1. INTRODUCTION
The dispersion of two immiscible liquids in a turbulent liquid flow is commonly found in many technical processes with major importance for chemical, pharmaceutical, petroleum, and food industry. The size distribution of the drops resulting from the opposed phenomena of drop breakage and coalescence plays an essential role in the overall performance of these processes. For example, in stirred tanks the mass transfer rate between the phases in liquid-liquid systems does not only depend on the dynamics of the motion between the two immiscible liquids, but even more on the particle size distribution of the drops. A quantitative understanding of drop breakage and coalescence mechanisms is essential for the development of predictive models for the mathematical description of drop size distributions. For that reason, both phenomena are, as different submodels, united in one model: The population balance equation. Currently simulations of dispersion properties like drop size distribution and interfacial area as a function of process and physical parameters are still inaccurate for an inhomogeneous flow field typical for a stirred tank. Therefore by variation of process parameters the model parameters must often be adapted [1, 5].

2. METHODS AND MATERIALS
2.1 Population Balance Equation
The population balance equation (PBE) is applied to predict the size distribution in stirred liquid/liquid systems. For this case transport terms are neglected, while the vessel is a batch reactor with high flow velocities inside the tank. These velocities cause a drop size distribution independent from the position in the tank. The source term of the PBE considers on the one hand that dispersed fluid particles can undergo break-up, implying death of the parental particle and birth of child individuals. On the other hand, it also happens that two particles coalesce. All these phenomena are described statistically by several sub-models for collision frequency, coalescence and breakage rate and daughter drop distribution, which have been proposed in the last four decades. The form used here is derived from the general form proposed by Hulburt und Katz [8]. The PBE describes the change of the number den-
sity function of particles in the reactor volume due to source and sink terms caused by breakage and coalescence incidents. The PBE does not neglect transport processes but in eq. (1) they are neglected:

\[
\frac{d f(V_p)}{dt} = \nu(V_p, V'_p) \beta(V_p, V'_p) g(V_p') f(V_p', t)dV_p - g(V_p)f(V_p, t)
\]

\[
- f(V_p, t)\int_{0}^{V_p} F(V_p', V_p') f(V_p', t)dV_p' + \frac{1}{2} \int_{0}^{V_p} F(V_p', V_p') f(V_p', t)f(V_p', t)dV_p'
\]

\[
v(V_p') - \text{number of daughter drops per breakage, } g(V_p) - \text{breakage rate}
\]

\[
\beta(V_p, V'_p) - \text{daughter drop size distribution, } F(V_p, V'_p) - \text{coalescence rate}
\]

For the solver PARSIVAL\textsuperscript{®} [20] the original model has to be transformed from the volume based form into the diameter based function via eq. (2). Here is \( V_p = k_V \cdot d_p^3 \) and \( k_V \) always \( k_V = \pi/6 \) as the volume factor for a sphere while all drops are assumed as ideal spheres.

\[
f_{d_p}(d_p, t) = 3k_V d_p^2 f_{V_p}(d_p, t)
\]

2.1.1 Modelling of coalescence phenomena within the PBE
A large number of models for breakage and coalescence exist in literature; the most important ones were analyzed recently by Lasheras et al. [12]. Most authors formulate the coalescence rate as a product of collision frequency of the drops \( h(d_p', d_p') \) and the collision efficiency \( \lambda(d_p', d_p') \):

\[
F(d_p', d_p') = h(d_p', d_p') \cdot \lambda(d_p', d_p')
\]

Since the collision frequency equation published by Coulaloglou & Tavlarides [2] was slightly erroneous the following corrected equation in diameter form is commonly used [18]:

\[
h(d_p', d_p') = c_1c \frac{e^{1/3}}{1 + \varphi_d} (d_p' + d_p')^2 (d_p'^{2/3} + d_p^{2/3})^{1/2}
\]

For the collision efficiency, Coulaloglou and Tavlarides [2] obtain:

\[
\lambda(d_p', d_p') = \exp \left( -c_2c \frac{\mu c \rho_c \epsilon}{\sigma^2(1 + \varphi)^3} \left( \frac{d_p' \cdot d_p}{d_p' + d_p} \right)^4 \right)
\]

The entire coalescence rate \( F(d_p', d_p') \) gives low values for the contact of two small or two large drops and high values for the contact of a small and a large drop. The coalescence rate by Coulaloglou and Tavlarides [2] is used for modelling here, as many applications have proven its reliability. For further simulations it has to be extended concerning pH-value and ionic strength to take results from [10] into account. They revealed that ionic strength and pH-value play a decisive role concerning both steady state and transient drop size distributions. This has to be considered in further model approaches by additional physical parameters.

