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Optimal design, dynamics and control of a reactive DWC for biodiesel production

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ABSTRACT

Reactive separation technologies were proposed recently for fatty acid methyl esters (FAME) production, providing significant benefits such as minimal capital and operating cost savings. One approach is to use a reactive dividing-wall column (R-DWC) for the biodiesel production process. However, since the R-DWC is designed for a quaternary reactive system – two reactants (one in excess) and two products – more difficulties concerning the process control may be expected considering the high degree of integration of the process.

This study is among the first to tackle the optimal design, dynamics and control of such an integrated unit and proposes an efficient control structure for a biodiesel process based on reactive DWC technology. AspenTech Aspen Plus and Aspen Dynamics were used as computer aided process engineering (CAPE) tools to perform the rigorous steady-state and dynamic simulations, as well as the optimization of the new R-DWC based biodiesel process. A key finding of this study is that it is imperative to use a vapor feed of alcohol in order to reach the product specifications. Singular value decomposition (SVD) was used to determine the sensitive trays for inferential temperature control. The control structure proposed here demonstrates the excellent performance of the system in the case of industrially relevant disturbances such as production rate changes or catalyst deactivation.

Keywords: Dividing-wall column; Reactive distillation; Biodiesel; SQP; Optimal design; Process control

1. Introduction

Employing waste and non-edible raw materials is nowadays mandatory to comply with the ecological and ethical requirements for renewable energy, such as biofuels. Biodiesel is a renewable fuel consisting of fatty acid methyl esters (FAME), currently produced from green sources such as vegetable oils, animal fat or waste cooking-oils (Van Gerpen, 2005; Bowman et al., 2006; Lee et al., 2011). The use of waste oils receives increased attention due to the high cost of the refined vegetable oils. Zhang et al. (2003) showed that using waste oils can have indeed a positive impact on the economics of biodiesel processes. However, the waste raw materials contain a substantial amount of free fatty acids (FFA) thus not being compatible with current processes. For that reason, the development of an efficient continuous process for FAME manufacturing is required, in which the use of a solid catalyst is able to suppress the costly downstream processing steps and the waste treatment (Zabeti et al., 2009). Note that all conventional biodiesel processes suffer from problems associated with the use of liquid catalysts, leading to severe economical and environmental penalties (Helwani et al., 2009).

Process intensification methods can be further employed in order to reduce investment and operating costs, simplify the downstream processing steps, and minimize the waste streams (Qiu et al., 2010). Several recent studies proposed the FAME synthesis from free fatty acids (FFA) or tri-alkyl glycerides (TAG) using reactive separation processes, such as reactive distillation (Kiss, 2010, 2011), reactive absorption (Kiss, 2009; Kiss and Bildea, 2011a; Bildea and Kiss, 2011), reactive extraction or membrane reactors (Kiss and Bildea, 2012). The more recent review of Kiss and Bildea (2012) covers in detail all these reactive separation technologies by which the equilibrium of the reaction can be completely shifted toward FAME formation by continuously removing the products.

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Nowadays technologies such as reactive distillation (RD) and dividing-wall column (DWC) are proven process intensification technologies that offer significant capital and operating costs savings (Kiss and Bildea, 2012; Yildirim et al., 2011). Remarkable, DWC is the only known large scale process intensification example where both capital and operating costs can be vastly reduced, with the additional benefit of reducing the required installation space (Dejanović et al., 2010; Asprion and Kaibel, 2010). Moreover, DWC is not limited to ternary separations only but it can be used also in extractive distillation (Bravo-Bravo et al., 2010), azeotropic separations (Kiss and Suszwalak, 2012a,b), and reactive distillation (Mueller and Kenig, 2007; Hernandez et al., 2009; Kiss et al., 2009; Kiss and Suszwalak, 2012a,b). By further integrating RD and DWC technologies, more benefits can be obtained with even fewer resources (Kiss et al., 2009; Gomez-Castro et al., 2010, 2011). However, the small amount of literature studies about R-DWC focused so far only on the rate-based modeling and the process design (Mueller and Kenig, 2007; Kiss et al., 2012). Taking into account the high level of integration in a reactive DWC, the dynamics of the system and the process control also play a key role, being just as important as the design.

This study undertakes the optimal design, dynamics and control of such a highly integrated R-DWC unit for a biodiesel production and proposes an efficient control structure based on inexpensive inferential temperature control. AspenTech Aspen Plus and Aspen Dynamics were used as rigorous CAPE tools to perform the steady-state and dynamic simulations, as well as the sequential quadratic programming (SQP) optimization of the new R-DWC based biodiesel process. A novel control structure is also proposed to test the performance of the system in the case of industrially relevant disturbances such as production rate changes.

