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ScienceDirect
Computers and Chemical Engineering 31 (2007) 1187–1198
Computers & Chemical Engineering
www.elsevier.com/locate/compchemeng

Production of isopropyl palmitate in a catalytic distillation column: Comparison between experimental and simulation studies

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Received 15 March 2006; received in revised form 10 October 2006; accepted 12 October 2006
Available online 20 November 2006

Abstract

Fatty acid esterification is increasingly realized as a reactive distillation (RD) process because of its formation being affected by the chemical equilibrium. The reactive distillation column performance for the production of isopropyl palmitate by esterification of the palmitic acid with isopropanol has been studied in the present research. The reaction was catalyzed in the presence of zinc acetate supported on functionalized silica gel catalyst. The process parameters such as total feed flow rate, reboiler temperature, palmitic acid feed composition, palmitic acid feed temperature, molar ratio of isopropanol feed to palmitic acid feed and reflux ratio were studied experimentally in the catalytic distillation column. Two types of models were used for the simulation of catalytic distillation column. These were (a) equilibrium stage model and (b) rate-based model. The predictions from the rate-based model matched with the experimental results qualitatively and quantitatively. The simulation study was also carried out to determine the effects of other important parameters and design factors such as the column pressure, distillate to feed ratio, feed location, catalyst weight, height of reactive zone and height of separation zones. A technically optimized RD process for the production of isopropyl palmitate has been proposed on the basis of the experimental and simulated data.

Keywords: Reactive distillation; Fatty acid esterification; Isopropyl palmitate; Heterogeneous catalyst; Experimental; Modeling; Simulation

1. Introduction

Reactive distillation (RD) is the simultaneous implementation of reaction and separation within a single unit of column. Reactants are converted to products in a reaction zone in the presence of catalyst with simultaneous separation of the products and recycle of unused reactants to this zone. This combined operation is especially suited for the chemical reaction limited by equilibrium constraints, since one or more of the products of the reaction are continuously separated from the reactants.

The commercial success of RD for the production of methyl tert-butyl ether (MTBE) and methyl acetate demonstrates its ability to render cost-effectiveness and compactness to the chemical plant (Sharma & Mahajani, 2003). As a consequence, RD has been explored as a potentially alternative for several other chemical productions and reactions. The methyl acetate system serves as a model esterification system for the reactive distillation process (Popken, Steingeweg, & Gmehling, 2001). Beside methyl acetate synthesis, the esterification of other alcohols such as *n*-butanol and 2-methylpropanol with acetic acid has been investigated (Smejkal, Hanika, & Kolena, 2001; Steinigeweg & Gmehling, 2002). In contrast of these systems, information about the esterification of long chain carboxylic acids such as fatty acids by reactive distillation can hardly be found in the literature.

The esterification of fatty acid with 2-propanol and methanol in a tray reactive distillation column is reported by Jeromin, Bremus, and Peukert (1981), Schleper, Gutsche, Wnuck, and Jeromin (1990) and Bock, Wozny, and Gutsche (1997). The homogeneous catalyst in their processes required neutralization and separation of catalyst. This leads to the development of heterogeneously catalyzed reactive distillation column.

Omota, Dimian, and Bliek (2003) carried out the theoretical study of the reactive distillation column for the production of 2-ehtylhexyl dodecanoate using solid acid catalyst based on sulphated zirconia, whereas Steinigeweg and Gmehling (2003)

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0098-1354/$ – see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.compchemeng.2006.10.008

reported their experimental and simulation studies for the esterification of decanoic acid with methanol in a heterogeneously catalyzed packed column.

A new process for continuous production of fatty acid isopropyl esters using a reactive distillation column with a heterogeneous catalyst and membrane module was proposed by Bailer, Fassler, Moritz, and Von Scala (2003). They reported that the use of reactive distillation column could reduce the energy requirements and the plant size. However, no results and data are available in the open literature.

To the best of our knowledge, no information about the reactive distillation for the production of isopropyl palmitate from palmitic acid and isopropanol is available in the open literature. Isopropyl palmitate is primarily used in personal care and cosmetic formulations as a dry and soft non-oily emollient. It can be used as an excellent solvent for mineral oil, silicone and lanolin (Bailey, 1996).

