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Dipropylene glycol as a solvent for the extraction of aromatic hydrocarbons. Analysis and evaluation of the solvency properties and simulation of the extraction processes

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ABSTRACT

Solvent properties, solvation power and selectivity, are calculated for dipropylene glycol (DPG). Additionally, the performances realized by DPG in extraction columns were evaluated by simulating in PRO/II software the extraction of aromatic hydrocarbon from a fraction of Catalytic Reforming naphtha based on the binary interaction parameters obtained from liquid–liquid and vapor–liquid equilibrium experimental data for the binary mixtures of DPG with representative aromatic and non-aromatic hydrocarbons with six up to eight carbon atoms, as determined in previous works. The simulation of the extraction columns was achieved for different operating conditions: solvent mass ratios from 1:1 up to 4:1 and different numbers of theoretical trays in simple columns, solvent mass ratios from 1:1 up to 4:1 and different reflux ratios in columns operated with reflux of extract, and in columns operated with reflux of raffinate. The results show that DPG has a good solvation power, and its utilization in extraction ensures a pure raffinate is obtained.

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1. Introduction

Removal of aromatic hydrocarbons from fuels, particularly from gasoline, is of great interest in the current context of environmental protection legislation. Taking this into account, there are developing research studies aiming to find new processes and/or new solvents that more efficiently extract aromatic hydrocarbons from their mixtures. Recently, researchers from DDBST (Dortmund Data Bank Software and Separation Technology) developed software (Gmehling and Schedemann, 2014) that allows for prediction of the solvent capacity and selectivity of solvents, starting from equilibrium data, physicochemical and transport properties data existing in DDB (Dortmund Data Bank) and using predictive thermodynamic models, such as UNIFAC (UNIQUAC Functional-group

Activity Coefficients) (Fredenslund et al., 1975), modified UNIFAC (Lohmann et al., 2001; Lohmann and Gmehling, 2001; Gmehling et al., 2002) and equations of state based on group contributions, such as PSRK (Predictive Soave–Redlich–Kwong) (Holderbaum and Gmehling, 1991; Gmehling, 1995) and VTPR (Volume Translated Peng–Robinson) (Schmid et al., 2014). The UNIFAC model was extensively used to predict phase equilibria in different mixtures of hydrocarbons and various solvents (Mukhopadhyay and Dongaonkar, 1983; Mukhopadhyay and Pathak, 1986; Wang et al., 1998; Radwan et al., 1997). The UNIQUAC (Universal-Quasi Chemical) (Abrams and Prausnitz, 1975) and NRTL (Non Random Two Liquids) (Renon and Prausnitz, 1968) models were also utilized in different studies to describe better phase equilibria in binary, ternary, and multicomponent mixtures of aromatic and non-aromatic

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hydrocarbons and tetraethylene glycol (Darwish et al., 2003), *n*-methyl-2-pyrrolidone (Al-Jimaz et al., 2007), and sulfolane (Mukhopadhyay and Sahasranaman, 1982).

The study presented in this paper is part of a wide research study developed in our department, which refers to the utilization of propylene glycols (monopropylene glycol (MPG), dipropylene glycol (DPG), tripropylene glycol (TPG) and tetrapropylene glycol (TePG)) as solvents for aromatic hydrocarbon extraction. Some assumptions regarding the solvent properties of MPG are presented by Oprea and Guțu (2008), and research studies were stopped because MPG was found to have weak solvent properties. Instead, the studies performed on dipropylene glycol revealed that it has a great affinity for aromatic hydrocarbons. Liquid–liquid equilibrium data between DPG and non-aromatic and aromatic hydrocarbons with six to eight carbon atoms are presented in a previous work (Nicolae and Oprea, 2012). During the developed experiments, it was found that DPG is completely miscible with aromatic hydrocarbons (benzene, toluene, ethylbenzene and xylenes). As consequence, vapor–liquid equilibrium data between DPG and the aromatic hydrocarbons mentioned below were determined (Nicolae and Oprea, 2014). For tripropylene glycol, the research is in progress, while for TePG, currently, only the physical and transport properties have been determined (Fendu and Oprea, 2013).

