

Accepted Manuscript

Distribution models for nitrophenols in a liquid-liquid system

A.L.C.V. Lopes, A.F.G. Ribeiro, M.P.S. Reis, D.C.M. Silva, I. Portugal,
C.M.S.G. Baptista

PII: S0009-2509(18)30270-7
DOI: <https://doi.org/10.1016/j.ces.2018.04.056>
Reference: CES 14188

To appear in: *Chemical Engineering Science*

Received Date: 30 March 2017
Revised Date: 22 March 2018
Accepted Date: 25 April 2018

Please cite this article as: A.L.C.V. Lopes, A.F.G. Ribeiro, M.P.S. Reis, D.C.M. Silva, I. Portugal, C.M.S.G. Baptista, Distribution models for nitrophenols in a liquid-liquid system, *Chemical Engineering Science* (2018), doi: <https://doi.org/10.1016/j.ces.2018.04.056>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Distribution models for nitrophenols in a liquid-liquid system

A.L.C.V. Lopes^{a,b,c}, A.F.G. Ribeiro^a, M.P.S. Reis^b, D.C.M. Silva^a,
I. Portugal^c, C.M.S.G. Baptista^{b,*}

^a CUF - Químicos Industriais S.A., Quinta da Indústria, Rua do Amoníaco Português
n.º.10, Beduído, 3860-680 Estarreja, Portugal

^b CIEPQPF - Department of Chemical Engineering, Faculty of Sciences and Technology,
University of Coimbra, Rua Sílvio Lima, Polo II, 3030-790 Coimbra, Portugal

^c Department of Chemistry and CICECO, University of Aveiro, Campus Universitário de
Santiago, 3810 - 193 Aveiro, Portugal

Abstract

The formation of nitrophenols by-products is still of major concern for the economics and environmental impact of the industrial process of benzene (Bz) nitration to mononitrobenzene (MNB) with mixed acid (sulphuric and nitric acids). The knowledge of nitrophenol (NP) distribution ratios in the liquid-liquid mixture (D_j , $j = \{NP\}$) is desirable for process optimization and for understanding the reaction mechanisms behind nitrophenols formation.

In this study, a data-driven approach was implemented to provide prediction models for D_j of 2,4-dinitrophenol (DNP) and of 2,4,6-trinitrophenol (TNP) in a biphasic liquid system with a composition representative of the industrial processes. In the first step, screening tests were performed to identify the main variables influencing the experimental equilibrium weight fractions of nitrophenols in the aqueous phase ($w_{j,e}^A$). Subsequently two independent data sets were built for development and external validation of prediction multivariate linear regression (MLR) models, at 30 °C. The fitting results (R^2 and $R_{ad}^2 \geq 0.90$) and the prediction results ($R_{pred,DNP}^2 = 0.931$, $R_{pred,TNP}^2 = 0.908$) confirmed the quality of the $w_{j,e}^A$

*Corresponding author: cristina@eq.uc.pt

Email addresses: alopes@eq.uc.pt (A.L.C.V. Lopes), alejandro.ribeiro@cuf-qi.pt (A.F.G. Ribeiro), marco@eq.uc.pt (M.P.S. Reis), dulce.silva@cuf-qi.pt (D.C.M. Silva), inesport@ua.pt (I. Portugal)

Download English Version:

<https://daneshyari.com/en/article/6588346>

Download Persian Version:

<https://daneshyari.com/article/6588346>

[Daneshyari.com](https://daneshyari.com)