2.2.1 Modelling of breakage phenomena within the PBE
Numerous authors proposed model equations for the drop breakage rate [1, 2, and 14]. In many cases the authors assume that drop breakage occurs due to drop-eddy collisions. The most widely used and discussed model for the drop breakage rate is the approach of Coulaloglou and Tavlarides [2], which is used for the simulation in this investigation. They
assume that breakage occurs if the kinetic energy of an eddy is larger than the surface energy of the droplet. For the breakage rate $g(d_p)$ (in diameter form) with two free parameters $c_{1,b}$ and $c_{2,b}$ they obtain:

$$g(d_p) = c_{1,b} \frac{e^{1/3}}{(1 + \varphi_d) d_p^{2/3}} \exp \left( - c_{2,b} \frac{\sigma(1 + \varphi_d)^2}{\rho e^{2/3} d_p^{5/3}} \right)$$

(6)

To determine the daughter drop distribution, it is necessary to specify the number of daughter drops. Most authors assume binary breakage of a mother drop into two daughter drops with a maximum probability of forming two equally sized daughter drops. This part of the model has to be discussed, because first experimental investigations analysing drop breakage carried out by Konno et al. [9] found a maximum probability for ternary breakage in a CSTR. Investigations on breakage have also been carried out by Galinat et al. [4]. They do also not show maximum probability for equally sized daughter drops. Kuriyama et al. [11] analyzed breakage events of highly viscous drops and investigated breakages with up to 30 daughter drops.

The daughter drop size distribution in the model of Coulaloglou and Tavlarides [2] is a standard Gaussian distribution with binary breakage. Several alternative models were proposed during the last decades with partly contradictory results [2, 18]; an overview is given in [19]. Analysing existing models for daughter drop size distributions an improved model should be based on the energy dissipation rate and the mother drop diameter. While analysing all sub models of the PBE is too extensive, our investigation started with analysing breakage phenomena. In the following chapters we will focus on analysing and modelling daughter drop size distribution after drop breakage.

### 2.2 Experimental Set Ups

Two different kind of experimental investigations were carried out: The whole application, a stirred tank is analysed and single drop experiments to determine physical laws of drop breakage were carried out.

In the stirred tank an optical measurement technique (Fig. 1, left) [15] was installed in order to determine the drop size distribution. Photos were taken from inside the vessel ($T = 150$ mm, Rushton turbine, $D/T = 1/3$, $h/H = 1/3$, $H/T = 1$). The drops were semi-automatically measured and counted by image analysis. The distributions are used for estimation of the numerical parameters and also to verify the modelling. This is done by the commercial software PARSIVAL®. Experimental and numerical results of drop size distributions of the stirred tank are given in [5].

For the investigation of the daughter drop size distribution a new experimental setup was developed in order to determine number and size distribution of the daughter drops (Fig. 1, right). This set-up consists of a single drop breakage cell where both the process of breakage (cam 2) and the daughter drop size distributions (cam 1) can be analyzed. The cell is build by a rectangular channel with a fixed single blade representative for a section of a Rushton turbine. A single petroleum drop with a clearly defined diameter between 300 \(\mu\)m and 2 mm is introduced into a continuous water flow by a Hamilton pump. This high accurate dosing pump produces mother drops with standard deviation of the diameter less than 0.05. The broken drops created in the vicinity of the blade were photographed using a CMOS camera (cam 1) with a flash. The breakage event is analysed with a high speed camera (cam 2) with 650 frames per second.
The experiments aim at representing a breakage of a single mother drop in the stirred tank. In order to simulate the flow field near the stirrer (Fig. 1, left) by the flow field around the blade in the channel (Fig. 1, right) the following approach has been made: In direct vicinity of the stirrer the highest local velocities inside the stirred tank exist [13, 16, 17], which are mainly responsible for the breakage processes. A correlation of the velocity at the stirrer tip and the effective local fluid velocity \( w \) in the vicinity of the stirrer is given by [13]:

\[
\bar{w} \approx 0.3 \, w_{\text{tip}}
\]

The velocity gradients close to the blade induce the breakage in the stirred tank. That implies that the difference:

\[
\Delta w = w_{\text{tip}} - \bar{w}
\]

has to be taken for the flow velocity in the channel. That implies the same relative velocity in the vessel and in the breakage cell. The correlation in eq. (8) gives the possibility to determine flow velocities in the breakage cell which characterise the impeller speeds in the stirred tank. Some results for the velocity are given in Tab. 1. The specific power input represents a second variable, which is very important for such model experiments. To compare this parameter in the stirred tank with the power input in the breakage cell, some CFD simulations using the commercial software STAR-CD® were carried out. Such simulations give the opportunity to control the local dissipation rate of turbulent kinetic energy (\( \varepsilon \)) in the breakage cell. These data are well known for a stirred tank using a Rushton turbine by many experimental investigations [6, 13, and 16].

