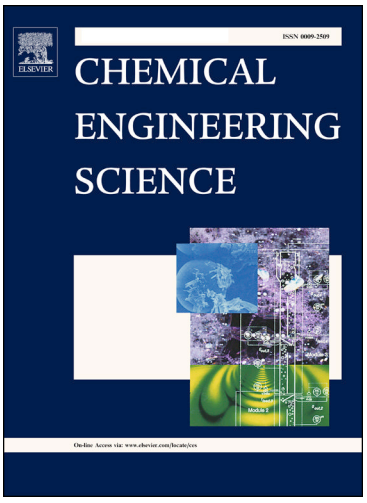

Distribution models for nitrophenols in a liquid-liquid system

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Distribution models for nitrophenols in a liquid-liquid system

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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 ($w^{\mathrm{A}}_{j,e}$). 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 $R^2_{ad} \geq 0.90$) and the prediction results ($R^2_{pred,\mathrm{DNP}} = 0.931$, $R^2_{pred,\mathrm{TNP}} = 0.908$) confirmed the quality of the $w^{\mathrm{A}}_{j,e}$

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