Design of Thermally Coupled Reactive Distillation Schemes for Triethyl Citrate Production Using Economic and Controllability Criteria

Miguel A. Santaella, Luis E. Jiménez, Álvaro Orjuela, Juan Gabriel Segovia-Hernández

PII: S1385-8947(17)31159-2
DOI: http://dx.doi.org/10.1016/j.cej.2017.07.015
Reference: CEJ 17281

To appear in: *Chemical Engineering Journal*

Received Date: 24 March 2017
Revised Date: 22 June 2017
Accepted Date: 5 July 2017

Please cite this article as: M.A. Santaella, L.E. Jiménez, A. Orjuela, J.G. Segovia-Hernández, Design of Thermally Coupled Reactive Distillation Schemes for Triethyl Citrate Production Using Economic and Controllability Criteria, *Chemical Engineering Journal* (2017), doi: http://dx.doi.org/10.1016/j.cej.2017.07.015

Design of Thermally Coupled Reactive Distillation Schemes for Triethyl Citrate Production Using Economic and Controllability Criteria

Miguel A. Santaella[1], Luis E. Jiménez[1], Álvaro Orjuela[1¥], Juan Gabriel Segovia-Hernández[2],

[1]Universidad Nacional de Colombia, Ciudad Universitaria, Departamento de Ingeniería Química y Ambiental, Bogotá DC, Colombia

[¥]Corresponding author: aorjuelal@unal.edu.co. (+57-1) 3165000 ext. 14303

[2] Facultad de Química, Universidad de Guanajuato, Noria Alta s/n, Guanajuato, Gto. 36050, México.

Abstract

This work describes a systematic process design for triethyl citrate production by direct esterification of citric acid with ethanol via simultaneous reaction-separation technologies. The design methodology includes simultaneous optimization of controllability and profitability criteria. With a novel approach, the conceptual feasibility analysis of the intensified processes was carried out by extending the reactive residue curve maps (RRCM) to mixtures with six components by implementing a substitution degree parameter. The RRCM have been also extended to the conceptual design of dividing wall columns. The configuration of both, traditional and dividing wall reactive distillation columns, were obtained from the conceptual analysis. The processes were simulated using experimentally validated models, and further optimized using a nature inspired multi-objective algorithm. A triethyl citrate production capacity of 10kTon/yr was used as process specification. Final designs evidenced citric acid conversions above 99.9%, energy consumption from 3-5MJ/kg, and a TEC production costs of c.a 1.5USD/kg. Controllability assessment was performed by evaluating the condition number of the proposed operating schemes. Pareto diagrams indicate that the minimization of total annual costs and controllability are conflicting goals in both production schemes. Nevertheless, both alternatives withstand large perturbations over the main process variables. The reactive dividing wall column scheme results in large energy and cost savings over a traditional reactive distillation process.

Keywords: triethyl citrate, reactive distillation, dividing wall column, controllability, optimization