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Graphical techniques for analysing and synthesising separation processes

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ABSTRACT

Recently, Column Profile Maps were developed as a generalized, graphically based distillation synthesis method. Unlike several other synthesis methods, it is not specific to any configuration and therefore allows the designer to devise almost any separation before being constrained by equipment. This thesis attempts to expand the theory of Column Profile Maps.

Specifically, it is shown how new, and somewhat counter intuitive, column sections may be designed by merely imposing a sharp split constraint on a particular system. This special mathematical constraint makes it possible to maneuver topological characteristics of the system in almost any imaginable direction. This could lead to new designs being sought to exploit these profile behaviors, specifically in columns that require internal column sections (complex columns).

Thermally coupled columns have received considerable attention for their ability to drastically reduce operating expenditures. Here, we have extended the Column Profile Map technique to encompass a systematic procedure for the design of single and multiple side rectifying and stripping units. It is shown how one may go about designing such columns rigorously without making simplifying assumptions with regard to the phase equilibrium behaviour and/or product specifications (as classical methods such as Underwood do), with the use of a Temperature Collocation method, as well as through a shortcut technique for rapid synthesis assuming ideal phase equilibrium behavior based on Column Profile Map eigenvectors. The efficacy of the shortcut technique is demonstrated with finding the best thermally coupled column comprising of a large main column and appending side-units. Naturally, the best structure is dependent on the objective function, and simple calculations presented here allow one to choose the best structure with regard to both heat quantity and quality. Furthermore, the eigenvector method allows one to construct an Attainable Region consisting of all potential designs for even the most complex column.

The Column Profile Map technique is also extended to Reactive Distillation, which allows one to graphically assess the complex interaction of phenomena. Valuable conclusions can be gleaned from this method, specifically that improving a single piece of equipment's performance may prove detrimental to the overall system's operation. The methods

developed here allow one to understand exactly why a complex process such as reactive distillation has some of the strange characteristics often reported in literature. Furthermore, it is shown how non-ideal phase equilibrium behavior may improve the column's operability and in fact improve the overall feasibility of the unit. Using this method, one may quickly assess desirable process chemistry, feed compositions, desirable phase equilibrium and equipment sizes. Again, an Attainable Region is presented which shows *all* possible modes of operation that would give rise to a predefined product specification.

Finally, computational techniques are presented which allows for swift calculation of stationary points in systems ranging from constant volatility to highly non-ideal, multi azeotropic systems. The importance of quickly and accurately knowing where pinch points are located, even in negative composition space, is demonstrated by critically looking at several design methods. Notably, it is shown that the Rectification Body Method is neither a necessary nor sufficient condition for design and cannot be safely extrapolated to complex column design. With knowledge of *all* pinch points and using the Column Profile Map technique it is shown how one may synthesise new and counter-intuitive column sections, so much so that azeotropes can be shifted outside the physically realizable space.