EXPECTATIONS FROM SIMULATION: PART ONE – REALISTIC AND RELIABLE

In part one of a two-part article, **Prashanth Chandran, Nathan Hatcher and Ralph Weiland, Optimized Gas Treating, Inc., USA,** detail the two perspectives that should be considered when setting expectations from simulation.

Process calculations and design used to be carried out with pencils, graph paper, and slide rules. Now this is done by computer. Results from a computer perhaps lend themselves an undeserved aura of authenticity, especially when reported to 8 or 10 figures. But if the methodologies remain the same and the calculations have only been relegated to a computer, then the computer merely takes the drudgery out of the work. So, what should be expected from a simulator, and what advantages does simulation offer?

Computer simulation affords: faster computation, the ability to look at interactions between process units, the ability to perform detailed sensitivity analyses, and the implementation of more realistic models – enabled by

greater computing power. That simulation offers increased speed is unquestioned, so unless the calculations are either trivial or superfluous, the first advantage is always realised. Today, one can run more simulations and carry out more computations on a laptop computer in a day than was once possible by slide rule and calculator in 10 years of 24 hour days. But if that is all that simulation provides, it falls well short of its real potential. Expectations from simulation can be viewed from two perspectives: realism of models, and reliability of results.

Both must be considered if a simulator is to deliver what it should.

Realism

A computational model of any unit operation is just a set of equations representing one or more principles underlying our understanding of the processes occurring within the operation. For example, a centrifugal pump can be conceptualised as a unit providing a pressure increase. At the process level, it is not necessary to model the pump using computational fluid dynamics (CFD) simply to provide the pressure rise and the associated temperature increase. Thermodynamics work nicely for that. However, a pump designer will want a much more realistic model of the pump, maybe even going to the extent of carrying out CFD analysis of the flows and potential cavitation within the casing.

Conclusion 1

The necessary level of complexity or realism of a model depends on one's needs, objectives and expectations.

If one is involved in specification and detailed design of heat exchangers, access to advanced software would be of great value. But if it is enough to know that an exchanger in a flowsheet is only there to raise or lower the temperature of a stream, all that needs to be computed is the duty required for a given temperature change (or the temperature change for a given duty), and possibly the pressure drop. Such a model can be extremely simple, involving nothing more than the computation of stream enthalpies. However, if the interest is in exchanger design, then one is in the business of predicting performance based on exchanger geometry, metallurgy, fluid properties, and the fundamentals of heat transfer. Heat exchangers have been designed in detail for well over 75 years, using a model based on heat transfer rates and additivity of resistances.[1]

The model uses individual film coefficients for heat transfer found from generalised charts that are constructed using parameters in the form of dimensionless groups. In today's software, those charts are digitised into correlations. Accurate provision is made for two-phase flows, boiling heat transfer, condensation in the presence of inert gases, and a host of other embellishments such as extended heat transfer surfaces and turbulence promoters. Models based on heat transfer rates use databases of fundamental information to allow one to actually predict performance with a high degree of reliability. As a concept, an ideal-stage heat exchanger is an absurdity – as is the efficiency of an exchanger modelled this way. Yet in mass transfer separations equipment, with its enormous cost, many consider ideal stages, stage efficiencies, and height equivalents to a theoretical plate to be state-of-the-art.

Conclusion 2

In parallel with heat transfer, if process or revamp guarantees must be made and design fat kept to a minimum, true mass transfer rate-based simulation is essential for column design.

To some extent, then, perhaps the question 'what do you expect from simulation?' should be turned around to read 'what do you need from simulation?' Matching what is wanted with what is given requires an operator to match the simulator to their requirements, i.e. to their expectations. To help answer this question, it may be worth pointing out that there are two types of models: those that perform automated heat and material balances (lumped parameter models); and those that predict performance (distributed parameter models). In the world of separations, ideal-stage-based column models usually must be viewed as little more than automated heat and material balancers, combined with a (maybe complex) thermodynamic model for the component distribution between the phases.[2] Truly predictive models must be based on mass and heat transfer rate principles, just like their heat exchanger brethren. They are essential to trimming excess fat from a design.

