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Design heuristics for semicontinuous separation processes with chemical reactions

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ABSTRACT

Semicontinuous processes have been studied in recent years for many purposes, including extractive, azeotropic, and reactive distillations, and reactive liquid–liquid extraction. In this paper, using a continuous process as a base case, heuristics are introduced to create semicontinuous process designs. The methodology for synthesizing a semicontinuous separation process (including the process units, connectivity, control system, integration with chemical reaction(s), and choice of transitional modes) is presented based on experiences involving prior case studies.

Keywords: Semicontinuous; Process intensification; Process synthesis; Heuristics

1. Introduction

Semicontinuous processes have been introduced in recent years as a process intensification technique that allows multiple separations to be performed in one separation column (Phimister and Seider, 2000a,b,c, 2001; Adams and Seider, 2006, 2008, in press). A middle vessel (MV) is tightly integrated with the separation column, where the MV receives a stream from the column (the distillate, bottoms, or sidedraw), while the column simultaneously receives a feed stream from the MV. Depending on the process objective, a chemical reaction(s) could be integrated into the separation process, either in an external vessel, in the separation column, or in a CSTR used as a MV. The process operates in a forced cycle (or campaign), that is, a predefined sequence of operating modes, which may include charge steps, product collection steps, and transitional modes.

Because semicontinuous processes require fewer separation units than their continuous analogs, the capital costs of semicontinuous processes are normally lower than those of continuous processes. On the other hand, because semicontinuous processes use approximately the same equipment items as in batch processes, their capital costs are normally comparable. However, the energy requirements of semicontinuous processes are normally lower because semicontinuous processes do not involve column startup or shutdown modes often required in batch processes. Continuous processes, on the other hand, often require even less energy since they involve no such transitional modes and are heat-integrated more easily, yielding additional energy efficiencies. Given these considerations, the choice of either batch, semicontinuous, or continuous designs is normally determined by the desired plant throughput, as shown schematically in Fig. 1.

Specialty chemicals are typically produced at throughputs above those for which batch designs are preferable, but below those for which continuous designs are preferable. Also, the demand for specialty chemicals continues to rise (Scott, 2004; Van Savage, 2004; Chang, 2005, 2007). Consequently, semicontinuous processing is becoming increasingly attractive at intermediate throughputs. In the following sections, several semicontinuous processes are reviewed to highlight the differences in their configurations. In Section 2, these processes are generalized and heuristics are introduced that are well-suited for the design of semicontinuous processes, beginning with traditional continuous processes. Then, in Section 3, generalized control system principles are presented, and in Section 4, heuristics for designing transitions between the modes and phases of semicontinuous campaigns are discussed.

Abbreviations: 24DMD, 2,4-dimethyl-1,3-dioxolane; 2ID, 2-isopropyl-1,3-dioxane; CSTR, continuous stirred-tank reactor; MV, middle vessel; PDO, 1,3-propanediol.

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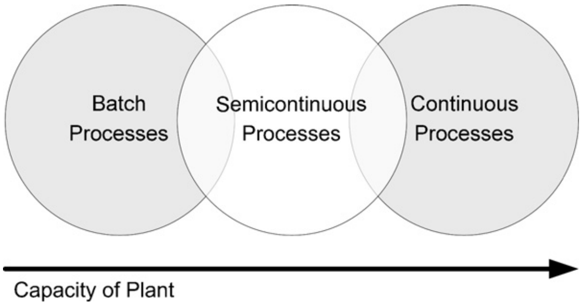

Fig. 1 – Desirable process design choices as plant capacity increases.

Continuous middle-vessel columns (MVCs) or batch middle-vessel columns (Bezzo and Barolo, 2005; Meski and Morari, 1995; Monroy-Loperena and Alvarez-Ramirez, 2004; Phimister and Seider, 2000d) are similar in configuration to the semicontinuous processes discussed herein. In MVCs, a middle vessel receives a sidedraw from the column, while simultaneously sending a feed stream to the column. It may also receive a parallel feed from upstream. The primary purpose of a MV in continuous or batch distillation is to adjust the dynamics of the process, usually to aid in control and disturbance rejection. However, in semicontinuous systems, the MV facilitates an extra separation step—without incorporating a second column. Other considerations involving MVCs are beyond the scope of this manuscript.

2. Process synthesis

2.1. Basic configuration

When creating a semicontinuous process, it is helpful to use a continuous configuration as a guide. For example, consider the separation of species A, B, and C, where species A has the highest volatility and species C has the lowest. In a typical continuous process, with no azeotropes, a mixture of species A, B, and C is separated using two distillation columns in series, as shown in the upper left panel of Fig. 2. This continuous scheme uses two process operations in sequence to: (1) separate A from B and C; and (2) separate B from C.

2.1.1. Scheme 1

An analogous semicontinuous design can be constructed using the same operations in one distillation column, with each operation occurring in a different phase of a cycle. In Scheme 1, shown in the upper right panel of Fig. 2, a semicontinuous process uses one distillation column and two middle vessels. In the first phase of operation (Phase I), the first MV

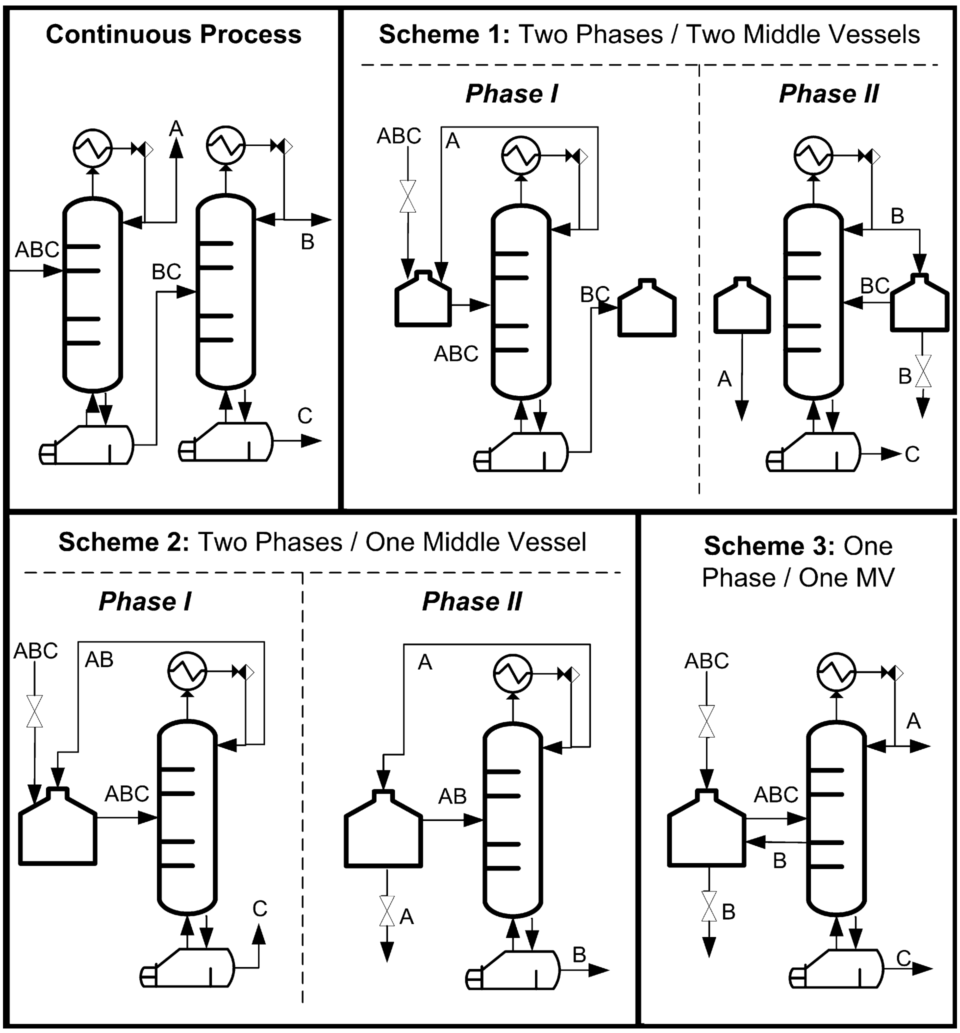

Fig. 2 – Design configurations for continuous and semicontinuous ternary separation systems. Upper left panel: a continuous process. Upper right (Scheme 1): a semicontinuous process with two MVs operating in two different phases of operation in a cycle. Lower left (Scheme 2): a semicontinuous process with one MV operating in two phases. Lower right (Scheme 3): a semicontinuous process with one MV operating in one phase of operation.