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A new model for estimating mass transfer coefficients for the extraction of ethanethiol with alkaline solutions in packed columns

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Abstract

The mathematical model for estimating the mass transfer coefficients for the ethanethiol extraction from gasoline, with alkaline solutions was established by processing the data obtained in a laboratory and in a pilot plant experiment. It allows the estimation of overall mass transfer coefficients, taking into account the dispersed phase velocity, the concentration of NaOH solution, the specific area and the porosity of the packing. The model's parameters were statistical tested in order to confirm the accuracy of the model.

Keywords: Mass transfer; Packed columns; Modelling; Residuals; Analysis

1. Preliminaries

The thiols extraction from sour petroleum fractions is an usual process in petroleum refining industry. The process is a liquid–liquid extraction accompanied by a chemical reaction of second order between the thiols and NaOH. Since the chemical reaction is very fast, the process is controlled by the mass transfer of thiols from the hydrocarbon phase into NaOH solution. So, the estimation of the mass transfer coefficients, as the expression of the process rate, could be useful for the design and the simulation of the industrial extraction process.

In the present work, the authors establish a mathematical model for the estimation of the mass transfer coefficients in the case of ethanethiol extraction with NaOH solutions, analyzing and processing original experimental data obtained in laboratory and in a pilot plant, in extractors equipped with structured packing. We chose the ethanethiol as the key-component of the caustic refining process because it is the heaviest thiol efficiently removable from LPG by simple extraction.

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2. Experimental results

The experiment was fulfilled in laboratory and pilot plant equipment.

In laboratory, an Elgin extractor was available. It has the dimensions: 26 mm – the interior diameter and 700–800 mm – the active height. The extraction column was used in two variants: as a dispersion column and packed with a handicraft-structured packing of metal gauze type, with the specific area $a_p = 60\ \mathrm{m^2/m^3}$ and the porosity $\eta = 0.98$. The pilot scale column has a diameter of 76 mm and an active height of approximately 1000 mm, from which the packing layer represents 840 mm. In this case, the structured packing was of corrugated metal sheet type (Sulzer SMV350Y), with the specific area: $a_p = 340\ \mathrm{m^2/m^3}$ and the porosity, $\eta = 0.98$.

Whatever the size of the column was, the experiment was led on the same manner: the feed was the hydrogenated gasoline enriched in ethanethiol. The ethanethiol extraction was performed with NaOH solution with the concentrations: 5 wt%, 10 wt% and 15 wt%. The solvent-to-feed ratio was variable. The two phases (gasoline and NaOH solution) flow in countercurrent and the concentration in raffinate (gasoline) and in extract (NaOH solution) was found by chemical analysis.

The steps followed to calculate the *overall mass transfer drop-side coefficients* $(K_{od} \cdot a)$ are:

(a) The calculation of the *theoretical extraction stages* NTT, where NTT is defined as the number of equilibriums needed to reach the concentration in raffinate, for a certain solvent-to-feed ratio (S/A).
The number of the theoretical extraction stages NTT was graphically determined using the distribution coefficient, K [1].

(b) The calculation of the *number of the transfer units related to the drop-side*, $\mathrm{NUT_{od}}$, where *the mass transfer unit* is defined as the height of the column along which the driving force of the mass transfer changes by a factor of e.
For systems following the Nernst law (a linear correlation between the concentrations of ethanethiol-solute in both the liquid phases) and for high values of the extraction factor ($E = K * S/A$), the number of the transfer units $\mathrm{NUT_{od}}$ can be calculated from the number of theoretical stages NTT, by [2–4]

$$\frac{\mathrm{NTT}}{\mathrm{NUT_{od}}} = \frac{1 - \frac{1}{E}}{\ln E}.$$

(c) The calculation of the mass transfer unit height $\mathrm{HUT_{od}}$, dividing the active height of the experimental column H to the number of transfer units $\mathrm{NUT_{od}}$.

(d) The calculation of overall mass transfer drop-side coefficients $(K_{od} \cdot a)$, from the $\mathrm{HUT_{od}}$ values, using the formula:

$$K_{od}a = \frac{v_d}{\mathrm{HUT_{od}}} \quad [\mathrm{s^{-1}}],$$

Table 1
The experimental data used for the calculation of the mass transfer unit height (HUT) at the ethanethiol extraction with NaOH solutions, in the dispersion column [2]

Conc. of NaOH solution and the repartition coefficient	Dispersed phase velocity, v_d (cm/s)	Thiol conc. in feed, x_j (ppm)	Thiol conc. in raffinate, x_e (ppm)	Thiol conc. in extract, y_e (ppm)	No. of theoretical stages, NTT	No. of transfer units, NUT	Transfer unit height, $\mathrm{HUT_{od}}$ (cm)
5%, $K = 48.9$	0.17	1204	662	743	0.46	1.67	41.8
	0.23		566	1118	0.36	1.31	53.5
	0.33		780	568	0.54	1.85	37.8
10%, $K = 92$	0.17	711	188	258	0.74	3.04	23.0
	0.23		205	319	0.72	2.30	30.5
	0.33		185	458	0.82	2.46	28.4
15%, $K = 102.4$	0.17	745	148	178	0.80	3.50	20.2
	0.23		159	223	0.79	2.76	25.4
	0.33		136	320	0.75	3.51	20.0