Conclusion 3

Match the simulator to its purpose. A sledgehammer is not required to crack a walnut, but rocks cannot be broken with a stick either.

If the model is not rate-based then it is in some sense fitted because adjustments are required. These might take the form of efficiency factors, kinetics factors, heat transfer efficiency, height of a theoretical stage, etc., to force a match between the simulation and known or expected performance. Fitted simulators are best used when tuned to an existing facility where an engineer wants to explore the potential effects of relatively modest operating parameter changes. However, the farther one moves from the set of fitted conditions, the less reliable the results become. The benefit of this type of simulator is that a user can apply adjustments that force the simulator to perfectly match their plant data, but in grassroots design this can be completely misleading – or even dangerous – if the deviation from fitted conditions falls outside of a stable operating range. They are certainly not predictive.

Predictive simulators are necessarily mass transfer rate-based and calculate results without user-specified adjustments. These simulators are best for designing new facilities, identifying unstable operating conditions, or determining how existing equipment or designs would perform in a new service or under a new set of operating conditions. Examples are revamp projects, or for selection of a modular plant for a given service. The advantage of a real mass transfer rate-based simulator is that it provides results based on sound engineering principles and thermodynamic properties rather than on the user (or software developer's) experience.

Conclusion 4

Predictive simulators, whether for heat transfer or mass separations, are necessarily truly rate-based. If there are stages, efficiencies, or stage calculations, it is not predictive.

Whether an idealised or mechanistic model is most suitable for a simulator's separations calculations depends on the intended use for the simulation results. If all that is needed is to fit the model to plant data and then run what-if studies over limited ranges of certain parameters, a fitted model may fulfil the need quite nicely. If one must offer process design guarantees or guarantee the outcome of a revamp, a predictive simulator is an absolute necessity – unless there is room to add quite a bit of fat (and cost) to the design.

Reliability of simulation data: what is data and what is not?

Engineers who use simulation tools are always concerned about whether the results of their simulations are correct or not, or whether they are even reasonably reliable. This kind of concern is only natural, and is certainly justified. After all, operators may be called upon to guarantee the design of a US$10 million column or a US$2000 million plant, the performance of certain tower internals, or indeed a solvent formulation. When troubleshooting, operators certainly do not want to be led unknowingly to a wrong solution – or even to no solution at all – because the simulation failed to model real behaviour. So, what are some of the approaches that people have used in trying to establish reliability of a simulator? What are you using for benchmarking, and is it valid?

Frequently, one hears of comparisons of one simulator with another, or with data from a solvent supplier or a process licensor. Sadly, comparisons between a simulator and real, measured plant performance data are made much less frequently. Most process simulators are intended to show what a column or unit should be doing if it has been correctly built and is operated properly. This is certainly the case for OGT's ProTreat® and SulphurPro® simulators.[3]

One of the most common reasons for making comparisons between simulators is lack of reliable data; perhaps the hope is that two of the simulators will be close to each other, the assumption being that democratically this makes them both right. However, each may be as wrong as the other. From the point of view of an EPC contractor who has been using a specific simulator for years, the reason may be that it has always been done that way, and it has worked, so why change? Thinking like this encourages plants that are twice the size they need to be to continue to be built, and until such time as the contractor takes a look at some real plant performance data (or starts winning fewer bids), that is the way that they will continue to be built.

Two simulators will seldom produce the same answers. Simulation software principally consists of models for various unit operations, together with numerical methods or procedures for solving the sets of equations that pertain to each, and to the flowsheet as a whole. These equation sets consist of more than just heat and material balances. Even for a simple heat exchanger, physical properties are a necessary part of the model equation set, and the physical properties calculated by the model depend on the database used to fit the properties' models in the first place. So, there are two factors that will almost certainly differ between simulators: the properties database (which, incidentally, every user of software should always check against real data), and the model (regression) equations used for numerically representing the properties – and that is just for a simple heat exchanger with a single phase.

