The CONTACTOR™

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Approaches to Simulating Distillation and Absorption

Distillation of spirits has been practiced since the time of the ancient Greeks who ascribed sacred powers to the liquids that resulted from refining wine using stills such as the one shown in Figure 1. Dionysian cults incorporated these early spirits into religious rituals. Distillation and other phase separation processes have come a long way since then, and so have the ways they've been analyzed and computed. Figure 2 shows the progression of models and computational approaches to the design, analysis, and optimization of stagewise separation processes.

Figure 1 Ancient Greek Still

Prior to 1925, distillation and absorption columns weren't really designed in the modern sense of the word. They were constructed using experience embodied in rules of thumb.

The work of McCabe and Thiele† changed all that, allowing designs to be done rationally, at least for binary systems. A group of new concepts evolved such as the notion of key components, that allowed even multicomponent systems to be handled graphically. Slide rules and graph paper yielded to programmable calculators allowing simple separations to be done digitally, although still on the basis of McCabe and Thiele's ideal-stage concept. With digital computers, it became possible to do these calculations extremely rapidly and efficiently; however, it also became possible to treat a tower full of trays or packing on a *mass transfer rate basis*, just like heat exchangers had been done for the better part of the 20th century.

This was a radically new concept and a huge advance in separation process simulation. The first mass transfer rate-based models were developed in the mid-1980's, about 35 years ago. Unfortunately, and probably for pedagogical reasons, undergraduate education has remained rooted in the McCabe-Thiele era with the regrettable result that for most chemical engineers the antiquated ideal-stage model still reigns, complete with the unjustified descriptor, "state-of-the-art". But, it's not.

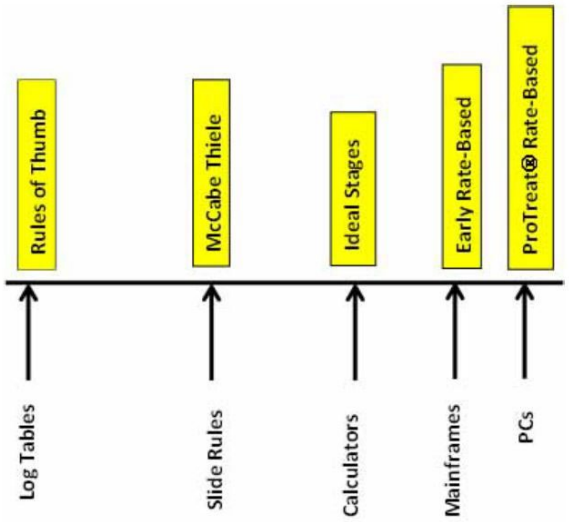

Figure 2 Paleontology of Separation Process Calculations

Ideal Stages

The ideal stage model requires only phase equilibrium and, for non-isothermal operations, enthalpy data. The Information needs are absolutely minimal—the model doesn't even need to know what, or even if, anything is in the column or, indeed, if there is even a column at all. In one sense, this is a distinct advantage—one has to know virtually

† W.L. McCabe & E.W. Thiele, *Graphical Design of Fractionating Columns,* Ind. Eng. Chem., **17**, 605–611 (1925).

nothing beyond phase equilibrium thermodynamics to arrive at an answer. Unfortunately, the practical value of the answer depends directly on the level of knowledge used to get it, and there are huge steps from an ideal stage to the realities of an actual column.

Ideal stage models can never be predictive, no matter how embellished by chemical reaction kinetics (an oxymoron to an *equilibrium* stage, in any case) and other accoutrements. *They can correlate, but they can never predict*. One might be led to believe that overall efficiencies are the way out, i.e., the connection between the ideal and the real. However, overall efficiencies are really nothing more than a disguised form of rules of thumb and operating experience. In distillation of similar hydrocarbons (e.g., alkanes), overall efficiencies are usually in the range 80-110%. But in absorption and gas treating, especially with reactions, efficiencies range from 5-80%, a 16-fold range, which *for a new situation* leaves the designer at sea in a storm aboard a dismasted rudderless ship. Prediction, let alone *reliable* prediction, is out of the question in new territory.

