Compartment-model for the simulation of the separation performance of stirred liquid–liquid-extraction columns

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Abstract
For detailed simulation and evaluation of stirred extraction columns a CFD based compartment-model was developed. Instead of simulating all effects in a computational expensive PBE-CFD-model, the velocity field calculation of the continuous phase is decoupled from the calculation of the dispersed phase (one-way coupling). In CFD only the continuous phase is simulated and the resulting velocity profile is used in the compartment-model to simulate the drop movement, coalescence, breakage and mass transfer for a representative number of drops (Monte-Carlo Method). This decoupling has a major impact on the calculated fluid-dynamics. Thus, the velocity profile of the CFD results is modified in the model to account for phase interaction. The compartment-model is applied for the simulation of a Kühni extraction column with the system toluene/water/acetone. The simulation results, namely holdup, drop size and concentration profiles over the column height, are in good agreement with experiments for different loads and different stirrer speeds.

KEYWORDS
CFD, compartment-model, multiphase, time-driven constant-number Monte-Carlo

1 | INTRODUCTION

For a model based design of liquid–liquid-extraction columns the movement of the drops as well as drop coalescence, breakage and mass transfer should be calculated. Especially models, which incorporate population balance equations (PBE), are capable of tracking the drop-property-distribution along the column height. PBE-based simulation tools for liquid–liquid-extraction columns can be classified in three approaches:

- One-dimensional simulation tools, which only describe the drop properties along the column height, such as ReDrop or PBELab.1-4
- CFD-models (computational fluid dynamics) with PBE, which calculate the fluid dynamics and mass transfer in an either two- or three-dimensional simulation domain.5-14
- Compartment-models, which decouple the fluid dynamic simulation from the calculation of the drop-property-distribution of the PBE.15,16

The advantage of one-dimensional models is the fast simulation of extraction columns. The model requires sub-models, which take the influence of the column geometry and energy input on drop movement, coalescence, breakage and mass transfer into account. Especially in stirred extraction-columns the retardation/slowing of drops caused by the stirrer-vortexes requires appropriate sub-models.17,18 However, such sub-models are only applicable for -column-designs, for which the correlations were developed.

The influence of novel column designs on the performance of extraction columns can be determined with CFD-models in combination with PBE. The coupled interaction of all phenomena can be modeled in detail. Nevertheless, each independent property, which
has to be considered in the PBE, increases the dimensionality of the PBE and therefore the computational effort. For example Attarakih et al. simulated an extraction column type RDC (rotating disc contactor) with a two-dimensional CFD-PBE model and required 4.63 days (without mesh refinement) to 27 days (with mesh refinement) to simulate the steady state operation point. The simulation with a three-dimensional CFD-PBE model would require even more simulation time. When simulating multiple mass-transfer components or reactions, which have to be included into the population balance, the simulation will become even more expensive.

Therefore, a hybrid model-approach was developed by Weber et al. The CFD-simulation is decoupled from the PBE by means of a compartment-model. The velocity profile of the continuous phase is modeled in CFD, accelerating the simulation time of the single phase CFD-model compared to a multiphase PBE-CFD-model. The resulting velocity and turbulent dissipation rate profile is used in the compartment-model to simulate all additional effects like drop movement, coalescence, breakage and mass transfer via PBE. The drop PBE is calculated with a Monte-Carlo method, simulating only a representative number of drops. The simulation of representative drops gives the opportunity to calculate drop movement, coalescence, and breakage on the basis of the finely resolved velocity and turbulent energy dissipation profile of the single phase CFD simulation. The drop calculation is therefore independent from the compartment resolution. However, a Monte-Carlo method requires more simulation time when calculating only single component mass transfer and is therefore often not used in CFD-PBE models for liquid–liquid extraction columns. The coupling between the continuous and disperse phase is one-way, since the effect of the disperse phase on the continuous phase velocity is neglected in the CFD-model. However, Weber et al. developed a method to approximate the effect of the disperse phase on the continuous phase velocity in the compartment model.

The advantage of the compartment-model is the calculation of the drop movement according to the velocity profile of the continuous phase. Consequently, the fluid dynamic in extraction columns with novel designs can be predicted, without the need to develop new sub-models for example, for the slowing factor which describes the retardation of the drops’ rise velocity due to stirrer induced vortices. Furthermore, the local energy input is calculated by the CFD-simulation. Consequently, drop breakage can be calculated according to the local turbulent dissipation rate, which is highest at the stirrer tip. The local turbulent dissipation rate is typically not used in one-dimensional simulation models, which apply an averaged energy input for the breakage models.

