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A comparison between drop size distributions derived from the probability distribution functions and maximum entropy principle. Case study; pilot plant Scheibel extraction column

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ABSTRACT

A new model for prediction of drop size distribution is proposed in an eleven stage Scheibel extraction column by the maximum entropy density approximation technique. In addition, the conventional probability distribution functions (Gamma, Inverse Gaussian, Weibull) have already been applied to estimate the drop size distribution. The experimental procedures were carried out by three different systems such as toluene–water, *n*-butyl acetate–water and *n*-butanol–water. The drop size distribution was measured with an image analysis technique as a function of the operating conditions and physical properties of the liquid–liquid systems. The results show that the agitation speed has the main effect on the drop size distribution in the column. However, the effects of phase flow rates are not significant. An empirical correlation is proposed for estimation of the Sauter mean drop diameter in terms of operating variables, column geometry and physical properties. The results show that the maximum entropy function describes the drop size distribution better than the conventional probability distribution functions. The Shannon maximum entropy method provided a novel prediction method for the drop size distributions in the liquid–liquid extraction columns. The latter that could be used for modeling approaches.

1. Introduction

The solvent extraction technique refers to the distribution of a solute between two immiscible liquid phases in contact with each other. This method is now very well established, featuring extensively as a selective separation process (Kislik, 2012).

The determination of drop size distributions and dispersion conditions is a common method that is used in the liquid–liquid extraction systems for the characterization and the optimization processes (Thornton, 1992). Knowledge of the drop size distribution is used for process monitoring, to control, to characterize and to improve product quality (Mjalli and Abdel-Jabbar, 2005; Rydberg et al., 2004). Maximum throughput and dispersed phase holdup can be dramatically affected by the drop size. In addition, the holdup and drop size are considered to determine mass transfer interfacial area (Chen et al., 2013; Godfrey and Slater, 1994). Indeed, the drop size distribution plays a key role in scaling up of an extraction column (Thornton, 1992). This is because the same mean drop size can be obtained from various drop size distributions which have different interfacial areas. Therefore, the change in the mean drop size and drop size distribution with agitation speed is very important in the liquid–liquid extraction columns (Rincon-Rubio et al., 1994; Zhang et al., 2009). The adequacy of various conventional proba-

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Nomenclature

AARE	Average absolute relative error (–)
d_{30}	Volume drop diameter (m^3)
d_{32}	Sauter mean drop diameter (m)
D	Blade length (m)
D_i	Droplet diameter (m)
d_e	Equivalent diameter of drop (m)
d_{ic}	Value of drop size from calculated correlation (m)
d_m	Mean value of drop size (m)
d_{max}	Maximum drop diameter (m)
d_R	Rotor diameter (m)
g	Acceleration due to gravity (m/s^2)
h_c	Compartment height (m)
m	Mass (kg)
N	Rotor speed (1/s)
n_i	Number of droplets of mean diameter d_i (–)
P	Probability of number density (–)
Pdf	Probability distribution function (–)
Q	Flow rate of the continuous or dispersed phase (m^3/s)
R^2	Coefficient of determination (–)
RSME	Root mean square error for drop size (m)
S	Shannon entropy (–)
V	Superficial velocity (m/s)

Greek

λ	Lagrange multipliers of probability maximum entropy function
α	Constant parameter of probability of density function
β	Constant parameter of probability of density function
γ	Interfacial tension (N/m)
$\Delta\rho$	Density difference between phases (kg/m^3)
μ	Viscosity (Pa s)
ρ	Density (kg/m^3)
σ	Standard deviation of drop size (m)

Subscripts

c	Continuous phase
d	Dispersed phase

bility density functions such as Normal, Log-normal, Gamma, Inverse Gaussian and Weibull functions was investigated by researchers for the prediction of drop size distribution in liquid–liquid extraction column. The description of these functions was shown in Table 1 (Montgomery and Runger, 1994).

The full potential of liquid extraction processes could not be realized because of the lack of suitable commercial equipment (Godfrey and Slater, 1994). The operation of all pieces of extraction equipment is a compromise between capacity and efficiency. The theoretical stage is based on mixing the countercurrent phases to achieve equilibrium and then separating them completely. The first step requires a long contacting time. The smaller droplets will move more slowly countercurrent to the continuous phase, thus reducing throughput and increasing contact time. The use of external power for mixing can provide the full range of capability up to stable emulsion formation.

