The CONTACTOR™

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What's Data and What's Not

People who use simulation tools are always concerned about whether the results of their simulations are correct or not, or whether they're even reasonably accurate. This kind of concern is only natural and it's certainly justified. After all, you may be called upon to guarantee a design, or the performance of certain tower internals, or a solvent formulation. If you're troubleshooting, you certainly don't want to be led up the garden path to a wrong solution or even to no solution at all because the simulation failed to model real behavior. So what are some of the approaches 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 vendor. Sadly, comparisons between a simulator and real, measured plant performance data are made much less frequently. Simulators are intended to show what a column or unit *should* be doing if it has been correctly built and it's being operated properly, and that's certainly the case for the ProTreat® simulator.

Probably the most common reason people make comparisons between simulators is because they lack reliable data—perhaps they're hoping that two of the simulators will be close to each other, the assumption being that this makes them both right; whereas, 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's the way we've always done it, it's worked, so why change?" Thinking like this allows plants to continue to be built that are twice the size they need to be and until such time as the contractor takes a look at some real plant performance data, that's the way they'll continue to be built.

It's a fact that no two simulators will ever give the same answers. Simulation software consists principally of models for various unit operations together with methods or procedures for solving the sets of equations that pertain to each such model and the flow sheet 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 model in the first place. So already we have two factors that will almost certainly differ between simulators: the properties database and the model (regression) equation used for fitting, and that's just for a simple heat exchanger with a single phase.

Two different simulators will calculate unit operations involving vapor-liquid equilibrium (VLE) quite differently because the phase equilibrium models will differ. Not only will there be differences in the VLE data themselves, but the models can span a huge range of complexity and accuracy, all the way from ideal gas plus ideal liquid solution models to VLE packages that use equations of state and activity coefficient models of various kinds. There is yet another, and perhaps more significant difference between models for columns in different simulators.

There are two fundamentally different models for columns: ideal stage and mass transfer rate based, and they will give different answers almost all the time. ProTreat uses the mass transfer rate-based model. Other commercial simulators use ideal stages, either with user-supplied efficiencies or with other modifications such as ideal stage residence times and thermal efficiencies in an attempt to make a connection between real trays or real packing and ideal stages.

In ProTreat's case a well-established database of tower internals (trays and packing) mass transfer performance data is used so there is

automatically a direct connection to real trays and packing. With other simulators the user has to supply a best guess for the missing parameters until a match with the intuitively expected performance (or less often with measured field data) is achieved. In any event, all the available commercial simulators will invariably give different answers to the same problem. Making comparisons between simulators, therefore, is an exercise in futility. At the end of the day all one can say with certainty is "They're different". On their own, comparisons between simulators tell you nothing more. So, are simulators data? Absolutely not! One cannot be used for benchmarking another. They're *models*, *not data*.

Comparisons are often made between a simulator and solvent vendor "data", but just what is this data? Solvent vendors, too, use simulators to estimate the performance of their particular solvent in a particular plant configuration. In fact, most of them use either ProTreat or an in-house simulator with a mass transfer rate basis. Solvent vendors have to provide performance guarantees for their solvent. The performance they are guaranteeing is not what their simulator says, but with the results of simulation after a sizable safety factor has been applied. For example, a solvent vendor may project that a solvent CO2 lean loading of, say, 0.01 moles/mole can be achieved when, in fact, the simulator says 0.003 would be reached. Is the value 0.01 moles/mole data? Indeed, is either value data? Absolutely not! The value 0.01 moles/mole is the guarantee. It's not data. In fact, it's a very rare occurrence when a solvent vendor provides a customer real data at all.

Comparisons between simulators and so-called solvent vendor data are to some extent meaningless as well, although perhaps not quite as meaningless as comparisons between simulators themselves. If your simulation gives better performance than the solvent vendor is guaranteeing, both may be right; but, if simulated performance is considerably poorer than the solvent vendor guarantee, something is wrong and further investigation is warranted. The main point though, is that vendor guarantees are most definitely not data. So just what is data?

Data is nothing more or less than what is measured in the field from an operating plant. That doesn't necessarily mean the data is *good* data, but by definition it is data. However, **if it hasn't been measured in the field it's not 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 zeroed and spanned *have **not** been calibrated*!). On-line analyzers must be calibrated, laboratory procedures validated, trays installed level without too many valves missing, packing properly installed with reliably-uniform liquid distribution. Measured pressure drop values should compare favorably with internals vendor calculations so as to minimize (but not eliminate) the possibility of foaming and fouling. So is reasonable material and energy balance closure. Those are some of the things that characterize good data.

As users of simulation tools, we all want to be convinced that the tool we're using is reliable and accurate. The only truly valid benchmark for a simulator is real data measured in the field on an operating plant in which

- All instrumentation has been shown to be reading correctly,
- On-line analyzers have been calibrated
- There are no leaking tube bundles in heat exchangers,
- Piping is lined up as expected for flow in the right direction,
- The solvent has been analyzed in detail, and the analysis includes heat stable salts,
- Tower internals details are actually known (tower drawings are often missing!),
- The internals themselves have all been properly installed, and
- Basic material and energy balances close to a reasonable degree.

In such circumstances, the simulator should compare reasonably closely with the measured performance data *without adjusting or providing any factors to force agreement* (in other words, the simulator should be truly predictive). But if all you're doing is comparing with another simulator, or comparing with so-called solvent vendor data, you do not have a valid benchmark, and this makes the comparison nearly worthless. Results from simulations and solvent vendor guarantees are *not* data. Only measured data is data!

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