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Editorial

Today's Distillation Modeling

For those of you wondering what exactly is on the cover of this month's *CEP*, step back nearly 500 years ago and think chymistry, the archaic spelling of chemistry, which was once synonymous with alchemy. The image is a distillation apparatus from the hand-colored title page of the 1512 edition of Hieronymus Brunschwig's *Liber de arte distillandi*, reproduced with permission from the Eddleman and Fisher Collections at the Chemical Heritage Foundation. We thought this would certainly catch your attention on what is probably the workhorse of all unit operations — distillation.

We've certainly come a long way since 1512. There are a multitude of textbooks available that discuss distillation, and, as the authors of this month's cover story (pp. 28–39), Ross Taylor, Rajamani Krishna and Harry Kooijman, point out, "Chemical engineers have been solving their distillation problems using the equilibrium stage model since Sorel first used the model for the distillation of alcohol over 100 years ago." However, the actual conditions of a column are often far from equilibrium. And as the authors note, "...chemical engineers have long been aware of the fact that the streams leaving a real tray or section of a packed column are not in equilibrium with each other. In fact, the separation actually achieved depends on the rates of mass transfer from the vapor to the liquid phases, and these rates depend on the extent to which the vapor and liquid streams are *not* in equilibrium with each other."

The obstacle in modeling the actual conditions stems from the the difficulty in solving non-equilibrium, or rate based, equations. The complexity of these equations was so great, that many considered them impractical to solve. But, computing power has increased to the point where equations that were once thought to be too complex to solve, can now be calculated relatively quickly. And this is the case in point for non-equilibrium modeling. Today's powerful computers now make it possible to model actual conditions, thereby enabling engineers to model more accurately than ever before. Taylor, Krishna and Kooijman mention a few software programs that already contain non-equilibrium models. These include RateFrac from AspenTech, ChemCAD from ChemStations and ChemSep from CACHE.

And just in case you're interested in alchemy, I would recommend reading, "Transmutations: Alchemy in Art," by Lawrence M. Principe and Lloyd DeWitt. It was quite an interesting and enjoyable read as I was researching for this editorial.

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