358e Feasibility Studies on Complex Batch Reactive Distillation

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Reactive distillation has become an attractive process technology in recent years because of the potential reductions in capital costs, operating costs, and environmental impact. It can be used to conduct processes that would be prohibitively complicated and unwieldy if handled in a conventional process consisting solely of many single-operation units. This is because conducting reaction and distillation simultaneously allows reaction to overcome the limitations of distillation (by circumventing azeotropes) and vice versa (by bringing reactions to near-completion)¹. The Eastman Chemical process for producing methyl acetate is a prime example of the benefits of reactive distillation².

When designing reactive distillation systems and before conducting numerous trial-and-error simulations and physical experiments, it is useful to understand under what circumstances reactive distillation can feasibly produce pure products. This paper builds upon previous feasibility studies on batch reactive distillation and adds new feasibility criteria to extend the applicability of batch reactive distillation. In previous work³, the feasibility criteria were determined for simple batch reactive columns conducting a single reaction of the form aK+bI \leftrightarrow cL+dH or bI \leftrightarrow cL +dH:

1) With an unstable node (UN) product that is reachable from the entire reaction equilibrium curve by simple distillation, a batch rectifier with a reactive pot can produce pure products regardless of the number of azeotropes or their dynamic properties. A symmetric result is obtained in a batch stripper with a stable node (SN).

2) If the products are an UN and a SN and are in the same distillation region as a part of the reaction equilibrium curve, then pure products can be produced in a batch reactive middle-vessel column (MVC).

Even though the above feasibility criteria apply to a wide range of azeotropic mixtures, there are many phase equilibrium systems that do not meet the criteria listed above for simple batch reactive columns (rectifier, stripper, MVC). The simple batch reactive columns are not feasible if no node products exist that are reachable by residue curves from the reaction equilibrium curve.

For combinations of reaction and phase equilibrium where simple homogeneous reactive batch columns cannot produce pure products, we present three alternative methods:

1) If an unstable node heterogenous azeotrope decants to an almost-pure product and that azeotrope is always reachable from the reaction equilibrium manifold, then a batch reactive rectifier can produce pure products with a decanter.

2) If a homogenous entrainer allows extractive section profiles to connect the reaction equilibrium manifold to an entrainer-product binary edge, then a homogenous batch reactive extractive distillation (BRED) column can produce pure product. The feasibility calculations for this system are based upon the feasibility calculations for continuous reactive extractive distillation⁴.

3) If the above two criteria are not met, then an entrainer that induces an unstable node heterogenous azeotrope between itself and one of the products should be used in a rectifier, a middle-vessel column, or a BRED column.

References

1. Malone MF, Doherty MF. Reactive distillation. Ind. Eng. Chem. Res. 2000; 39: 3953-3957.

2. Agreda VH, Partin LR, Heise WH. High purity methyl acetate via reactive distillation. Chem. Eng. Prog. 1990; 86(2): 40-46.

3. Guo Z, Ghufran M, Lee JW. Feasible products in batch reactive distillation. AIChE J. 2003; 49: 3161-3172.

4. Guo Z, Chin J, Lee JW. Feasibility of continuous reactive distillation with azeotropic mixtures. Ind. Eng. Chem. Res. 2004; 43: 3758-3769.