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Using maximum entropy, Gamma, Inverse Gaussian and Weibull approach for prediction of drop size distribution in a liquid–liquid extraction column

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ABSTRACT

In this study, drop size distribution and Sauter mean drop diameters were measured and correlated under operating variables and physical properties of the systems using a 113 mm diameter Kühni column. Three systems including toluene-water, *n*-butyl acetate-water and *n*-butanol-water were experimented in this column. The countercurrent flow pattern of the liquid phases was characterized regarding the Sauter mean drop diameter and drop size distribution; a photographic method was used to assess drop sizes. The following operating variables were studied: rotor speed, flow rate of both liquid phases and interfacial tension. The drop size distribution and Sauter mean drop diameter were found to depend largely on the rotor speed and interfacial tension, albeit, only partially dependent on the phase velocities. The maximum entropy principle and the conventional probability distribution functions (Gamma, Inverse Gaussian, Weibull) have already been applied to estimate the drop size distribution. Experimental results show that the maximum entropy function describes the drop size distribution better than the conventional probability distribution functions for three systems in a Kühni column extractor. An empirical correlation is proposed for the estimation of the Sauter mean drop diameter. The acquired information would be useful in design of liquid–liquid extraction columns.

1. Introduction

Liquid–liquid extraction is an important separation process. Various types of solvent extraction columns have been used for a range of applications in the chemical, petroleum, nuclear, hydrometallurgical industries and other areas for many years (Aguailar and Cortina, 2013; Kislik, 2012). Knowledge of the hydrodynamic parameters including drop size is of fundamental importance in the design of liquid–liquid extraction columns (Asadollahzadeh et al., 2016b; Yuan et al., 2014). In solvent extraction processes, for instance, the interfacial area of the dispersion, controls the mass transfer rate and it is a key parameter for the design and scaling-up of gravity settlers that ensure the ultimate liquid phases separation (Asadollahzadeh et al., 2016a,c; Godfrey and Slater, 1994).

Mechanically agitated extraction columns, are widely used in industry. For this type of extractor, there are two different methods of phase agitation: rotary agitation by discs, turbines etc. and agitation by pulsators. The Kühni column is one type of extraction column in which the necessary interface for mass transfer is achieved with turbines placed one above the other compartments (Hemmati et al., 2015a). The agitated

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Nomenclature

AARE	Average absolute relative error (–)
d_{32}	Sauter mean drop diameter (m)
D_i	Droplet diameter (m)
D_c	Column diameter (m)
d_R	Rotor diameter (m)
C_Ψ	Constant parameter in Eq. (3) (–)
C_{II}	Constant parameter in Eq. (3) (–)
C_Ω	Constant parameter in Eq. (3) (–)
e	Power dissipated per unit mass ($m^2 s^3$)
g	Acceleration due to gravity (m/s^2)
H	Effective height of the column (m)
h	Compartment height (m)
N	Rotor speed (1/s)
n_i	Number of droplets of mean diameter d_i (–)
m	Mass (kg)
P	Probability of number density (–)
Q	Flow rate of the continuous or dispersed phase (m^3/s)
V	Superficial velocity (m/s)
V_i	Impeller tip velocity (m/s)
V_k	Characteristic velocity (m/s)
S	Shannon entropy (–)

Greek letters

λ	Lagrange multipliers of probability maximum entropy function
ρ	Density (kg/m^3)
ρ_m	Density of dispersion (kg/m^3)
$\Delta\rho$	Density difference between phases (kg/m^3)
μ	Viscosity (Pa s)
σ	Interfacial tension (N/m)
φ	Dispersed phase holdup (–)
ε	Cross sectional area (–)

Subscripts

c	Continuous phase
d	Dispersed phase

column is universally suitable for all types of liquid–liquid extraction applications. Therefore, the change in mean drop size and drop size distribution with agitation speed is very important in these extractors (Hemmati et al., 2015b; Oliveira et al., 2008). The unified correlations for prediction of the drop size in mechanically agitated columns are shown in Table 1.

A unified correlation for prediction of the drop size in mechanically agitated columns, namely Kühni, rotating disc, asymmetric rotating disc and Wirtz-II is reported by (Kumar and Hartland, 1996).

As a general trend, the Sauter mean drop diameter decreases everywhere in the extraction column with agitation, while the drop size distribution becomes narrower. On the other hand, an increase in the flow rates results in larger drops, an effect which has been found to be more significant for the dispersed phase flow rate in comparison with the continuous one (Tsouris et al., 1990).

Oliveira et al. (2008) studied the experiments in a short Kühni column extractor and observed that smaller drops and more uniform drop size distributions were obtained with the increase of rotor speed and column stage number, thus indicating the predominance of the drop breakage phenomena in the short columns.

The adequacies of various conventional probability density functions such as Normal, Log-normal, Gamma, Inverse Gaussian and Weibull functions were investigated by researchers for the prediction of drop size distribution in the liquid–liquid extraction column. The description of these functions is shown in Table 2 (Montgomery and Runger, 1994).

Other general features of size distribution for dispersed systems are investigated by (Mugele and Evans, 1951). A modification of the log-probability equation, called the upper-limit equation and Nukiyama–Tanasawa equation were used for dispersed spray data. The results obtained the mean diameters accurately and it indicated the type of distribution function that may be derivable from mechanical principles (Mugele and Evans, 1951).

There are many innovative and exciting statistical methods now being developed and applied to predict experimental data. The maximum entropy principle (MEP) has been successfully applied to many problems arising in a wide variety of fields such as physical, chemical, biological, computer science, etc. The maximum entropy method allows determining the least biased probability distribution function when the information available is limited by some macroscopic constraints. Nonetheless, no research work for using statistical maximum entropy method was reported in the Kühni pilot plant column for determination of drop size distribution.

In this study, the drop size of the dispersed phase was measured over a wide range of operating conditions using a 113 mm diameter Kühni column. The experimental data were then compared with the literature correlations. The maximum entropy method according the previous research work in the multi-impeller extraction contactor (Asadollahzadeh et al., 2015) and stochastic density function (Weibull, Inverse Gaussian, Gamma) were used for prediction of drop size distributions in the Kühni pilot plant column. In the process of making these comparisons, estimates will be made of the constant parameters in the maximum entropy approach as a function of effective variables. In addition, an empirical correlation was developed to predict the mean drop size based on the experimental data and the literature data for different liquid systems.

2. Fitting performance evaluation

The coefficient of determination (R^2) is used to evaluate the performance of the probability distribution functions. This coefficient defined as a percentage indicates how much of the total variation in the dependent variable can be accounted for by the experimental distribution. A higher R^2 represents a better fit using the theoretical or empirical function. The definition of the R^2 is:

$$R = 1 - \frac{\sigma_{d,x}}{\sigma_d} \tag{8}$$

where R is the correlation coefficient and σ_d is the standard deviation of the experimental data from its own mean value d_m, and is defined as:

$$\sigma_d = \left[\frac{\sum_{i=1}^{n} (d_i - d_m)^2}{n-1} \right]^{1/2} \tag{9}$$