<table>
<thead>
<tr>
<th>( N ) [U/min]</th>
<th>( \Delta w ) [m/s]</th>
<th>( \varepsilon ) [m(^2)/s(^3)]</th>
<th>( \varepsilon_{\text{loc,max}} ) [m(^2)/s(^3)]</th>
<th>( \varepsilon_{\text{loc,max}} ) [m(^2)/s(^3)]</th>
<th>( \varepsilon_{\text{loc,max}} ) [m(^2)/s(^3)]</th>
<th>( \varepsilon_{\text{loc,max}} ) [m(^2)/s(^3)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>0.5</td>
<td>0.3</td>
<td>17.0</td>
<td>3.4</td>
<td>0.03</td>
<td>0.04</td>
</tr>
<tr>
<td>550</td>
<td>1.0</td>
<td>0.8</td>
<td>44.2</td>
<td>26.1</td>
<td>0.05</td>
<td>0.06</td>
</tr>
<tr>
<td>700</td>
<td>1.5</td>
<td>1.8</td>
<td>91.1</td>
<td>88.0</td>
<td>0.07</td>
<td>0.08</td>
</tr>
</tbody>
</table>

Tab. 1 – Results of \( \varepsilon \) and \( \varepsilon_{\text{loc,max}} \) for the used Rushton turbine according to [16] compared to values found for the breakage cell by CFD.
Table 1 shows the results of $\bar{\varepsilon}$ and $\varepsilon_{\text{loc},\text{max}}$ for the used system. The values for $\varepsilon_{\text{loc},\text{max}}$ represent the highest local dissipation rates, which can be found close to the blade [13, 16]. Both values, the experimental data from literature listed in Tab. 1 and the calculated CFD results of the breakage cell, have to be compared. An example for such CFD simulation results is given in Fig. 2 for a velocity of 1.5 m/s. The agreement with the example from Schaefer [16] listed in Tab. 1 is excellent. It is also significant that with decreasing the velocity the accordance of the Simulation with the experiments is also decreasing. It is known that $k-\varepsilon$ turbulence models like the used one for the simulations are more accurate for high than for low velocities. That would explain, why the CFD data of the highest velocity fits the experimental data from Schaefer [16]. It can be assumed that a better model would produce better accordance even at low velocities. Nevertheless, the results proof that the breakage cell is an appropriate experimental set up to simulate single drop breakage, occurring to them in the stirred tank.

![Fig. 2 – Simulation results of $\varepsilon_{\text{loc},\text{max}}$ for a flow velocity of 1.5 m/s in the breakage cell.](image)

![Fig. 3 – Pictures of the daughter drops in the breakage cell under image processing: a – reference picture, b – original picture, c – picture after image subtraction, d – binary picture.](image)

The drop size analysis is carried out automatically with the commercial software ImageProPlus®. The first step of picture analysis is the subtraction of a reference picture from the picture with drops. To get a binary picture a threshold is set. The final picture only contains black drops (see Fig. 3). These areas are analysed and associated with a diameter. For volume conservation reasons the sum of detected daughter drop volumes is related to the mother drop volume. If the deviation of the volumes is more than 15% the breakage event is neglected and not counted. Thus a drop is not counted twice the image capturing is lim-
ited to a maximum of 15 frames per second with the applied system. With this acquisition frequency some drops are not recorded or the drops are too small to get recorded. The smallest diameter which can be detected with the used set-up is 50 µm.

A statistical analysis shows the significance of the measured data. With increasing mother drop size the number of statistically required samples is growing because the probability for high number of daughter drops is increased. For the technical relevant diameters ≤1 mm we analyzed the statistical necessary number of break up’s: 284 measurements for a 560 µm mother droplet, 503 events for 1 mm droplet.