2. Problem statement

The biodiesel process based on a reactive DWC offers significant advantages such as the use of only ~15% excess methanol to ensure the completely conversion of FFA, and important capital and operating cost savings (Kiss et al., 2012). However, the problem of dynamics and process control is just as important as the optimal process design. At a first glance, the control of a reactive DWC may not pose to be an issue, as several efficient control structures are available for DWC (Kiss and Rewagad, 2011). Nonetheless, it is worthwhile mentioning that DWC units are designed for ternary separations and therefore, the already proposed control structures are applicable to multi-component separations without reaction. Moreover, in case of reactive distillation, the performance of the control structure strongly depends on the process design and on the type of chemical reactions that occur in the column.

The R-DWC unit studied here is designed for a quaternary system, two products and two reactants, with one of the reactants in excess. A critical aspect of the process is to ensure the full conversion of the FFA by having an excess of methanol and therefore, avoiding that unreacted FFA becomes an impurity in the bottom stream. However, the excess methanol can become an impurity in the side stream. The reason is that the prefractionator of the R-DWC is operated with multiple feeds (with lightest component fed at the lower part) and therefore unable to perform the sharp split between the light and the heavy components of the system like, as typically the case in a standard DWC. To solve these problems, this study proposes an optimal design and an efficient control strategy for a reactive DWC for FAME production.

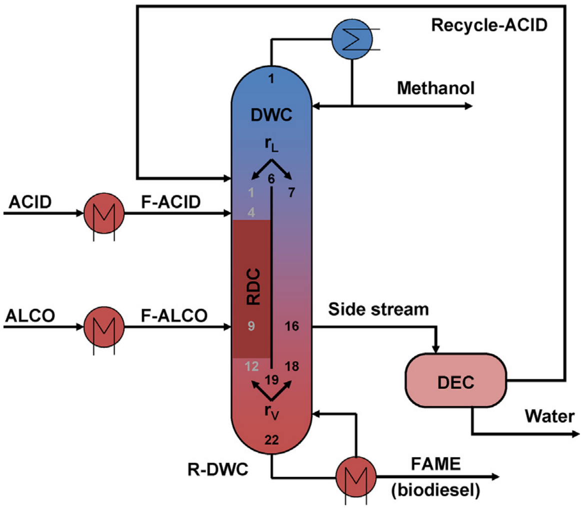

Fig. 1 – Reactive DWC used for the FAME synthesis from free fatty acids and methanol.

3. Results and discussion

Significant savings in the operating and capital investment cost can be achieved by combining RD and DWC technologies, but the high degree of integration can raise more difficulties in the process control. This study is based on a previously reported idea about FAME synthesis in a reactive DWC (Kiss et al., 2012), but it is among the first to present a novel optimal design while tacking the dynamics and control of this highly integrated process.

Fig. 1 shows the proposed R-DWC design, based on reported RD synthesis and design methods (Schembecker and Tlatlik, 2003; Jantharasuk et al., 2011). FAME is produced as pure bottom product, water as side stream, while the methanol excess is recovered as top distillate and recycled. The alcohol to acid ratio plays a crucial role in the design and operation of the integrated R-DWC unit. All products can be obtained at high purity only in a narrow optimal range of the alcohol to acid ratio. At smaller ratio, methanol is fully converted but the excess of FFA becomes an impurity in the FAME stream, while at high ratio the FFA are fully converted and the excess of methanol becomes an impurity in the side stream (Kiss, 2011).

The R-DWC column was simulated using two rigorous RADFRAC units, as no off-the-shelf DWC unit is available in the current commercial process simulators. The physical properties required for the simulation and the binary interaction parameters for the methanol–water and acid–ester pairs were available in the Aspen Plus database of pure components, while the other interaction parameters were estimated using the UNIFAC – Dortmund modified group contribution method (Aspen Technology, 2010). The fatty components were conveniently lumped into one fatty acid and its fatty ester, according to: $R{-}COOH + CH_3OH \leftrightarrow R{-}COO{-}CH_3 + H_2O$. Dodecanoic (lauric) acid/ester was selected as lumped component, and sulfated zirconia was considered as solid acid catalyst, due to the availability of experimental results, VLLE parameters and kinetics for this system (Kiss et al., 2006; Dimian et al., 2009). More details about the system are presented by Kiss et al. (2012).