Similar compartment-models were developed, for example, for homogeneous reactors, loop-reactors, crystallizers, and bubble columns. Weber et al. simulated an extraction column type Kühni with a compartment-model. The model is capable to simulate the fluid dynamic in the column. However, mass transfer was not considered and the applicability for different energy inputs was not shown. Furthermore, fitting parameters were required to calculate the coalescence in the dense packed layer under stators. Therefore, the model was further improved by including sub-models for mass transfer and simplifying the modeling of the coalescence below the stators.

In the following, the improved compartment-model is presented. With the model the fluid dynamics and mass transfer of the extraction system toluene/water/acetone is simulated in a Kühni extraction column. The model is used to calculate various column loads and energy inputs. At the beginning of the article, we will present the simulated extraction column and the properties of the extraction system. The CFD-model is explained briefly and following the compartment-model, the implemented sub-models and the simulation setup are described. The simulations are compared to published extraction column experiments. We will first present the calculation of the holdup and sauter drop-diameter in the extraction column and afterwards the simulated concentration profiles of the disperse and continuous phase. The paper finishes with a conclusion and outlook.

2 MATERIALS AND METHODS

2.1 Set-up of stirred liquid–liquid extraction column

The column experiments of Garthe for the extraction system with toluene as dispersed phase, water as continuous phase and acetone as transfer component are compared with the simulation results of the compartment-model. The internals of the extraction column are of type Kühni and the column has a diameter of 80 mm and a height of 2.95 m. The internal design is given in Figures 1 and 2.

The chemical properties of the extraction system depend on the acetone concentration in the phases. The concentration dependent chemical properties were determined by Henschke and are given in Table 1. $x$ represents the concentration in the continuous water phase and $y$ the one in the dispersed toluene phase.

For the distribution coefficient of the transfer component acetone, the correlation of Henschke is used (Equation 1), since it compares well with the experimental values of Garthe.

$$K = 0.6442 + 2.6814x - 5.9026x^2$$

2.2 CFD-model

The velocity profile of the continuous phase is calculated with ANSYS Fluent. The CFD-model consists of a single phase Euler-Model using the standard $k$-$\varepsilon$ turbulence model. The Kühni extractor of Garthe consists of total 53 stirred sections. When simulating only the continuous phase, the velocity profile of the stirred sections in the column is comparable. Buchbender showed at single drop experiments, that only five stirred section are required for a representative velocity profile. Therefore, five stirred section are simulated in the CFD-model.
For the compartment simulation the velocity profile of the whole column is generated by duplicating the velocity profile of the middle stirred section 49 times.

2.3 | Multidimensional compartment-model

In the compartment-model the disperse phase is modeled via a representative amount of drops with a volume-constant time-driven Monte-Carlo Method. For each drop its movement, mass transfer as well as coalescence and breakage probabilities are calculated. The models for drop movement, coalescence and breakage require data from the CFD simulation such as the velocity and turbulent dissipation rate at the position of each drop. These data are stored in a three-dimensional grid. The grid represents the flow profile of the continuous phase. Therefore, the grid discretizes the continuous phase via cylindrical grid cells, which are called compartments. Between adjacent compartments, the exchange volume-flow is calculated with a surface integral according to the velocity profile of the CFD-simulation results. Internals like stirrers, stators or rods. In case of a collision between internals and drops an elastic reflection is calculated.

A volume and material balance are implemented to calculate the exchange volume and mass of the continuous phase between the compartments. These balances include displacement effects of the continuous phase volume in the compartments caused by mixing effects during drop coalescence, the drop movement and mass transfer.
In the following sections, an overview on the calculation of the drop movement and the implemented sub-models is presented. Furthermore, the modification of the continuous phase velocity to account for the effect of the dispersed phase is explained. For the calculation of the exchange volume flows between the compartments and for a more detailed explanation of the simulation of the drop movement refer to Weber et al.16

### 2.4 Drop movement in 3D velocity field

The drop movement is calculated in the 3D domain of the compartment grid. For each representative drop a force balance is solved, considering drag, gravitational and buoyancy forces. However, the coupling to the continuous phase is one-way, neglecting the influence of the dispersed phase on the continuous velocity profile. The drag force is calculated with the single drop velocity model of Henschke.1 The model requires three fitting parameters, which describe the transition of rigid spherical drops to deformed drops with a mobile interface. The model parameters were derived from single drop experiments with simultaneous mass transfer from Henschke1 for the extraction system toluene/water/acetone ($\text{dum} = 4.366 \, \text{mm}, \ a_{15} = 2.239, \ a_{16} = 1.824$).

