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Interpreting the dynamic effect of internal heat integration on reactive distillation columns☆

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ABSTRACT

In this work, the impact of internal heat integration upon process dynamics and controllability by superposing reactive section onto stripping section, relocating feed locations, and redistributing catalyst within the reactive section is explored based on a hypothetical ideal reactive distillation system containing an exothermic reaction: $A + B \leftrightarrow C + D$. Steady state operation analysis and closed-loop controllability evaluation are carried out by comparing the process designs with and without the consideration of internal heat integration. For superposing reactive section onto stripping section, favorable effect is aroused due to its low sensitivities to the changes in operating condition. For ascending the lower feed stage, somewhat detrimental effect occurs because of the accompanied adverse internal heat integration and strong sensitivity to the changes in operating condition. For descending the upper feed stage, serious detrimental effect happens because of the introduced adverse internal heat integration and strong sensitivity to the changes in operating condition. For redistributing catalyst in the reactive section, fairly small negative influence is aroused by the sensitivity to the changes in operating condition. When reinforcing internal heat integration with a combinatorial use of these three strategies, the decent of the upper feed stage should be avoided in process development. Although the conclusions are derived based on the hypothetical ideal reactive distillation column studied, they are considered to be of general significance to the design and operation of other reactive distillation columns.

1. Introduction

Research outcomes have demonstrated that distributing reactive section (RXS) strictly between rectifying section (RS) and stripping section (SS) is not always a good design option for the reactive distillation columns (RDCs) involving reactions with highly thermal effect, because the potentials of internal heat integration (IHI) between the reaction operation (RO) and the separation operation (SO) involved cannot be fully exploited [1–3]. Based on the second law of thermodynamics, we therefore devised three strategies, *i.e.*, extending the RXS onto the RS (for the RDCs containing endothermic reactions) or the SS (for the RDCs containing exothermic reactions), relocating feed locations, and redistributing catalyst within the RXS, for the reinforcement of IHI during process development [4–8]. Further studies have also indicated that these strategies, if cautiously used in a combinatorial way, are not only effective for enhancing the thermodynamic efficiency of the RDCs having reactions with highly thermal effect but also likely to yield favorable influences to process dynamics and controllability [6–9]. With regard to the detailed impact of each individual strategy on process dynamics and controllability, no systematic studies have been conducted, yet.

Recently, Kumar and Kaistha in a series of two papers addressed the influences of IHI (*i.e.*, through feed stage relocation and catalyst redistribution by superposing the RXS onto the SS) upon the controllability of an ideal RDC (involving a hypothetical exothermic reaction: $A + B \leftrightarrow C + D$) and a methyl acetate RDC [10,11]. They found that while IHI always presented favorable impact upon the controllability of the latter, unfavorable effect could be observed to the former. Based on these results they claimed that the impact of IHI upon the process dynamics and controllability of a RDC was case dependent. Although their interpretation on process dynamics and controllability appeared reasonable, almost no comprehensive explanations were given on the underlying interplay between process development and process dynamics and controllability. Moreover, their reinforcement of IHI in the ideal RDC was actually not well established. In fact, two places could be questionable and they are: (1) No necessary compensation for mass transfer driving forces was made to the SS after the extension of the RXS; and (2) an adverse IHI was introduced into the process design by descending the upper feed stage. For the first issue, the deficiency of

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mass transfer driving forces caused by the IHI between the RXS and the SS can present certain negative influences to the separation of the reacting mixture and consequently the reaction conversion, intensifying the interaction between the RO and the SO involved. For the second issue, the adverse IHI between the RXS and the RS can restrain considerably the attainable quality of the top product due to the pinch effect aroused, intensifying the interaction between the RO and the SO involved. These two issues might have been the main reasons that made IHI unfavorable to process dynamics and controllability. To gain a deep insight into the effect of IHI on process dynamics and operability, one has therefore to conduct correctly the reinforcement of internal heat integration before its impact on process dynamics and operability is studied.

The current article focuses on the dynamic effect of these three strategies, *i.e.*, extending the RXS onto the SS, relocating feed locations, and redistributing catalyst within the RXS, for deepening IHI between the RO and the SO involved in a hypothetical ideal RDC with an exothermic reaction: $A + B \leftrightarrow C + D$. With regard to each of the three strategies, its impact upon process dynamics and operability is examined through steady state operation analysis and close-loop controllability evaluation. Intensive comparison is also made in the aspect of static and dynamic behaviors between the process designs with and without the consideration of IHI. The underlying interplays between the three strategies for IHI and their impact on process dynamics and operability are analyzed, and some useful guidelines are generalized for IHI through the carefully combinatorial application of these three strategies.

