The CONTACTOR™

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So What Simulator Should I Use? How to Decide

The short answer to the question posed by the title is to use the one that is consistently closest to the truth. But there are several subtleties embedded in this response.

The literature is replete with authors who insist on comparing simulators A, B, C and D with each other and invariably they conclude that they're all different, and they all give different answers. A recent work by Nagpal (2010) concluded that accurate "rate-based" process simulators are required for optimal design of SRUs and TGTUs but that there is considerable variability among commercial simulators. Nagpal's main conclusion was that reliable operating data from existing units are required to validate the simulator results. We applaud that conclusion wholeheartedly, but unfortunately the paper presented no data and therefore reached no conclusion with regard to which one of simulators 1, 2, 3 or 4 was better than the others.

A column simulator cannot be truly predictive unless it is *mass transfer* rate-based. This does not mean just "rate based". It means that the simulator must be based on treating the columns (both absorbers and regenerators) as pieces of equipment whose performance is determined by *mass transfer rates*. All too often the term "rate based" is applied to simulators that use equilibrium stages and attempt to incorporate reaction kinetics by using an inappropriate (wrong) model such as modeling the reacting liquid on a tray as a CSTR. This has been addressed in some detail in a previous issue of the Contactor™ (Volume 4, Number 3). Suffice it to say that if a simulator relies on the user providing the residence time on a theoretical tray (whether realistic or not) to obtain a match with plant data, it is obvious that (1) the simulator is built on incorrect physics and (2) it is not really predictive because *it has to be fitted* to plant data.

Vendor proposals are commonly used as benchmarks for comparing simulations for new designs. But vendor proposals are themselves based on simulation so this approach once again boils down to comparing tools with tools. After all, solvent vendor runs are not data — only plant performance or field data or VLE data are data. Any data, whether it be simple VLE data or the plant performance or field data must first be *validated* before they can be used reliably to benchmark a simulation tool.

The reliability of solvent vendor runs depends on the simulator the vendor used and sometimes on specifically who performed the simulations. It seems to be a common practice for solvent vendors to assume amine lean loading values and then proceed with absorber simulations as though the lean loadings were chiseled in stone when, in fact, they may be quite erroneous values.

There's no benefit from using the results of one simulation tool as "data" for benchmarking another because the tools are just that: they're tools whose purpose is to approximate reality. With any process model, the *best* that can be hoped for is a reasonably accurate representation of the real plant operations. If you measure the results from one tool against those from another, you're implicitly assuming one of them is right when in fact neither may be. The proper way to test a simulator is against real, measured, and validated, plant or unit ***performance*** data. There is just no other way.

The first requirement of any simulation tool is that it's based in sound, solid science and good engineering. If your tool uses ideal or equilibrium stages, no matter how embellished, it simply doesn't qualify as reliable in new situations, because there is always the chance that the column is mass transfer rate controlled and there is no way for an equilibrium stage model to know this *a priori*. Reliable prediction is a critical requirement, unless the engineer wishes to play Russian roulette with the design.

The second requirement is that the simulator should ask for no data that cannot be directly measured in the plant. Asking the user to input tray efficiencies, HETPs or ideal stage residence times is an immediate disqualification. Such information (estimates) are used to force the simulator to match plant data. But if you have no plant data, there's not much to match against except maybe performance data from a "similar" plant operating under "similar" conditions. Know-how and rules-of-thumb can be helpful, but by definition can never be predictive.

The third requirement is that the simulator has been thoroughly test for its ability to predict a large amount of actual plant ***performance*** data. This means the simulator has been run on the basis of known plant parameters but without knowing beforehand what the actual performance is. Performance is revealed only ***after*** the simulations have been run. To be useful *and* reliable, the simulator must be able to predict performance without already knowing the answers.

The fourth requirement is for the simulator to be capable of predicting both regenerator and absorber performance. This is critically necessary because absorber performance leans so heavily on the quality of the solvent the regenerator is actually producing. If you can't simulate regenerator performance, the whole simulation is up in the air.

The fifth requirement is for the simulator to be capable of accurately predicting the performance not just of trays, but of random and structured packing as well, and without recourse to fitting parameters such as HETPs. Packed column performance quite obviously depends on the packing type (random vs. structured, and brand) as well as on packing size. This must be the case simply because the surface area of the packing determines the wetted area, and the type of packing affects the separation performance.

If your amine treating simulator uses equilibrium stages *in any form* it is using out-of-date technology and it should be leaving you with a very unsettled feeling about the certainty of your designs. Mass transfer rate-based commercial simulation has been around since the mid-1980s. In the ensuing 25 years it has proven itself time and again to be reliable and fully predictive, not just in amine treating but in reactive and catalytic distillation, azeotropic distillation and complex extractive distillation applications.

Mass transfer rate-based simulation is used by all the leading amine solvent vendors in North America, Europe and Asia to generate proposals for gas plants, refinery systems, ammonia plants and LNG facilities. And in most cases ProTreat™ is the foundation for simulation. ProTreat is the only mass transfer rate-based commercial simulator designed *specifically* for gas treating. ProTreat has been thoroughly tested by others against an enormous amount of plant data collected during plant testing, optimization and benchmarking in every corner of the world. As one licensee has stated more than once, "It's uncanny how close ProTreat comes to what we see in the field no matter where we are".

The tremendous amount of pre-design work being done in post-combustion carbon capture is providing us with the opportunity to demonstrate the power of mass transfer rate-based modeling as embodied in ProTreat™. By providing merely a few vapor-liquid equilibrium measurements for a new solvent and an estimate for the reaction kinetic rate between CO_2 and the active ingredient, we have shown (Weiland et al., 2010a, 2010b) how it is possible to build a *virtual pilot plant* to test out various ideas and explore the limits of a proposed process. There is no longer a need to go to the expense of actual pilot planting until a really promising candidate solvent or process is identified.

References

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