### 2.5 Adaption of the continuous phase velocity

Since the CFD-simulation neglects the disperse phase, the coupling between the continuous and disperse phase is principally one-way. However, it is necessary to modify the continuous phase velocity according to the local holdup in the compartment simulation, to obtain reliable results. Two modifications are used and introduced in the following. The first is applied for the areas under the stators and the second for the rest of the column (Figure 3).

Below the stators, Weber et al16 observed drop layers of up to 3 mm height (chemical system butyl acetate as dispersed phase and water as continuous phase). The accumulated drop reduce the continuous phase velocity under the stators.26 Therefore, in the compartment-model the velocity of the continuous phase under the stators is reduced proportional to the holdup $\alpha$.

$$v_{c,\text{mod}} = v_c (1 - \alpha) \tag{2}$$

Equation (2) is applied only in the areas under the stators, the so-called coalescence regimes (see Figure 3). The height coordinate of the drops which enter these areas is randomly distributed so that a packed layer is formed with a holdup of approximately 74% (gray area in Figure 3). This represents the holdup value for the case of the closest packing of uniform spheres. In the simulations, the drop layer thickness varies according to the amount of drops in the coalescence regime, which in turn results from the fluid dynamic column load, operation point and chemical system.

For the simulation of the dense drop layer, the compartment model has to know, when Equation (5) has to be applied. Therefore, a maximum possible layer thickness is defined in advance to the compartment-model simulation. For the extraction system butyl acetate/water/acetone Weber et al16 experimentally observed a maximum layer thickness of 3 mm. However, due to different properties of the extraction system, operation points and different coalescence behavior larger dense packed layers could arise. Therefore, a height of 7 mm is chosen allowing the calculation of layers with up to 7 mm height.

In the other parts of the column a different modification is applied. When the drops move through the column they will accumulate according to the drop rise velocity, the counter-current flow of the continuous phase and the vortexes induced by stirrers. This accumulation leads to less space for the continuous phase volume flow increasing the continuous phase velocity as shown in Figure 4. This

| Property                  | Formula                           | Unit    | Validity  |
|---------------------------|-----------------------------------|---------|-----------|
| Density water             | 998.3 – 138.7x                    | kg/m³   | x < 0.33  |
| Density toluene           | 865.6 – 67.65y                    | kg/m³   | y < 0.4   |
| Viscosity water           | (1.009 + 2.477x) · 10^{-3}       | Pas     | x < 0.2   |
| Viscosity toluene         | (0.5828 – 0.3804y) · 10^{-3}     | Pas     | y < 0.3   |
| Diffusion coefficient in toluene | (2.786 – 4.608y) · 10^{-9} | m²/s    | y < 0.044 |
| Interfacial tension       | 0.04639x – 0.8439y²              | N/m     | x < 0.4   |

**TABLE 1** Chemical properties at 20 °C and ~100 kPa

![Figure 3](image-url)  
**FIGURE 3** Application of continuous phase velocity modification in the compartment model

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idea is implemented into the compartment-model using a continuity balance. Assuming a relative velocity $v_{rel}$ between the continuous and dispersed phase entering the control volume, following volume balance can be derived, with $A$ representing the free area, $A_{red}$ the reduced area for the continuous phase due to the holdup $\alpha$ and $v_{rel,mod}$ the modified velocity due to the reduced space.

$$
V = A \cdot v_{rel} = A_{red} \cdot v_{rel,mod}
$$

(3)

The reduced area $A_{red}$ is calculated according to the local holdup.

$$
A_{red} = A (1 - \alpha)
$$

(4)

When applying Equation (4) in Equation (3) and with $v_{rel} = v_c - v_d$ the modified continuous phase velocity can be calculated.

$$
v_{rel,mod} = v_{rel} + v_d = v_{rel} \frac{1}{1 - \alpha} + v_d = (v_c - v_d) \frac{1}{1 - \alpha} + v_d
$$

(5)

For Equation (5) the local holdup $\alpha$ is calculated for each representative drop in a search radius (25 mm). All neighbor drops in this search radius are determined with the Matlab function "knnsearch." Since the drops are tracked as moving points they can overlap and the holdup could be calculated to high. Therefore, the local holdup is limited to 50% in the simulation.

