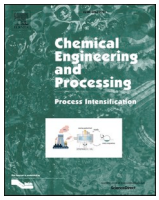
Chemical Engineering & Processing: Process Intensification 191 (2023) 109435

Contents lists available at ScienceDirect

Chemical Engineering and Processing - Process Intensification

journal homepage: www.elsevier.com/locate/cep



Intensification of esterification reaction microbubble mediated reactive distillation

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ARTICLE INFO

Keywords:
Acid catalysis
Esterification
Methyl acetate
Mass transfer
Microbubbles

ABSTRACT

The current study is based on the microbubble mediated reactive distillation by converting conventional homogeneous liquid-liquid system into a heterogeneous vapour-liquid system. Microbubbles owing to their higher surface area to volume ratio provides better mass transfer as well increasing the conversion and rate of reaction. To prove the hypothesis, production of methyl acetate was investigated because of its industrial importance. The experimental plan was designed using Response Surface Methodology (RSM). It allowed analysing the effects of operational parameters simultaneously. The kinetics investigation demonstrated that the esterification reaction occurs, indeed, on the vapour liquid interface at the skin/surface of the bubble and follows pseudo-first order kinetics. The maximum conversion of the process was found to be 91% in 20 min which is significantly higher than any previous study. Furthermore, RSM and Gated Recurrent Unit (GRU) were employed to develop models to analyse the correlations among parameters and to predict the responses. The GRU produced higher R^2 = 0.9981 as compared to R^2 = 0.9715 produced by RSM. The results depict that GRU model is more robust and reliable than Response Surface Methodology for parameter interaction study and response prediction.

1. Introduction

Esterification is one of the most important reactions in chemical synthesis. It has several numerous industrial application such as biodiesel, pesticides, cosmetics, paints and dyes etc., [1]. Esterification reaction has a low conversion and a low reaction rate and requires an acid catalyst to increase the reaction rate [2]. The low conversion and reaction rate is caused by establishment of equilibrium and poor mass transfer between the reactants [3]. Consequently, the separation of product becomes energy intensive and the overall cost of the process is increased [4]. For instance, the cost for the separation of the product in a distillation column is US$ 0.1345 Million/ton is very high as compare to the cost of catalyst or cost to maintain temperature and pressure [5]. The cost of the separation of the product for different process is given in supplementary data Table S-I.

To overcome the establishment of equilibrium, several methods have been investigated. Esterification process was carried out in reactive distillation (RD) columns in which reaction and separation occur simultaneously [6]. Initially RD was commercially used for the production of methyl acetate in 1983 by Eastman company [7]. The main challenges of the RD are; handling of large size of distillation columns, and low conversion [8]. As the reaction and separation process occur in the same unit due to this azeotropes form in the column and also it increases the design complexity and handling in reactive distillation column [9]. Pressure swing distillation has also been employed for MeOH production. It is carried out in two stages. The column is operated at atmospheric pressure. The esterification reaction is carried out in liquid phase. However, the presence of acetic acid (AcOH), water, methanol and acetate creates adverse equilibrium conditions and consequently reduce the production and purity of the product [10]. Then two column system was purposed-one column for rectifying and the other for the stripping section. However, to increase the purity (%) to 99.5%, a third column had to be introduced [11]. Reactive distillation with divided wall column has been reported for esterification. The reactants were fed

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https://doi.org/10.1016/j.cep.2023.109435
Received 14 February 2023; Received in revised form 10 May 2023; Accepted 20 May 2023
Available online 21 May 2023