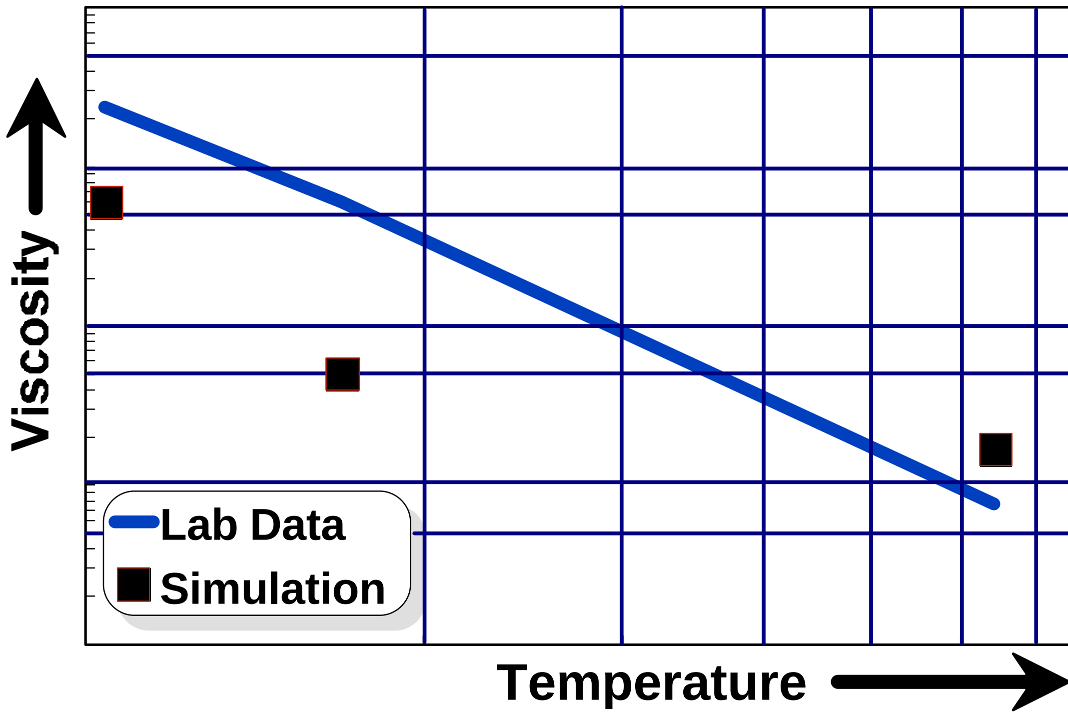
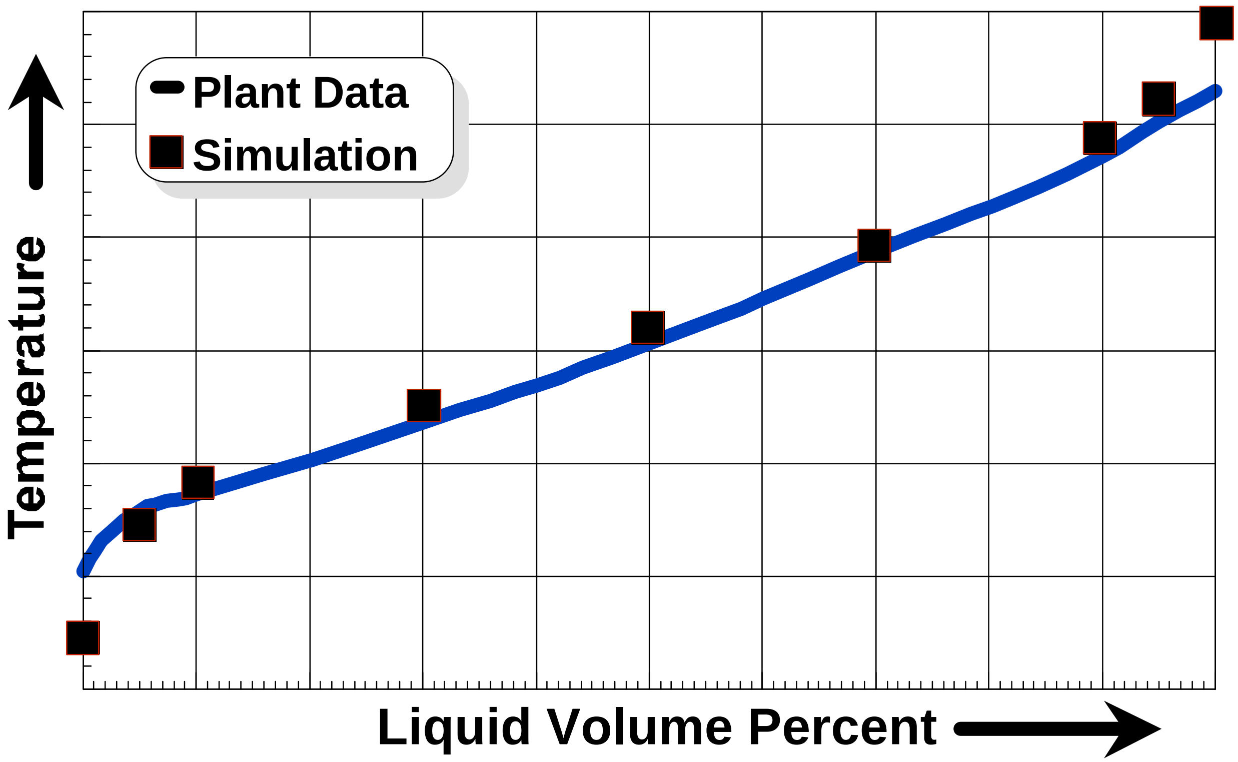


Figure 4 - Comparison of Simulation and Lab Data Product Distillations



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 increase the likelihood that results will meet expectations.

Please contact the author at:

Stratus Engineering, Inc.
PMB 339
2951 Marina Bay Drive #130
League City, Texas 77573
Phone: (281) 335-7138 Fax: (281) 335-8116
E-Mail: dfsstratus@aol.com Website: www.stratusengr.com

References

"PRO/II Reference Manual," Simulation Sciences Inc., 1994.
"HYSIM User's Guide," Hyprotech Ltd., 1994.