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# From single drop coalescence to droplet swarms – Scale-up considering the influence of collision velocity and drop size on coalescence probability

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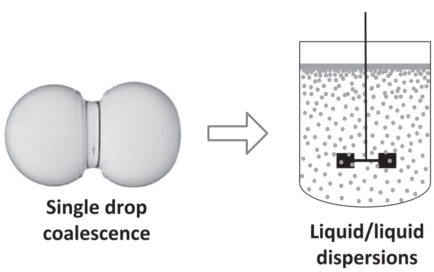
## G R A P H I C A L  A B S T R A C T

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Coalescence modelling in liquid/liquid dispersions is a challenging task and field of investigations up to now, which becomes apparent when comparing the various existent models with their different and partly even contradictive implementation of influencing factors. In this work, systematic investigations of single drop coalescence were used to compare and validate different coalescence efficiency models regarding the important influencing parameters relative collision velocity and drop size. The impact of these parameters could be analysed independently from each other for the first time and used to identify the best modelling approach. Moreover, the numerical parameter of the coalescence efficiency model could be obtained based on single drop experiments. Using this determined parameter the simulation of drop size distributions within a lab scale stirred vessel was possible. The presented method offers the possibility of independent parameter estimation for population balance equation simulations based on single drop experiments. The application of this systematic approach allows the separate validation of submodels and reliable parameter determination by small scale investigations. On this basis a sound scale-up is possible using population balance equation simulations.



## 1. Introduction

In many technical applications liquid/liquid systems are an integral part of the production process, i.e. in extraction columns or stirred tanks. The drop size distribution within these apparatuses is formed by drop breakage and coalescence and determines the overall efficiency of the process. Hence, a similar drop size distribution is the main goal for scale-up from lab scale to production scale. However, empirical scale-up rules are used up to

*Abbreviations:* C&T: Coulaloglou and Tavlarides (1977); CAV: critical approach velocity; CFD: computer fluid dynamics; Chen: Chen et al. (1998); Hen: Henschke et al. (2002); L&M: Lehr and Mewes (2001); MIBK: methyl isobutyl ketone; P&B: Prince and Blanch (1990); PBE: population balance equation(s); PTFE: polytetrafluoroethylene; RMSD: root-mean-square deviation; Sov: Sovova (1981)

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**Nomenclature**

*Latin letters*

| | |
|---|---|
| $A_{1,2,3}$ | Hamaker constant [N m] |
| $c_{1,b}$ | numerical parameter in PBE: breakage rate [–] |
| $c_{2,b}$ | numerical parameter in PBE: breakage rate [–] |
| $c_{1,c}$ | numerical parameter in PBE: collision frequency [–] |
| $c_{2,c}$ | numerical parameter in PBE: coalescence efficiency [various] |
| $c_\beta$ | standard deviation tolerance [–] |
| $C_D$ | drag coefficient [–] |
| $d_{32}$ | Sauter mean diameter [m] |
| $d_{bot}$ | bottom droplet diameter [m] |
| $d_{eq}$ | equivalent droplet diameter [m] |
| $d_i$ | impeller diameter [m] |
| $d_\mu$ | mean diameter of Gaussian drop size distribution [m] |
| $d_\sigma$ | standard deviation of Gaussian drop size distribution [m] |
| $d_p$, $d_p'$, $d_p''$ | particle/droplet diameter, differentiation between several drops by apostrophe(s): ′ [m] |
| $d_{p,max}$ | maximal particle/droplet diameter [m] |
| $d_{top}$ | top droplet diameter [m] |
| $D_t$ | tank diameter [m] |
| $f$ | number density function [m$^{-3}$] |
| $F$ | coalescence rate [m$^3$/s] |
| $g$ | breakage rate [s$^{-1}$] |
| $g$ | gravitational acceleration [m/s$^2$] |
| $h$ | drop rise height [m] |
| $h_{coll}$ | drop rise height at collision [m] |
| $h_i$ | height of impeller installation (from bottom) [m] |
| $H_t$ | tank height [m] |
| $m$ | number of values [–] |
| $M$ | mass [kg] |
| $n$ | stirrer frequency [min$^{-1}$] |
| $n_d$ | number of daughter drops after breakage event: 2 [–] |
| $Ne$ | Power/Newton number [–] |
| $P$ | power input [W] |
| $Re$ | Reynolds number [–] |
| $s_{collision}$ | drop separation distance at collision [m] |
| $t$ | time [s] |
| $t_{contact}$ | contact time of two drops [s] |
| $v$ | velocity [m/s] |
| $v_{coll}$ | relative collision velocity between drops [m/s] |
| $v_{crit}$ | critical collision velocity [m/s] |
| $v_{flow}$ | absolute flow velocity [m/s] |
| $v_{max}$ | maximal collision velocity [m/s] |
| $v_p$ | particle/droplet rise velocity [m/s] |
| $v_{rel}$ | relative velocity between drops (at collision) [m/s] |
| $v_t$ | terminal rise velocity [m/s] |
| $V_p$ | particle/droplet volume [m$^3$] |
| $V_\mu$ | mean value of daughter drop volume distribution [m$^3$] |
| $V_\sigma$ | standard deviation of daughter drop volume distribution [m$^3$] |
| $V_t$ | tank volume [m$^3$] |
| $X_i$ | experimental value [various] |
| $\hat{X}_i$ | simulation result [various] |