3. RESULTS AND ANALYSES

3.1 Experimental Results

First of all, the experiments had the aim to record the number of daughter drops per breakage. Fig. 5 shows the probability of the daughter drop number for different mother drop diameters. The maximum number of daughter drops was observed for a 2 mm mother drop with 97 daughter drops. Fig. 4 shows an example for such a multiple break- age of a 2 mm mother drop. The turbulence and the flow acceleration in the wake of the stirrer blade deform the drop and disrupt it into several pieces. The images represent a total time of 10 ms.

![Fig. 4 – Highspeed photographs of a breaking 2mm mother drop.](image)

With decreasing mother drop volume the average number of daughter drops also decreases. The most frequent breakage event for smaller drops is the binary breakage. The 560µm mother diameter shows a probability for binary breakage of nearly 60 percent. For larger drop diameters (2 mm) the tertiary breakage is the most probably one. Since drops in stirred liquid/liquid applications for the analyzed systems are around a size of 500µm and smaller [5], it is an acceptable assumption to use \( \nu = 2 \) for simulations of drop size distribution using the population balance equation. If the mean diameter of investigated drop size distribution is larger than 1 mm, values larger than 2 should be used for the simulation of such systems.

Decreasing the flow velocity (Fig. 6) for a constant mother drop size, the probability for binary breakage is, as expected, increasing. These results reflect the influence of the power input on drop breakage. This is the second parameter besides the mother drop diameter which should be taken into account for modelling of drop breakage and daughter drop size distributions.

![Fig. 5 – Probability of different numbers of daughter drops: Varying the mother drop diameter \( \nu \) for 1 m/s flow velocity.](image)
Fig. 6–Probability of different numbers of daughter drops: Varying the flow velocity for 1 mm mother drop.

Fig. 7 shows the number density distribution of single breakage events from 2 up to 10 daughter drops for 1 mm mother drops. The upper abscissa marks the mean diameter for equally sized daughter drops, as assumed by many authors in the literature. The results show, that such an assumption is significantly wrong. The mean diameter for binary breakage of the experiments is larger than the theoretical assumption and for higher numbers then ternary breakage it is significantly smaller.

All together, these results about number probabilities and number density distributions of daughter drops are a solid basis for further developments of drop breakage models. They will be used for modelling of the number of daughter drops \( \nu \) and the size distribution \( \beta \).

**3.2 Modelling**

Firstly the numerical investigations aim on the development of a new model for the daughter drop size distributions \( \beta \) as a function of \( \nu \). For the modelling a daughter drop probability density function (pdf) is used, which is similar to a particle density distribution (pdd). Thus pdf’s provide probabilistic values, whereas pdd’s provide deterministic values. Efficient daughter drop size pdf’s used within the PBE problem must satisfy some important requirements: Besides the necessity that mass is conserved before, during and after the breakage process, the candidate function should have no singularity points and it should fall to zero as the ratio between the daughter and the mother diameters goes to zero and to one \([19]\). Furthermore, it is important that the model is meaningful from a physical point of view. This means that, since the distribution of breakage products, as confirmed by all experimental observations, is influenced by both, turbulent energy dissipation rate and mother drop diameter, such parameters should be contained in the pdf as parameters. Finally the function should be positive on the whole
domain and upper bounded (required for successful implementation in PARSVIAL®).

Many statistical models show a maximum for equally sized drops, like the normal distribution suggested by Coulaloglou and Tavlarides [2] or the Beta-pdf by Konno et al. [9]. These models do not contain any dependency on physical parameters. Another model by Dieemer and Olson [3] is a very flexible one. It is a generalized function, so that nearly all daughter drop distributions in the literature are captured by varying the two free parameters q and υ (see eq. (9)). These parameters are defined as functions of a shape parameter q and of the mean number of daughter drops per breakage event υ. The pdf can be formulated as:

\[
\beta(z) = \nu \left( \frac{\Gamma(q \nu)}{\Gamma(q)\Gamma(q(\nu - 1))} \right) z^{q-1} (1-z)^{q(\nu-1)-1} = \nu \frac{z^{q-1} (1-z)^{r-1}}{\beta(q, r)} ,
\]

By keeping the physical parameters (θ, ρ, η, σ) constant, it is possible to identify the dependency of q on the Weber number. Therefore the Dieemer and Olson pdf was transformed into diameter coordinates and extended taken the energy dissipation rate into account. Our new model is expressing q as follows:

\[
q = \alpha \text{ We}^a \left( \frac{d_{cr}}{d_p} \right)^b \tag{10}
\]

\[
d_{cr} = \frac{0.206}{\epsilon^{2/5}} \left( \frac{\sigma}{\rho} \right)^{3/5} \text{ - critical diameter,}
\]

\[\text{We} = \frac{\rho n^2 D^3}{\sigma} \text{ - Weber number.}\]

The parameters for q were fitted against the presented experimental data more information can also be found in [11]. While υ is constant for a simulation and q changes only for different number of daughter drops, no additional parameter for the simulation of the drop size distribution is introduced.

