Modelling of a pervaporation membrane reactor during esterification reaction coupled with separation to produce ethyl acetate

Ayça Hasanoğlu*, Salih Dinçer

Yıldız Technical University, Department of Chemical Engineering, Davutpaşa Campus, 34210 Istanbul, Turkey
Tel. +902123834780; Fax: +902123834725; email: aycameric@yahoo.com, dincer@yildiz.edu.tr

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ABSTRACT

As a follow up to the previous report on the experimental study of esterification reaction to yield ethyl acetate in a pervaporation membrane reactor (PMR), in this study; modelling of PMR during esterification reaction coupled with separation is presented. The analyzed system is the esterification reaction catalysed by sulfuric acid and Amberlyst 15 in a batch PMR in the temperature range of 50–70°C using polydimethylsiloxane (PDMS) membranes permselective to ethyl acetate. In this way, conversions were increased by continuous removal of ethyl acetate from the reaction medium. The theoretical model was developed taking account permeation of the all components in the reaction mixture. The kinetic calculations were made on the assumptions that the reaction obeyed second order kinetics. The model satisfactorily agrees with the experimental results obtained in the previous work, thus allowing the prediction of the conversion variation with the pervaporation time. The coefficient of determination, $R^2$, was in the range of 0.9798 to 0.9991. This modelling methodology could be used to extrapolate or to scale-up this type of systems as it provides assistance to analyze the effect of the operating parameters on the conversions during the esterification process.

Keywords: Membrane reactor; Pervaporation; Esterification; Ethyl acetate; modelling; PDMS

*Corresponding author.