2. IHI versus Process Dynamics and Operability

For a simple conventional distillation column, thermodynamic analysis reveals that its RS needs to release a certain amount of heat to approach reverse operation and functions generally as a heat source [12]. On the contrary, its SS needs to absorb a certain amount of heat to approach reverse operation and functions generally as a heat sink. The interpretations have served as useful guidelines for the development of various heat-integrated distillation columns so far [13]. For a RDC involving a reaction with highly thermal effect, the interpretations can still be applied for process synthesis and design and evolve recently into three strategies for process development, *i.e.*, extending the RXS onto the RS (in case of an endothermic reaction) or the SS (in case of an exothermic reaction), relocating feed locations, and redistributing catalyst within the RXS. These three strategies work to strengthen IHI between the RO and the SO involved and secure consequently great improvement in thermodynamic efficiency.

For a RDC, its dynamics and controllability are mainly determined by the combination between the RO and the SO involved. Inappropriate combination between these two operations is the primary reason that gives rise to complicated process dynamics and worsens consequently process controllability. Although IHI is aimed at the enhancement of thermodynamic efficiency, it is likely to modify the inherent process dynamics and controllability. Two reasons can be listed here. One is the resultant combination between the RO and the SO involved. A high thermodynamic efficiency is yielded with the more coordinated relation between the RO and the SO involved. The same can also be true for the resultant process dynamics and operability. The other is the reduction in the size of RDCs because IHI abates vapor and liquid flow rates and thus stage holdups, leading to a smaller time constant. Obviously, the former is much more prominent than the latter.

It should be indicated here that two characteristics of the scheme for IHI could degrade substantially the dynamics and controllability of a RDC. One is the sensitivity of the thermodynamic efficiency to the changes in operating condition, and the other is the occurrence of adverse IHI. For a derived scheme for IHI, if its thermodynamic efficiency appears sensitive to the changes in operating condition (*e.g.*, variations in throughput and/or product specifications), then the process gains are subject to changes, presenting definitely negative influences to process dynamics and controllability. In cases when favorable IHI is aroused along with adverse IHI (*e.g.*, relocations of the upper and/or lower feed stages), the resultant adverse IHI can restrict the RO and thus intensify the conflict between the RO and the SO involved. Therefore, interpreting the inherent characteristics of the three strategies for IHI is essential to ascertain their impact on process dynamics and controllability.

One fact should be pointed here that IHI (*i.e.*, extending the RXS onto the RS or the SS) reduces actually the mass transfer driving forces. The degradation in process dynamics and operability thus caused should not be attributed to IHI itself. To ensure the resultant process design with a satisfactory redundancy, the process designers have to make

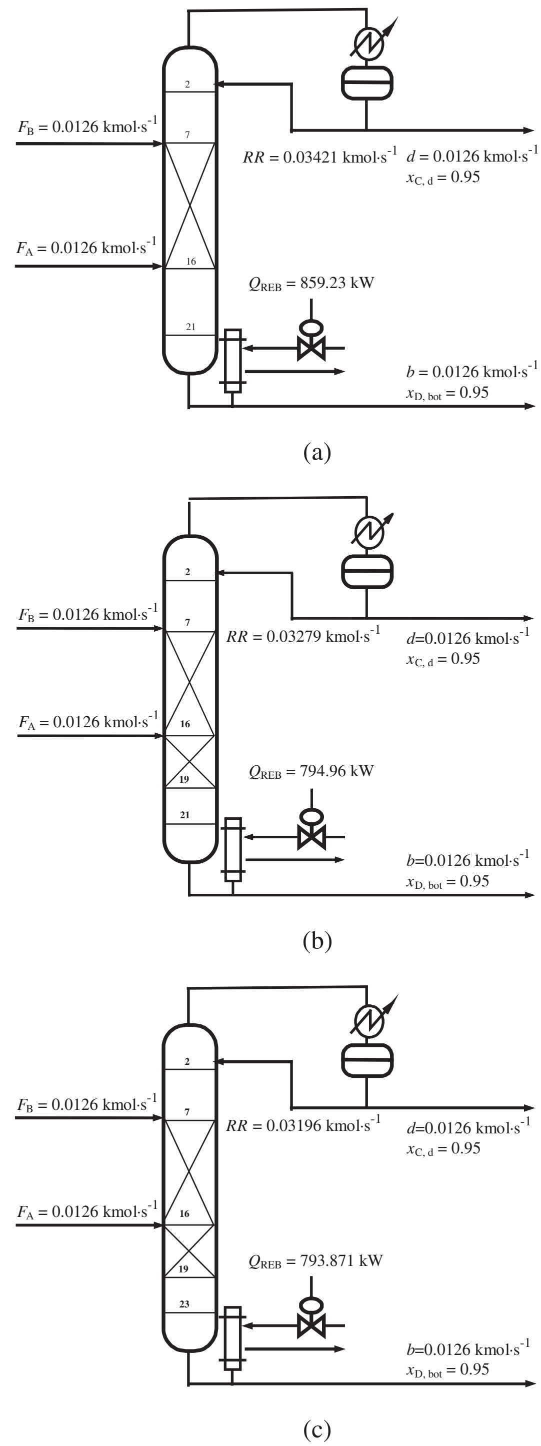

Fig. 1. Schematic of the ideal reactive distillation columns: (a) 5/10/5, (b) 5/10/5(3), (c) 5/10/7(3).