All commercial simulators will invariably provide different answers for the same problem. As such, making comparisons between simulators is an exercise in futility. At the conclusion of the exercise, all one can say with certainty is that they are different. On their own, comparisons between simulators tell you nothing more. So, are simulators data? The answer is no; one cannot be used for benchmarking another. They are models, and are most assuredly not data.

Conclusion 5

Simulations are not data, they are models. One cannot be used to benchmark another. Trying to do so makes the implicit assumption that the benchmark standard is right. If it is indeed right, why would anyone benchmark anything else against it; after all, one already has the 'right' simulator.

Comparisons are often made between a simulator and solvent supplier or process licensor data, but just what is this data? Solvent suppliers and process licensors, too, use simulators to assess the likely performance of their solvent or design in a particular plant configuration. In fact, many of them use a simulator with a mass transfer rate basis. In most cases, suppliers and licensors must provide performance guarantees. The performance they are guaranteeing is not what their simulator says, but with the results of simulation after a conservative safety factor has been applied.

For example, a solvent supplier may project that a solvent carbon dioxide (CO_2) lean loading of 0.01 moles/mole can be achieved, for instance, when the simulator says 0.003 would be reached. Is the value 0.01 moles/mole data? Indeed, is either value data? The answer is that neither one of them is data. The value 0.01 moles/mole is the guarantee. It is not data; rather, it is a very rare event when a supplier or licensor provides a customer with real data at all.

Comparisons between simulators and so-called supplier data are to some extent meaningless, although perhaps not quite as meaningless as comparisons between simulators themselves. If your simulation has better performance than the solvent supplier (or process licensor) is guaranteeing, both may be right; but, if simulated performance is considerably poorer than the solvent supplier's guarantee, something is wrong and further investigation is warranted. The main point is that supplier guarantees should not be mistaken for data, which they most definitely are not.

Conclusion 6

Comparisons against solvent supplier and process licensor data are almost as meaningless as comparisons against another simulator. Commercially, suppliers and licensors tend to be conservative. They have to provide guarantees, and they do not want to have to replace the new solvent or equipment with another. Supplier reports, however long and official looking, are not data.

So just what is data? Data is nothing more or less than what is measured in the field from an operating plant. This does not necessarily mean that the data is good data, but by definition it is data. However, if it has not been measured in the field (or the laboratory), it cannot be called data. At a minimum, data to be used for benchmarking a simulator must have been measured using reliable flow, temperature and pressure instrumentation, preferably calibrated (instruments that have been merely zeroed and spanned have not been calibrated). Piping line-ups must be correct, online analysers must be calibrated, laboratory procedures validated, trays installed level without too many valves missing, and packing properly installed with reliably-uniform liquid distribution. Measured pressure drop values should compare favourably with internals supplier calculations so as to minimise (but not eliminate) the possibility of foaming and fouling. Reasonable material and energy balance closure is a requirement. These are some of the things that characterise good data.

Conclusion 7

Data is what is measured in the field from an operating plant. Heat and material balances must be close to within reasonable tolerances for data to be strictly valid as a benchmark. Users of simulation tools want to be convinced that the tool that is being used is both reliable and accurate. The only truly valid benchmark for a simulator is real data measured in the field.

Conclusion 8

The simulator should agree reasonably closely with the measured performance data, without adjusting or providing any factors to force agreement (in other words, the simulator must be truly predictive).

If all that operators are doing is comparing with another simulator, or comparing with solvent-supplier or process-licensor data (or simulations), then they do not have a valid benchmark. This makes the comparison worthless for the intended purpose of validation. Results from simulations and solvent supplier guarantees are not data; only measurements are data.

To be continued

Part two of this article will present several case studies involving real process and performance data as measured in operating plants, and compared with simulations that have not been fitted in any way. The comparisons will reinforce the conclusions enumerated here.

Notes

1. Taken from ‘Process Heat Transfer’, McGraw-Hill Book Co., New York, (1950).
2. There are exceptions, one being distillation involving three phases where the computations to determine even the existence of a third phase can be quite complex. Indeed, for many chemical systems, the phase equilibrium models are complex enough that high-quality computer models of the thermodynamics are necessary for accurate results.
3. ProTreat is a registered trademark of Optimized Gas Treating, Inc.