Mass Transfer Rate Models and Reliability

In a previous issue of The Contactor (Vol. 4, No. 3, May, 2010, *Conflicted Meanings of Rate Based*) we discussed various interpretations of the term "rate based" without ever describing the anatomy of a mass transfer rate model itself. Suddenly, in the last few months various simulation software vendors have laid claim to having mass transfer rate-based models. Here, we point out (1) what a model's characteristics must be to qualify as rate based, (2) why it is a retrograde step to offer a multitude of mass transfer coefficient correlations, and (3) why selecting packed column segmentation doesn't have to be confusing and is *not* a source of uncertainty.

As the user of any simulation tool that applies the mass transfer rate-based approach, you will be unable to take full advantage of the power of such a model unless you have some understanding of how the model is constructed. Figure 1 is a conceptualization of the absorption process when it is accompanied by chemical reaction, e.g., in an amine-based process. The absorbing gases reach

Figure 1   Mass Transfer from Gas to Liquid

the gas-liquid interface by diffusion; they cross the interface by absorption; then they diffuse into the bulk liquid while reacting with the amine. Reaction products are formed, generating heat which diffuses back into the gas (a) by sensible heat transfer, and (b) by the transport of evaporated water. In simple terms, the transfer rate of a component, A, *through the gas to the interface* is

$$R_A = k_{A,g} a (p_A^b - p_A^i),$$

and *from the interface into the liquid* it is

$$R_A = k_{A,l} a E_A (c_A^i - c_A^b)$$

At steady state these rates are equal. The terms $k_{A,g}$ and $k_{A,l}$ are gas- and liquid-side mass transfer coefficients, a is the interfacial area, i and b refer to the interface and the bulk phase, and p and c are partial pressures and concentrations. The quantity E_A accounts in precise mechanistic terms for the effect of the chemical reaction on mass transfer.

With apologies for using equations, the first requirement for a model to be considered truly rate-based is that it uses the above equations for the **direct** calculation of the mass transfer rate (absorption or stripping). If a model uses equilibrium stage calculations and *then* estimates an efficiency or HETP using these equations, it is completely illegitimate to claim it to be rate based. At least two recent entrants into the rate-based field use this approach—they are not really rate based at all, and any such claims are at best disingenuous.

Other commercial simulation software packages offer mass transfer rate-based models. However, in doing so, they offer five or six different correlations for the mass transfer coefficients, usually developed from data taken in very small scale equipment. These vendors refer to each as a separate model, but offer no guidance as to which correlation (if any) is the *right* one, or even the better one, to use. As recent entrants to rate
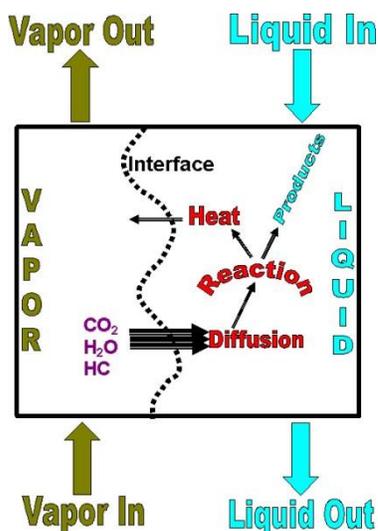
modeling, perhaps they simply do not know? But the result is that the user must guess which correlation to use, leaving the simulation results with unacceptable (and unnecessary) uncertainty. Indeed, it could be said that if you don't like one answer, all you have to do is choose another correlation until you get an answer you like. This argument has mistakenly been used by some to assert that a mass transfer rate-based model is analogous to guessing the efficiency or an HETP for use with ideal stages. On the contrary, performing the computation wrong five times is no substitute for doing it right the first time. All that's needed to do it correctly is the *right* mass transfer coefficient correlation.

ProTreat® uses correlations for mass transfer coefficients that, over a 12 year period, have been finely tuned to a very large amount of commercial performance data under a wide range of operating conditions, and in a variety of amine and physical solvent treating as well as other services (e.g. SWS and caustic). Although the correlations used in ProTreat's model are proprietary, we know that they are the *right* correlations simply because the results predicted by the model are invariably validated by actual commercial performance data in detail, including performance measurements on plants using random and structured packing.

Unlike trays, a packed column is a continuous contacting device. It has been stated by others that there is uncertainty in packed column simulation because there is no way to choose the number of segments into which the packing should be vertically subdivided for simulation. The implication is that segmentation is just another adjustable parameter, not much different from an efficiency, an HETP value, or a residence time on a theoretical stage. Nothing could be further from the truth. An early and very elementary lesson in Calculus I is to find the area under a curve, $y = f(x)$, by dividing the area into narrow slices and taking the limit as the width of the slices, Δx, becomes small and their number becomes large. Solving a packed column is similar to finding the area under a curve—the column is solved from one end to the other using an increasing number of smaller steps until further subdivision doesn't change the results significantly. It's not a question of uncertainty or expertise in selecting the correct segmentation; it's just a matter of improving accuracy until nothing further is gained by finer segmentation. One needs expertise to select an

HETP value for an ideal stage model—no expertise is needed to segment a packed column!

Figure 2 shows how the treated gas CO_2 content in a carbon-capture absorber containing 50 ft of FLEXIPAC® 3Y metal structured packing responds to segmentation. The 13 mole % CO_2 gas is treated with 30 wt % MEA. We simulated this 50 ft packed bed with segmentation ranging from 5 to 500 segments (10-ft to 0.1-ft segments).
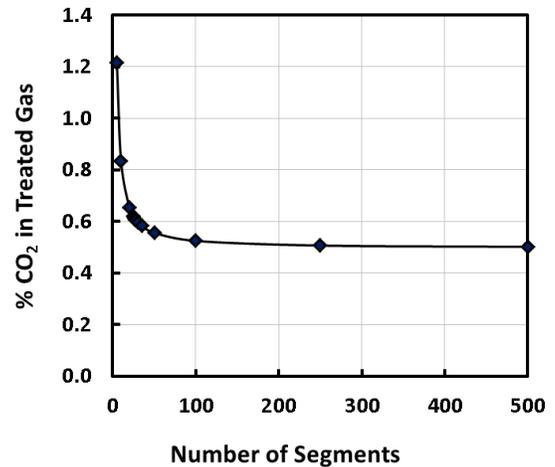

Figure 2   **Effect of Packing Segmentation on Carbon Dioxide in Treated Gas**

The figure shows that, just as expected, as the segmentation is made increasingly finer the treated gas CO_2 level asymptotes to a limit, in this case 0.500 mole % CO_2. Rough work can be done with as few as 25 segments (2 feet of packing per segment) but for a final simulation, 2.5 to 6 inches of packing per segment is preferred. Obviously there is nothing magic or requiring expertise to pick the right segmentation—getting it right is easy.

To summarize, (1) Any model must have certain well-defined characteristics to qualify as truly rate-based, (2) Mass transfer coefficients can be adequate or wrong—ProTreat's correlations are backed by 12 years of plant data and decades of research; they're right, (3) Knowing how to segment a packed column requires no expertise. Refuse to be misled by obfuscation.

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