The CONTACTOR™

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Confidence in Design — Are All the Parameters Real?

There's been a lot of chatter lately about rate based versus equilibrium based column models for amine plant simulation, but no one seems to have defined the terms. The distinctions can be made quite clear, however, by being a bit more specific. So before we compare and contrast these two classes of models, let's define exactly what we mean.

An equilibrium stage model is obviously one that uses or calculates the number of ideal or theoretical stages required to do a specified separation. The McCabe-Theile stepping-off-stages approach is the quintessential example of an ideal stage model, one that can be used graphically. Chemical reactions complicate things, but it might be possible to modify the ideal stage calculations to account in some way for reaction kinetics. This was discussed in some detail in *The Contactor*, Vol. 4, No. 3. To accommodate reaction kinetics in the solvent within a theoretical stage requires one to invoke a reactor model, and the CSTR is the obvious choice for the often well-mixed liquid on a tray. This leads naturally to the requirement that one specify the residence time of the theoretical stage, i.e., of the CSTR. But does the inclusion of a CSTR sub-model entitle the resulting column simulation to call itself rate based? Perhaps, but only at the risk of being disingenuous. After all, such a model does not calculate transfer rates of components between phases in order to *determine* the separation (simulation's main objective). At the very best, mass transfer rates are calculated only *after the fact* when the number of ideal stages has been estimated and an efficiency has been applied. Therefore, we posit that any model that uses ideal stages *in any way at all,* with or without a reaction kinetics correction, is inherently *not* truly, genuinely, rate-based, and it is not legitimately entitled to advertise itself as such.

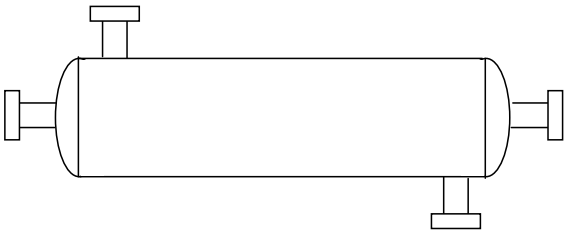
The terms rate model and rate-based model are thrown around rather loosely. We opine that these terms should be reserved for models that are based on calculating and using mass transfer rates between the phases *to determine the separation*. They are not quantities calculated after-the-fact.

A genuine mass and heat transfer rate-based simulation model uses sub-models for the transfer of components through the interface dividing the two phases to calculate the transfer rate of the component. Of course, the mass transfer rate model uses phase equilibrium because this sets the maximum possible separation, and it takes part in determining the driving force for absorption or stripping. It uses reaction kinetics, too, because reactions enhance the mass transfer. But it does **not** require the user of the model to propose values for artificial parameters or to adjust anything at all to achieve a "***match***" to column performance data. There is simply nothing to adjust and often there are no data to adjust against anyway, e.g., in a new design. A mass transfer rate-based model determines transfer rates between phases *to calculate directly the separation* achieved by a real tray. To match temperature profiles, the thermal efficiencies used by the ideal stage method are not required by true mass transfer rate models. Temperatures are matched automatically—thermodynamics and mass transfer see to that. In other words, the temperatures are a direct consequence of heat release by reaction and the transport of water between the phases (a mass transfer rate process), not some conjured up thermal efficiency.

In a nut shell, ideal stages completely ignore mass transfer, the very process that determines the ultimate separation achieved on a set of real trays or a height of real packing. There is no connection with what is real; instead, most aspects are simplified and extremely idealized. Mass transfer calculations, on the other hand, focus on the mass transfer process itself, and on real trays or packings. The two kinds of model are at

completely opposite ends of the spectrum. The mass transfer rate model uses engineering science and reveals the process in fine detail—the ideal stage model (modified for kinetics or otherwise) simplifies things to the extent that all detail and all connection with reality are lost.; so are the predictive ability and the confidence one can place in results.

A fairly close analogy that helps explain the elements of a mass transfer rate model is a conventional heat exchanger, say a water heater with steam on the shell side. The shell-side temperature is constant but on the tube side (one-pass) the water temperature gradually rises. Following the equilibrium stage tower model, if this were an ideal stage heat exchanger, the outlet water temperature would equal the steam temperature. Specifying an ideal exchanger efficiency would allow one to ***match*** the observed outlet temperature. But the efficiency would be the value needed to achieve a match. The idealization of an equilibrium stage exchanger had to be corrected empirically. This certainly cannot be called predictive—it just allows a match to be made. Could this model be used to design another exchanger? Yes, but only if the conditions were the same. Could it be used to "predict" performance at other operating conditions (different water flow rate, different steam temperature)? Yes, but with decreasing reliability as conditions move away from the matched case.



Mass transfer is much harder for ideal stages—there are many components, and complex equipment that ideal stages ignore. If the design engineer is required to know or estimate number of ideal stages, residence time (i.e., volume) of an ideal stage, mass transfer efficiency, the thermal efficiency of trays, or the packed height equivalent to a theoretical stage, the design will be only as reliable as the estimates. Even if one can fit a given set of plant data, the reliability of extrapolation to other conditions is questionable because the model inherently does not contain any information on the reality of how plant parameters affect performance The fault lies in the inadequacies of theoretical stages and the inability of reaction kinetics alone to cover the shortfall. Such models are not predictive, they are not rate based, and calling them such obscures their true nature as much as the models themselves obscure the details of column behavior. When a model must first be force matched to plant data, the answer is already known so one wonders why the simulator is even needed, apart from doing material balances.

Real heat exchangers are designed using shell- and tube-side heat transfer coefficients correlated with baffle size and spacing, tube Reynolds numbers, and thermal conductivities to name a few. One can use either charts such as exist in the classic heat transfer books such as Kern's *Heat Transfer*, or using HTRI or equivalent software. By assuming continuity of heat flux across the tube walls (steady state) the individual heat transfer coefficients and the tube wall resistance are combined into an overall heat transfer coefficient. Using this with a log mean temperature difference (LMTD) one calculates the heat transfer rate. In other words, one predicts the heat exchanger's performance. The approach is a **heat transfer rate-based model**, but it's not generally known by that name. The parallel with mass transfer is extremely strong. Heat transfer rate-based exchanger models are fully predictive and we're so used to that fact we don't even question it. Mass transfer rate based models are equally predictive, albeit computationally a lot more intensive.

A genuine mass transfer rate-based column model uses (1) internals details such as tray construction or packing brand, material, and size, (2) tower diameter, (3) number of actual, real trays or physically packed height, (4) inlet stream compositions, temperatures, pressures and flow rates, and a database of physical properties, plus phase equilibrium and kinetics correlations, ***to predict mass transfer rates, from which column performance itself is predicted.*** There are no adjustable parameters and the answers aren't known beforehand so there's nothing to fit. The model is used to calculate directly transfer rates and performance, not to fit it, and not to calculate mass transfer rates after the fact. The parameters are real and predictions are reliably accurate.

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