*Greek letters*

| | |
|---|---|
| $\alpha$ | virtual mass acceleration factor [–] |
| $\beta$ | daughter drop size distribution [–] |
| $\epsilon$ | energy dissipation rate [m$^2$/s$^3$] |
| $\epsilon_{max}$ | maximum energy dissipation rate [m$^2$/s$^3$] |
| $\epsilon_{mean}$ | mean energy dissipation rate [m$^2$/s$^3$] |
| $\gamma$ | interfacial tension [N/m] |
| $\lambda$ | coalescence efficiency/probability [–] |
| $\mu_c$ | dynamic viscosity of continuous phase [Pa s] |
| $\mu_d$ | dynamic viscosity of disperse phase [Pa s] |
| $\mu_{disp}$ | dynamic viscosity of dispersion [Pa s] |
| $\mu^*$ | dynamic viscosity ratio [–] |
| $\varphi$ | phase fraction [–] |
| $\varrho_c$ | density of continuous phase [kg/m$^3$] |
| $\varrho_d$ | density of disperse phase [kg/m$^3$] |
| $\varrho_{disp}$ | density of dispersion [kg/m$^3$] |
| $\vartheta$ | temperature [°C] |
| $\xi$ | collision frequency [m$^3$/s] |

now which require geometric similarity and constant impeller tip speed or power input (Ghotli et al., 2013). Apart from that, a mechanistic approach using population balance equations (PBE) (Liao and Lucas, 2010, 2009) was established in the past years using single drop investigations to describe the fundamental phenomena breakage and coalescence in PBE (Bart et al., 2006; Kamp and Kraume, 2015; Kopriwa et al., 2012; Maaß and Kraume, 2012; Villwock et al., 2014b). Using PBE, which describe the breakage and coalescence rate by separate submodels, a bottom-up approach from small scale single drop experiments to droplet swarms in technical applications can be performed directly omitting empirical scale-up and pilot plant scale investigations. As drop breakage was investigated in detail by several authors (Ghotli et al., 2013; Lasheras et al., 2002; Maaß, 2011; Maaß et al., 2011a; Solsvik et al., 2013) and the bottom-up approach was applied successfully focussing on the drop breakage (Maaß and Kraume, 2012), this work focusses on drop coalescence and its modelling in PBE.

### 1.1. Drop coalescence

Coalescence describes the confluence of two disperse droplets or a drop with the corresponding continuous phase. Before coalescence between two droplets occurs, the interfaces approach each other and a thin film of surrounding continuous phase has to drain between the interfaces. At a certain critical distance the continuous phase film ruptures and the drops confluence. However, a collision of droplets does not end in coalescence necessarily, but may also results in a repulsion or agglomeration of the droplets. The probability of coalescence after droplet collision is described by the coalescence efficiency in PBE. The coalescence efficiency is influenced by numerous factors especially surface active components in already small amounts (Kamp et al., in press). Due to the involved complex interactions in distances of several orders of magnitude, numerous modelling approaches can be found in literature (Liao and Lucas, 2010) which implement influencing factors differently and in parts even contradictorily (Kamp et al., in press; Kopriwa et al., 2012).

### 1.2. Drop rise velocity and surface mobility

To determine the purity of a system and the interface of investigated droplets in particular, the drop rise velocity is a very sensitive parameter. Already small changes at the interface result in an altered surface mobility and, thus, increased friction coefficient which again diminishes the rise velocity (Villwock et al., 2014a; Wegener et al., 2014). A force balance of a single drop with diameter $d_p$ leads to the terminal drop rise velocity: