**An investigation of the controllability of optimal reactive
distillation processes**

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**Highlights**

* The reactive distillation column superstructure is solved based on an economic objective function
* The impact of the reaction kinetics on the final process design and associated cost is investigated
* The controllability of the design alternatives is evaluated in the frequency domain
* This work provides a methodology on how to synthesize a reactive distillation process, including its control system

**1. Introduction**

Over the last few decades, there has been an increasing focus on process intensification in an effort to reduce environmental impact and to improve the economic performance of chemical processing plants. Reactive distillation combines reaction and separation into one single unit, offering significant energy and capital savings as well as improvements in reaction selectivity and yield1-2. The combination of the two different phenomena in a single unit, however, makes the design, operation and control of the process more demanding due to the interactions between the reaction and the separation3. Although research has shed light on many aspects of reactive distillation, the extension of conventional distillation design techniques to reactive systems is still a challenge and thus, a rigorous method of reactive distillation systems design, which also includes consideration of the controllability of the system, has not yet been fully established4.

**2. Methods**

The concept of distillation column superstructures has been successfully applied in the past for the design of distillation columns5. In this work, this approach will be extended to consider reactive distillation column superstructures6 in order to determine structural and operational decisions, including but not limited to, total number of stages, feed stages location, reactive zones, existence of additional units (pre/side/post reactors) etc. Case studies are considered with different kinetic characteristics. The Mixed-Integer Non-Linear Optimization Problem (MINLP) formed aims to minimize the total (capital and operational) cost of the process, subject to constraints such as maximum number of stages, product purity etc. gPROMS ProcessBuilder is used for the simulation and the optimization due to its rigorous optimization capabilities. The optimal design is then considered in dynamic mode and the controllability indices of the dynamic system are finally generated within the frequency domain in MATLAB in order to investigate the controllability and stability of the optimal design alternatives.

**3. Results and discussion**

It will be shown how the existence of fast or slow reaction kinetics inside the distillation column impacts on the optimal process design and control. In addition, the difference in the optimal total cost found for the various systems will be evaluated in order to explore how reaction kinetics impact on the total cost of the process and whether this can be a reason to render reactive distillation less economically attractive for systems with certain reaction characteristics. Moreover, the controllability analysis in the frequency domain will demonstrate how fast or slow kinetics impact on the stability and controllability of a process, and how controllability can determine whether a process alternative is selected for further investigation or not.

**4. Conclusions**

In this work, a Mixed-Integer Non-Linear Optimization Problem (MINLP) is solved, based on the superstructure method, for the synthesis of an economically optimal design of a reactive distillation column given a specific separation duty (target product purity). Different case studies are considered (slow/fast kinetics) and the impact of reaction kinetics on the optimal process design and cost is evaluated. The controllability and stability of the design alternatives are also evaluated. This work provides a methodology for how to select the most suitable reactive distillation process design, based on the minimum total cost as well as on the controllability of the process, especially in cases when more than one process design configuration exists.

**References**

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