Efficiencies depend strongly on the species being transferred, and on conditions for the particular tray in the column. This may not be fatal in total acid gas removal applications for example, but in selective treating, ideal-stage simulation is unable to predict conditions properly anywhere inside the tower. The deficiencies of the ideal-stage model are a direct result of ignoring the very information necessary to make the simulator predictive. Surely, it's what's actually in the tower that matters—tower internals are critically important to determining performance, and ideal stage models ignore them.

Mass Transfer Rate-Based Models

The superficial difference between mass transfer rate-models and ideal stage models is that the mass transfer model uses the actual number of trays or packed bed depth in the tower but the distinguishing features go far beyond that. The critical parameters in the rate model are *mass and heat transfer coefficients and interfacial area*. These depend on physical properties and phase flow rates, as well as tray design details and the type, brand, size, and material of the random or structured packing. Transfer coefficients are tied up with the tower internals. The internals are responsible for the separation, so the simulator should be expected to know about the internals.

One might view it as a disadvantage to have to input all this information into a simulator. However, *without it one simply cannot predict performance*. It's not a disadvantage; it's an absolute necessity. One hears it said that this or that simulator has six or eight mass transfer rate models. However, such is not really the case. The real situation is that simulators use several different *correlations* for mass transfer coefficients and most offer the user a selection amongst them. OGT | ProTreat® presents such a selection but only amongst correlations based, not on small-scale laboratory data, but on large-scale data correctly representing actual commercial operations. These correlations *predict* with remarkable accuracy numerous sets of tower performance data for crossflow trays and an extensive list of commercial random and structured packings, developed *from commercial tower data*.

Having correlations for pressure drop and hydraulic capacity does not provide the simulator with enhanced credibility when it comes to mass transfer performance. In reality, of course, hydraulics and mass transfer are intimately connected, but in a simulator, there is a real connection only if the tool's developer ensures the connection is actually made.

Another common misconception relates to the discretization of packed bed heights into a number of small Segments. *The number of segments is not an adjustable parameter* used to tune the results. Just as in numerical integration to find the area under a curve, columns are segmented finely enough to minimize numerical discretization errors. However, discretization must be *coarse enough to account for axial dispersion (mixing)*. Each segment is treated as a well-mixed cell. Thus, as the number of segments is increased (by making them ever finer) the series of segments approaches plug flow with no back mixing whatsoever—not a good representation of a device with significant axial mixing. Likewise, mixing models for the liquid flow across trays do not become problematic when tower diameters get large. Instead, as tower diameter increases number of tray-passes increases, keeping flow path length roughly fixed, along with cross-tray back mixing.

Connection between Ideal-Stage and Rate-Based Models

A mass transfer rate model of a column necessitates providing a lot of information about tower internals. Some information may not be available; after all, sometimes tower drawings go missing or they may not reflect changes made during a revamp. However, it is always possible to supply reasonable values for missing parameters such as weir height, percent active area, and tray spacing. Certainly, providing an estimate for some parameters is far superior to not recognizing the tower has any internals at all. And a solid mass transfer rate model can even be used for backing out a value for the overall efficiency or the Murphree tray efficiency needed by an ideal stage model to reproduce known performance. The reverse is impossible—truly reliable prediction from ideal stages is only possible when the answer is already known!

If the mass transfer rate-based simulator you are being offered uses a thermal efficiency, or mentions stages, it is either unreliable, or under the hood it's not a true mass transfer rate-based model. Mass transfer rate-based simulation results do *not* need to be checked against an ideal stage model.

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To learn more about this and other aspects of gas treating, plan to attend one of our training seminars. For details visit www.ogtrt.com/seminars.