Summing up, the developed algorithm for the velocity modification has following parameters: search radius for local holdup calculation, maximum local holdup value, maximum area of coalescence regimes and holdup in the dense packed layer. The area of the coalescence regimes was chosen according to experimentally measured layers (3 mm) and a security factor of 2.3 is applied. The holdup in the dense packed layer was chosen according to the closest dense packed layer of uniform spheres. In the end, the search radius for the local holdup calculation and the maximum holdup value were determined with parameter studies in comparison to the column experiments of Garthe. This parameters influence the calculated overall holdup. It is noteworthy, that the compartment model fails to predict the holdup in an extraction column by a factor of up to ~4, when the modification of the continuous phase velocity is neglected. Especially at high column loads, the dispersed phase has a major impact on the continuous phase velocity profile as also reported by CFD simulations and PIV measurements.

2.6 Modeling of coalescence and breakage during drop movement

Coalescence is determined with random numbers between 0 and 1. When the random number is smaller than the coalescence probability, the drop is marked and coalesces with another marked drop. The probability for drop coalescence $Z_c$ is calculated with the time-step size $\Delta t$ and the statistic lifespan $\tau_c$ until the drop coalesces with another drop.

$$
Z_c = \frac{\Delta t}{\tau_c}
$$

(6)

For $\tau_c$, the model of Henschke is applied, which was developed for liquid–liquid extraction columns.

$$
\tau_c = \frac{\xi}{\alpha^2 \cdot H_d \cdot (\Delta t/\rho) \frac{d^{1/3}}{}}
$$

(7)

Here $\xi$ represents the coalescence parameter, which needs to be fitted to column experiments, $\mu_c$ the viscosity of the continuous phase, $d$ the drop-diameter, $\alpha$ the local holdup calculated in the compartment-model, $\gamma$ the interfacial tension, $H_d$ the Hamaker coefficient (for organic-aqueous systems $\sim 10^{-20}$ Nm), $\Delta t$ the density difference and $g$ the constant of gravitation.

Instead of simulating the coalescence layer below the stators explicitly introducing several new model parameters as done by Weber et al., coalescence below the stator is calculated with the same coalescence model (Equations (6) and (7)) as in the free sedimentation. Only the local holdup is calculated differently by detecting all drop in one coalescence regime and determining the holdup there.

Drop breakage is modeled with the model of Han et al., which does not require any adjustable parameters. The model is capable to calculate binary, tertiary and quaternary breakage. However, triple integrals have to be solved. These integrals are solved before the actual compartment simulation. For a fixed set of physicochemical properties the breakage rates and daughter drop size distributions are calculated for all possible holdup, mother drop sizes and turbulent dissipation rate values. This procedure saves simulation time. The

\[ \text{FIGURE 4} \quad \text{Control volume for continuity balance, visualization of the velocity increase around a drop} \]
drawback is that the physicochemical properties are assumed to be constant along the column height. The change of chemical properties due to changing concentration of acetone along the column height is therefore neglected for drop breakage. As stated by Schmidt et al.\textsuperscript{29} especially interfacial tension and to less extent viscosity has a major impact on the drop breakage probability. In the case of the simulated toluene/water/acetone system the concentration of acetone varies between 0.9 and 6.3 wt% resulting in a change of interfacial tension of 32% between 32.2 and 21.9 mNm. In future investigations, this effect of concentration dependent properties will be included into the breakage model. At this stage, the resulting inaccuracy is fitted into the coalescence parameter $\xi$.

2.7 | Modeling of mass transfer

The mass transfer from continuous into disperse phase is calculated according to Equation (8)

$$\Delta m = \Delta t \cdot \pi d^2 \frac{1}{\rho_{d} \beta_d + \rho_{c} \beta_c} \cdot (Kx - y),$$  \hspace{1cm} (8)

where $\Delta t$ is the time step, $\rho_d$ and $\rho_c$ the disperse and continuous phase density, $\beta_d$ and $\beta_c$ the mass-transfer coefficients, $K$ the distribution coefficient and $y$ and $x$ the concentrations of the disperse and continuous phase. In single drop experiments with mass transfer from (excess) continuous phase into dispersed phase, Henschke et al.\textsuperscript{30} showed that mass transfer resistance in the continuous phase is can be neglected, due to the drop rise velocity and continuous renewal of the boundary layer in the continuous phase.\textsuperscript{1}

Henschke et al.\textsuperscript{30} developed a model for the mass-transfer coefficient of the dispersed phase, which includes mass transfer enhancement effects due to convective flux, inner circulation and instabilities at the drop interface. The mass transfer enhancement is modeled with an effective diffusion coefficient $D_{\text{eff}}$, which is applied for the calculation of the mass transfer coefficient of the dispersed phase.