Passing from binary to ternary breakage, the pdf becomes wider and the maximum is shifted towards a smaller diameter ratio, meaning that the probability of formation for

![Fig. 8 – Comparison between single drop experimental data and the Beta pdf by Diemer&Olson (2002). Mother drop diameter: 1 mm, binary (left) and ternary (right) breakage.](image)
large drops decreases. The distributions derived from single drop experiments show no trend characterized by a maximum in correspondence with equally sized drops contrary to popular models from the literature. In Fig. 9 the new model for daughter drop size distribution is compared with other models, predicting a maximum probability for equal size breakage in the case of three daughter drops generated per breakage event.

that binary breakage is the most probable breakage event for single drops. Therefore the number of daughter drops per breakage which were used for both presented simulations of drop size distribution (see Fig. 10) is \( \nu = 2 \). Further more the introduced breakage and coalescence model of Coulaloglou and Tavlarides [2] were used for both simulations. The models only differ in the daughter drop size distribution. The results using the standard Gaussian distribution are compared using our own developed model (see also Tab. 2 for the numerical parameters). The parameters in Tab. 2 were all fitted against the experimental data presented in Fig. 10. There it is shown that the extended Beta function based on Diemer and Olson [3] shows better results than the common model.

The normal distribution, suggested by Coulaloglou and Tavlarides [2], and also the advanced Beta pdf used by Konno et al. [9] are definitely too narrow in comparison with the experimental data. The pdf by Martinez-Bazan et al. [14] provides a distribution which is wide in comparison with the experimental data, although it approaches them much better than the ones previously considered. But the model is not mass conserving and could not be satisfactorily implemented in PARSIVAL® [20].

The extended model was successfully implemented in PARSIVAL® to simulate the drop size distribution in the investigated stirred tank. Fig. 10 shows the comparison between two simulations with PARSIVAL® and experimental data after 80 minutes for pH 13, toluene/water and a stirrer speed of 400 rpm in a probability net. Experiments have shown

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5. DISCUSSION AND CONCLUSIONS
In the present work a mathematical formulation is developed for the daughter drop size pdf, which occurs in the breakage source term within the PBE framework for the description of drop size distributions in stirred tanks. The Beta function by Diemer and Olson (2002b) has been extended in a way that a dependency on important physical parameters ($W_e, d_p$) is considered. This model fulfills all the requirements needed to be an efficient daughter drop size pdf. The agreement with the experimental pdf’s was found to be very good, especially in comparison with other models most cited in the literature.

The developed model is empirical and needs further experimental investigations. Nevertheless, it certainly represents an advance in accuracy and is more based on physical parameters which are relevant in stirred tanks.

ACKNOWLEDGEMENTS
The authors gratefully acknowledge the financial support of the project within the framework of the Research Training Group “Transport phenomena with moving boundaries” provided by the German Research Foundation (DFG).

NOMENCLATURE
- $a, b, c$: numerical model parameter
- $B$: Euler’s Beta function
- $D$: stirrer diameter
- $d_p, d'_p, d'_p$: mother, daughter drop diameters
- $F(d_p, d'_p)$: coalescence rate
- $g(d_p, d_p)$: breakage rate
- $h(d_p, d'_p)$: collision frequency
- $h$: stirrer height
- $n$: stirrer frequency
- $H$: fill level
- $q$: shape parameter
- $T$: vessels diameter
- $w_{tip}$: flow velocity at the tip of an impeller blade
- $\bar{w}$: effective velocity of the fluid close by the tip of an impeller blade
- $\Delta w$: flow velocity
- $W_e$: Weber number
- $\alpha$: proportionality constant for $q$
- $\beta$: daughter drop size distribution
- $\epsilon$: power input
- $\phi$: phase fraction of the dispersed phase
- $\lambda(d_p, d'_p)$: collision efficiency
- $\mu_c$: viscosity of continuous phase
- $n$: number of daughter drops per breakage
- $\sigma$: surface tension
- $\rho$: density

REFERENCES