The experimental and simulation studies for the production of isopropyl palmitate in the heterogeneously catalyzed reactive distillation column have been reported the present work. The zinc acetate supported on silica gel was employed as the heterogeneous catalyst. The effect of variables such as total feed flow rate, reboiler temperature, composition of palmitic acid feed, temperature of palmitic acid feed, molar ratio of isopropanol to palmitic acid and reflux ratio were studied experimentally. The simulation of reactive distillation column was carried out using the RADFRAC and RATEFRAC modules of Aspen Plus 12.1 process simulation software. The experimental data were compared with the simulation results. Finally, a technically optimized reactive distillation process for the production of isopropyl palmitate is proposed. The flowsheet for the development of a RD process for the production of isopropyl palmitate is shown in Fig. 1.

2. Experimental

A reactive distillation column containing solid catalyst was used for the esterification of palmitic acid and isopropanol to produce isopropyl palmitate. The zinc acetate supported on functionalized silica gel was used as heterogeneous catalyst. The RD column was made of stainless steel with packing height of 3 m, total height of 6 m and internal diameter of 102 mm. The rectifying and stripping zones of the column were packed with Sulzer-BX packing while the reactive zone was packed

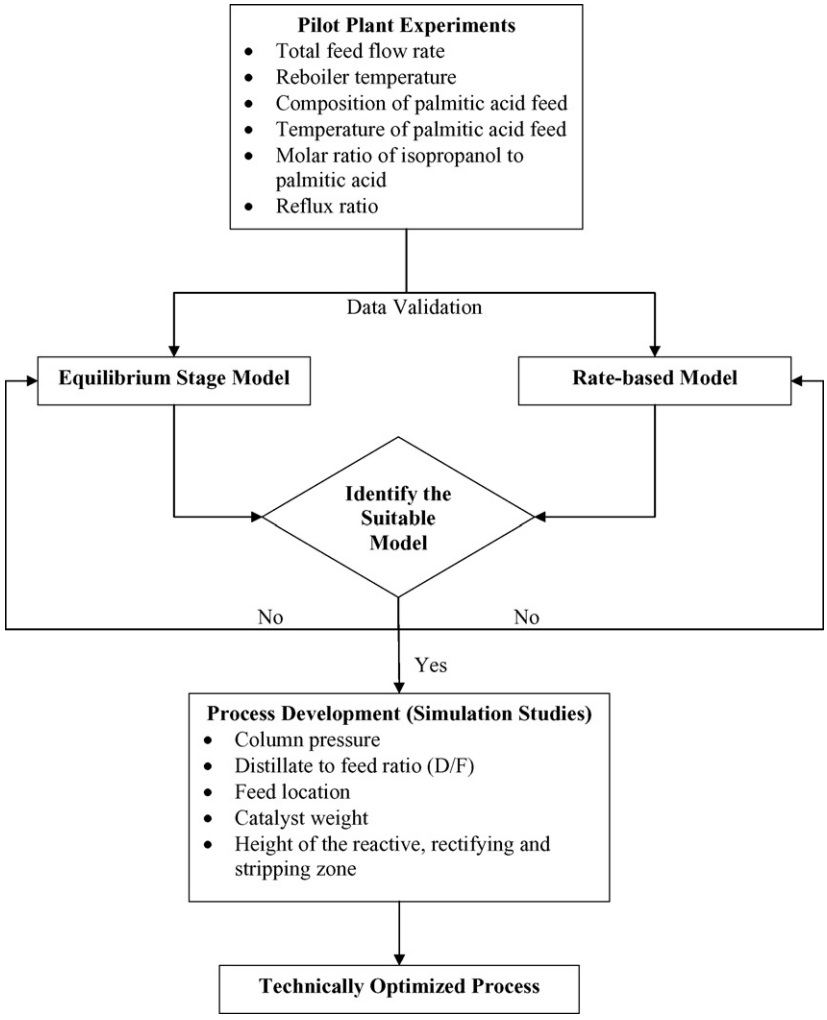

Fig. 1. Flowsheet for development of a RD process for the production of isopropyl palmitate.