This paper presents the results of the calculations performed to obtain the variation of selectivity and solvation power of DPG with temperature and solvent ratio. In addition, data regarding the performances of DPG during counter-current liquid–liquid extraction in columns are presented: the recovery grade of aromatics in the extract, the recovery grade of non-aromatics in the raffinate and the purities of the extract and the raffinate products in the case of the simple column operation (column without reflux) and in columns with reflux of extract and the corresponding case with reflux of raffinate. All of the calculations were performed using PRO/II simulation software and based on binary interaction parameters determined through the regression of liquid–liquid and vapor–liquid equilibrium data for the binary mixtures formed by DPG and hydrocarbons with six to eight carbon atoms (*n*-hexane, cyclohexane, *n*-heptane, *n*-octane, 2,2,4-trimethylpentane, benzene, toluene, ethylbenzene, *o*-xylene, *m*-xylene, *p*-xylene) (Nicolae and Oprea, 2012, 2014). These binary interaction parameters can be found in the Supplementary material (Tables S9 and S10). The equilibrium data for binary mixtures of DPG with the hydrocarbons mentioned above were necessary because the simulation software does not contain a complete thermodynamic model that could correctly characterize these binaries. This way, the NRTL thermodynamic model was completed with binary interaction parameters for the studied binaries and was utilized for calculations of the liquid–liquid extraction process in this work.

2. Solvent properties estimation

Evaluating the possibility of using a new compound as a solvent for the extraction of aromatic hydrocarbons implies the knowledge of the most important properties of the solvent: the capacity and the selectivity. There are some investigations on the prediction of the selectivity and the capacity of the most well-known and utilized solvents, starting from a small amount of equilibrium data and physical properties of the solvents: the first work (Deal and Derr, 1964) was published in

1954, and the most recent was published last year (Gmehling and Schedemann, 2014).

In addition, the performances realized by the solvent in the extraction column, recovery grades of hydrocarbons in the product phases (extract and raffinate), are important, as well as the purities of these phases that the solvent achieve in given conditions of temperature, pressure and solvent ratio. All of these performances are dependent on the capacity and selectivity of the solvent. The solvation capacity is defined as the capability of the solvent to solubilize the solute in the presence of a carrier solvent. The capacity is often also named power solvation and is expressed through the distribution coefficient of the solute (K_S) or the reverse of the activity coefficient at infinite dilution. The selectivity represents the capability of the solvent to preferentially solubilize one compound or a group of some compounds from a mixture with the carrier solvent. The selectivity is quantified through the selectivity coefficient (β) expressed as the ratio between the distribution coefficients of the solute and carrier solvents in the extraction solvent. In particular, for the aromatic extraction process, the distribution coefficients for aromatic and non-aromatic hydrocarbons are described by Eqs. (1) and (2), while the selectivity is described by Eq. (3).

$$K_{Ar} = \frac{X_{Ar,E}}{X_{Ar,R}} \quad (1)$$

$$K_{NAr} = \frac{X_{NAr,E}}{X_{NAr,R}} \quad (2)$$

$$\beta = \frac{(X_{Ar,E}/X_{Ar,R})}{(X_{NAr,E}/X_{NAr,R})} \quad (3)$$

where K_{Ar} is the distribution coefficient of aromatic hydrocarbons; K_{NAr} is the distribution coefficient of non-aromatic hydrocarbons; $X_{Ar,E}$, $X_{Ar,R}$ are the concentrations of aromatic hydrocarbons in the extract phase and in the raffinate phase, respectively, and $X_{NAr,E}$, $X_{NAr,R}$ are the concentrations of non-aromatic hydrocarbons in the same phases.

2.1. Solvation power and selectivity estimation of DPG and DEG

From Eqs. (1)–(3), the capacity and selectivity of a solvent can be estimated if the concentrations of the solute and the carrier solvent in the extraction solvent are known. The most realistic results are obtained when the experimental data are used for calculations; however, data obtained with simulation process software can also be used if complete equilibrium data are available for the mixtures implied. Starting from this second assumption, we performed the calculations for the capacity and selectivity of diethylene glycol (DEG) and dipropylene glycol (DPG) using PRO/II simulation software. Considering a mixture with a composition similar to a reformed naphtha and using different solvent mass ratios (2:1 up to 10:1), a single step extraction operation was simulated (in separators, as shown in Fig. 1). Equilibrium in the multicomponent system formed by hydrocarbons and DEG was calculated using NRTL thermodynamic model completed with the UNIFAC model for those binaries for which there are no equilibrium data in the databank of the utilized simulation program. The extraction process in a single step was simulated, and the composition of each resulted phase (extract and raffinate) was utilized to calculate the distribution coefficient (solvation power) using Eqs. (1) and (2), and the selectivity was calculated using Eq. (3). The

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