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## Investigations of mass transfer with chemical reactions in two-phase liquid–liquid systems

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### A B S T R A C T

A new method based on experimental determination of the product distribution of a set of complex test reactions has been introduced and applied to study mass transfer in liquid–liquid systems. The test reactions consist of two parallel reactions, one of them being instantaneous and the second fast relative to mass transfer. Two reactants are transferred from the dispersed, organic phase (phase volume 1% vol) to the continuous aqueous phase, where the third reactant is present. Experiments were carried out in a batch system agitated with either a six-blade paddle impeller or a high-shear rotor–stator LR4 Silverson mixer to disperse drops and increase the mass transfer rate. The product distribution and the drop size distribution were measured using gas chromatography–mass spectroscopy and Malvern MasterSizer, respectively with pH variation recorded during the process. The results show that the focused supply of energy in the Silverson mixer is effective for the short term irreversible drop break-up process producing smaller droplets than the six-blade paddle impeller. However for the long term mass transfer process the paddle impeller is more effective due to more uniform supply of energy and better mixing throughout the tank compared to the more localized mixing of the Silverson.

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### 1. Introduction

The inability to mix reagents rapidly retards a single fast chemical reaction, which may result in a larger vessel or longer mean residence time to achieve a particular conversion compared to well mixed reagents. Similarly in complex reactions the conversion rates will also be reduced by poor mixing when the reaction rate is fast relative to observed mixing rates. Even more important are the reduced yields and the distribution of the reaction products (Bałdyga and Bourne, 1999). In this work we are interested in rotor–stator mixers that belong to the group of high-shear devices which are expected to be more energy efficient because of the focused delivery of energy. Consequently they are used in many industries including chemical, pharmaceutical, biochemical, agricultural, cosmetic, health care and food processing for homogenization, dispersion, emulsification,

grinding, dissolving, performing chemical reactions with high selectivity, cell disruption and shear coagulation. High stresses and large values of deformation rate are generated in the rotor–stator mixers because the rotor is situated in close proximity to the stator and high rotor speeds are used. This requires a very high agitation power and hence, development of methods that can predict agitation power and efficiency of mixing is of the highest importance. In this context the opinion presented by Atiemo-Obeng and Calabrese (2004) is often cited, namely that “the current understanding of rotor–stator devices has almost no fundamental basis”, which has obvious consequences for design methodologies. However, considerable work has been done since 2004 on power draw during agitation (Bałdyga et al., 2007; Kowalski et al., 2011; Jasińska et al., 2012). In the present work a method that can be used to characterize mixing efficiency in a two-phase liquid–liquid system is proposed. The method is based on application of

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## Nomenclature

A, B, R, S	reactants
$A_d$	drop surface, $m^2$
$a$	specific surface area, $m^{-1}$
$a_v$	intermaterial area per unit volume, $m^{-1}$
$C_i$	concentration of $i$ , $mol\ m^{-3}$ , $mol\ dm^{-3}$
$D_{Ci}$	molecular diffusivity of $i$ in continuous phase, $m^2\ s^{-1}$
$\bar{D}$	deformation tensor, $s^{-1}$
$d_d$	drop diameter, $m$
$E$	engulfment parameter, $s^{-1}$
$eff$	efficiency of mixing
$Ha$	Hatta number
$k_1, k_2$	reaction rate constants, $dm^3\ mol^{-1}\ s^{-1}$
$k_L$	mass transfer coefficient, $m\ s^{-1}$
$N_C$	number of C moles, $mol$
$R_i$	reaction rate, $mol\ dm^{-3}\ s^{-1}$
$Sh$	Sherwood number
$t$	time, $s$
$V$	volume, $m^3$
$V_d$	drop volume, $m^3$
$v$	velocity, $m\ s^{-1}$
Greek letters	
$\varepsilon$	rate of dissipation of kinetic energy of turbulence per unit mass, $m^2\ s^{-3}$
$\varepsilon_T$	total rate of energy dissipation per unit mass, $m^2\ s^{-3}$
$\varepsilon_{N,Q}$	total rate of energy dissipation per unit mass for rotor–stator mixer, $m^2\ s^{-3}$
$\nu$	kinematic viscosity, $m^2\ s^{-1}$
$\sigma$	interfacial tension, $N\ m^{-1}$
$\tau_{Mi}$	time constant for mass transfer, $s$
$\tau_{Ri}$	time constant for reaction $i$ , $s$

