A Novel Hybrid Simulation-Optimization Approach for the Optimal Design of Multicomponent Distillation Columns

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Summary

This work presents a hybrid tray by tray simulation-optimization approach for the optimal and rigorous design of multicomponent distillation columns where, for a given feasible separation, convergence is almost always guaranteed in calculation times comparable to those used by commercial simulation packages. However, in this case the total number of stages and the optimal feed location are simultaneously determined. The distillate flow rate and the reflux ratio can be optimized in an outer loop providing the method a great flexibility. The commercial process simulator Hysys® has been used to solve the rigorous VLE using the available thermodynamic models such as NRTL, and MatLab® to implement the optimization algorithm.

Introduction

Whether simulate a distillation column can be a challenging problem, especially for high non ideal mixtures, design a distillation column is even a much more complex problem. While in simulation problems it is necessary to specify the total number of stages, all the feeds locations, all the side draws as well as the operating conditions, when we design a distillation column we are interested in calculating the distillate and residue flows, the number of stages and the optimum feed(s) location for a specified separation of components in products, that is to say that the design methods focus on the best column configuration for a specified separation.

Due to the inclusion of very efficient simulation algorithms in commercial packages the design of distillation columns has been usually performed by successive simulations [1,2]. However, this procedure is very time consuming and of doubtful utility when trying to evaluate optimal sequences of interrelated columns.

Methodology

Generalized scheme of a distillation column

Schematic representations of the internal existing streams at the zone connecting consecutive sectors in the case of a generalized feed side stream (GFK) for different thermal conditions:

Hysys Flowsheet: a) condenser calculation b) tray by tray calculations

Conclusions

A direct design method has been suggested and applied to different cases of ternary mixtures with very satisfactory results. This procedure, which can be easily completed and combined with other algorithms proposed to calculate distillation boundaries [3,4], is based on very simple concepts of tray by tray calculations methods, such as the extended Ponchon-Savarit method [5,6], and has the following characteristics:

- ✓ It is a design method very robust. The convergence, if the postulated separation is feasible, is almost always guaranteed.
- ✓ A near optimal design is obtained at each iteration, with their distillate and residue flows and composition, optimum feed stage location as well as the number of stages for the specified separation.
- ✓ Its extension to multiple feed, saturated liquid or vapour product, and heat addition or removal ($V_{GFK} = E_{GFK}/\lambda_n$ and $L_{GFK} = -E_{GFK}/\lambda_n$) side streams is immediate.
- ✓ The speed of convergence is similar to those in standard simulation packages.

References

- [1] Douglas JM. Conceptual Design of Chemical Processes. McGraw-Hill. 1988.
- [2] Doherty MF; Malone MF. Conceptual Design of Distillation Systems. McGraw-Hill. 2001.
- [3] Reyes-Labarta JA; Serrano MD; Velasco R; Olaya MM; Marcilla A. Approximate calculation of distillation boundaries for ternary azeotropic systems, Ind. Eng. Chem. Res. 2011, 50, 7462-7466.
- [4] Reyes-Labarta JA; Caballero JA; Marcilla A. Numerical determination of distillation boundaries for multicomponent homogeneous and heterogeneous azeotropic systems. ESCAPE20 (Computer Aided Chemical Engineering). 2010, 43, 3908-3923 (<http://hdl.handle.net/10045/14203>).
- [5] Marcilla A; Gómez A; Reyes J. New Method for Designing Distillation Columns of Multicomponent Mixtures. Latin American Applied Research International J. on Chem. Eng. 1997, 27, 51-60.
- [6] Reyes JA; Gómez A; Marcilla A. Graphical concepts to orient the Minimum Reflux Ratio Calculation on Ternary Mixtures Distillation. Ind. Eng. Chem. Res. 2000, 39, 3912-391.

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