The residence time of the dispersed phase in an agitated column is a function of the power input. High power inputs increase the approach to equilibrium between the phases by increasing the interfacial area for mass transfer and residence time of the droplets in the mixing and settling zones. In the industry, various types of commercial rotary agitated columns are used in the extraction processes (Aguailar and Cortina, 2013; Hemmati et al., 2015; Torab-Mostaedi and Asadollahzadeh, 2015).

Table 1 – Probability distribution functions (Montgomery and Runger, 1994).

Function		Parameter
Normal	$\frac{1}{\beta\sqrt{2\pi}}e^{-\frac{(x-\alpha)^2}{2\beta^2}}$	$\alpha \in R$, $\beta^2 > 0$, $x \in R$
Log-normal	$\frac{1}{x\beta\sqrt{2\pi}}e^{-\frac{(\ln x-\alpha)^2}{2\beta^2}}$	$\alpha \in R$, $\beta > 0$, $x \in (0, \infty)$
Inverse Gaussian	$\left[\frac{\beta}{2\pi x^3}\right]^{1/2}e^{-\frac{\beta(x-\alpha)^2}{2\alpha^2 x}}$	$\alpha > 0$, $\beta > 0$, $x \in (0, \infty)$
Gamma	$\frac{1}{\beta^\alpha\Gamma(\alpha)}x^{\alpha-1}e^{\frac{-x}{\beta}}$	$\alpha > 0$, $\beta > 0$, $x \in (0, \infty)$
Weibull	$\begin{cases}\frac{\beta}{\alpha}\left(\frac{x}{\alpha}\right)^{\beta-1}e^{-\left(\frac{x}{\alpha}\right)^\beta} & x \geq 0 \\ 0 & x < 0\end{cases}$	$\alpha > 0$, $\beta > 0$, $x \in (0, \infty)$

The Scheibel extraction column is one of the available countercurrent agitated contactors, consisting of an alternate series of mixing sections and packed sections in a vertical column. Its design was first proposed by Scheibel in 1946 that proved to be highly effective in laboratory, pilot plant, and small commercial scale processes (Bonnet and Jeffreys, 1985; Ma et al., 2014). There are at least three designs. This column consists of a vertical shell divided into a number of compartments by annular partition discs. A central agitator shaft has a set of double-bladed paddle or turbine impellers, one for each compartment. In the older version, a wire mesh packing filled a part of the compartment. The packing helps in drop coalescence but makes the column prone to fouling (Alatiqi et al., 1995; Godfrey and Slater, 1994).

Honekamp and Burkhart (1962) used the MIBK–water system to investigate the effect of different heights of packing on the mean drop size in the Scheibel extraction column.

The effect of dispersed phase holdup, rotor speed, and column height on the Sauter mean drop size in mixing sections was reported by Chiang and Mak (1990). Bonnet and Jeffreys (1985) reported that the dispersed phase mean drop size in mixing sections of Scheibel column was affected by packing pad height, phase flow rates, rotor speed.

Yuan et al. (2012) proposed a correlation for calculating the dispersed phase mean drop size in the Scheibel extraction column with no mass transfer, by the following relation:

$$\frac{d_{32}}{D} = 0.509\left(\frac{Q_d}{ND^3}\right)^{0.093}\left(\frac{\mu_c}{\mu_d}\right)^{0.246}\left(\frac{\Delta\rho}{\rho_d}\right)^{-2.40}\left(\frac{ND^2\rho_d}{\mu_d}\right)^{-0.63}\left(\frac{\gamma}{ND\mu_d}\right)^{0.456} \quad (1)$$

An improved correlation of the mean drop size in the modified Scheibel extraction column with no mass transfer was derived by Yuan et al. (2014). The correlation was divided into three sections in terms of the Reynolds number.

In the present paper, the influence of operating conditions and physical properties of the three systems (toluene–water, n-butyl acetate–water, n-butanol–water) on the drop size distribution in the Scheibel pilot plant column was investigated. A new methodology for estimation of drop size distribution based on the maximum entropy approach was examined in this column. The relevant Lagrange multipliers in the maximum entropy approach were correlated with effective variables such as operating parameters and physical properties of the three systems. In addition, the conventional probability distribution functions (Gamma, Inverse Gaussian, Weibull) have already been applied to compare the results with maximum entropy approach.