complex test reactions and follows the methodology that is traditionally used to study mixing in homogeneous systems (Bałdyga and Bourne, 1999). In this method the effects of process conditions on the product distribution from complex reactions are investigated, and the product distribution is afterwards linked to mixing energy efficiency using appropriate models. Using this method one can compare the energetic efficiency of mixing in systems of different geometry (Malecha et al., 2009). The method is based on the observation (Ottino, 1981) that the process of mixing between elongated but not completely mixed slabs can be represented by the rate of creation of the intermaterial area per unit volume,  $a_v$  [ $m^{-1}$ ], and is expressed by:

$$\left| \frac{1}{a_v} \frac{da_v}{dt} \right| = eff(t) (\bar{D} : \bar{D})^{1/2} \quad (1)$$

where  $\bar{D}$  [ $s^{-1}$ ] represents the deformation tensor that is defined using the velocity gradient,  $grad(v)$ .

$$\bar{D} = \frac{1}{2} [grad(v) + grad(v)^T] \quad (2)$$

Eq. (1) depicts the fact that orientation of the interface between different materials with respect to the principle axes of deformation determines effectiveness of mixing. Namely, not all the energy is dissipated due to flow and resulting fluid

deformation increases intermaterial area; their effect can be opposite as well.

Using this concept one can define efficiency of mixing by

$$eff(t) = \frac{1}{a_v} \frac{da_v}{dt} \left( \frac{\varepsilon_T}{3\nu} \right)^{-1/2} \quad (3)$$

where  $\varepsilon_T$  [ $m^2\ s^{-3}$ ] represents the total rate of energy dissipation per unit mass (Ottino, 1981; Rožeń, 2008). The procedure includes modelling of the effects of mixing on the course of the test chemical reactions using the E-model of micromixing (Bałdyga and Bourne, 1999). When micromixing is controlled by the viscous-convective engulfment process, then the concentration history can be calculated from the engulfment equations

$$\frac{dC_i}{dt} = E((C_i) - C_i) + R_i \quad (4)$$

$$\frac{dV}{dt} = E \cdot V \quad (5)$$

with the engulfment parameter,  $E = 0.058(\varepsilon/\nu)^{1/2}$ , that depends on the rate of energy dissipation,  $\varepsilon$ . We use then the rate of energy dissipation,  $\varepsilon$ , as a reference value, characterizing the pure effect of elongation of structures present in eddies of the length scale equal roughly to  $12\lambda_K$  (Bałdyga and Bourne, 1999) in isotropic, homogeneous turbulence. When as a system of test reactions comprising of a simultaneous diazo-coupling between 1- and 2-naphtols and diazotized sulphanilic acid is used, then there are two measures of product distribution, one concentrating on the yield of the secondary product S (a bisazo dye) and the other on the yield of the competitive product Q (a single monoazo dye).  $X_Q$  is the fraction of the diazotized sulphanilic acid converted into Q and similarly  $X_S$  presents the fraction of the diazotized sulphanilic acid converted into S. Effects of energy dissipation on  $X_S$  and  $X_Q$  are presented in Fig. 1, left; clearly in this case one should use  $X_Q$ .

Comparing now the theoretical rate of energy dissipation,  $\varepsilon$ , necessary to obtain the same product distribution,  $X_Q$ , as observed in considered experiment characterized by the rate of energy dissipation equal to  $\varepsilon_T$ , one can express the average efficiency of mixing,  $eff$ , by

$$\overline{eff} = \left( \frac{\varepsilon}{\varepsilon_T} \right)^{1/2} \quad (6)$$

The overbar in Eq. (6) denotes the value averaged over the residence time  $t$  in the mixer and  $\overline{eff}$  means this fraction of the real rate of strain that is used directly to increase the intermaterial area. The rate of strain is expressed here using a root square of the second invariant of the deformation tensor.

In the case of the rotor–stator system the rate of energy dissipation depends on both the rotor speed  $N$  and the flow rate  $Q$ , so we express the observed value of the rate of energy dissipation as  $\varepsilon_T = \varepsilon_{N,Q}$  (Jasińska et al., 2012). Fig. 1 explains the procedure applied to identify efficiency of mixing. Applying this procedure to experimental data of Jasińska et al. (2012) one obtains results shown in Fig. 1, down. It shows that the efficiency of mixing in the rotor–stator for homogeneous system, where micromixing controls the course of chemical reactions, is between 6% and 35%, and decreases with increasing rotor speed. Such a decrease results from the fact that for smaller rotor speeds the reaction zone is localized close to the screen in the region of high dissipation rate, whereas for higher rotor speeds the reaction zone shrinks and is localized closer to

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