$$\beta_d = D_{\text{eff}} \frac{1}{d} \sqrt{\frac{4d^2}{\pi D_{\text{eff}}} + \frac{x^4}{d^4}},$$  \hspace{1cm} (9)

$t$ is the drop age (= actual simulation time $-$ simulation time of dispersion). The formula includes an enhancement of the diffusion in the drop due to convective flux (inner circulation) and instabilities and is determined by

$$D_{\text{eff}} = D_d + \frac{V_{\text{rel}} d}{C_{IP} \left(1 + \frac{\mu_d}{\mu_I}\right)}$$  \hspace{1cm} (10)

with $D_d$ as the diffusion coefficient of the dispersed phase, $C_{IP}$ the instability parameter, $\mu_d$ the dispersed phase viscosity and $V_{\text{rel}}$ the relative velocity between drop and continuous phase. The instability parameter was determined by Henschke\textsuperscript{1} with single drop experiments to 9,445.

2.8 | Simulation plan

In this study, all column experiments of Garthe\textsuperscript{17} are simulated with the extraction system toluene/water/acetone, which were performed in a Kühni extractor. Therefore, the compartment-model is applied for a different extraction system compared to the previous publication of Weber et al.\textsuperscript{16} Furthermore, the accuracy of the compartment-model to simulate operation points with two different energy inputs (stirrer speeds) is determined. Finally, the measured concentration profiles are compared to the simulated concentration profiles. In Table 2 the simulated operation points are summarized. Garthe\textsuperscript{17} explained that his measured operation points with the highest load were close to the flooding point. Therefore, in Table 2 also the distance to the flooding load is given.

Before each operation point is simulated with the compartment-model, the velocity profile of the continuous phase is calculated with the CFD-model. Following, the drop movement, coalescence, breakage and mass transfer are calculated in the compartment-model. For each operation point the extraction column is simulated for 3 h assuring steady state operation. The coalescence parameter is fitted to the column experiments of Garthe\textsuperscript{17} so that the simulated sauter drop-diameter is in the range of the experimental measured diameter ($\xi=1,700$). The coalescence parameter is in the range of the coalescence parameter derived by Henschke\textsuperscript{1} for sieve trays ($\xi=2,500$). The difference is probably caused by different column internals and by the application of the local holdup, which is not averaged over the total column diameter in one height element as done by Henschke.

For the choice of the required amount of representative drops, time step size and compartment resolution sensitivity analysis were performed. As a result more than 2,000 drops per meter column should be simulated, the time step size should be 20 ms for the calculation of the drop movement and 5 ms for the calculation of the material balances between the compartments. The compartment grid should be chosen according to the velocity profile in the column. In general a grid resolution of three cells over the radius and two over the height of one stirred section was chosen. However, for the simulation of the operation points close to the flooding load, the holdup is high. This causes the exchange volume flow of one compartment to exceed the compartment volume. As a result the implemented volume and material balance becomes faulty. In that case only one compartment per stirred section is simulated. This resolution is still sufficient.

| Stirrer speed (rpm) | $V_c$ (l/h) | $V_d$ (l/h) | Flooding load |
|---------------------|------------|------------|---------------|
| 150                 | 40         | 48         | 57%           |
| 150                 | 60         | 72         | 86%           |
| 150                 | 70         | 84         | 100%          |
| 200                 | 40         | 50         | 69%           |
| 200                 | 50         | 60         | 85%           |
| 200                 | 60         | 70         | 100%          |
since such coarse compartment resolution had only a minor effect during pulse simulations. The error is in the domain of 10% between a resolution of 1 compartment and 64 compartments per stirred section.

3 | RESULTS AND DISCUSSION

In the following sections, the simulation results are compared with the experimentally measured holdup, sauter drop-diameter and concentration profiles. In the end, the compartment model is compared to one-dimensional simulation results of the same data set, which were published by Weber et al.4

3.1 | Fluid dynamic in DN80 extraction column

In the compartment-model, the drop movement is calculated in the three dimensional domain of the extraction column. A screenshot of the drop position in the compartment model is shown in Figure 5. On the left the velocity contour of the CFD-simulation is shown and on the right the simulated representative drops are projected on a 2D domain and shown as circles. The coalescence regimes below the stators are represented as a rectangle in magenta and the internals with green lines. The upper vortex drags drops back to the stirrer, so that some drops accumulate and circulate in the upper vortex. As a result the holdup in the upper stirrer section is higher as below the stirrer.

The simulated holdup and sauter drop-diameters in the extraction column are compared to the experiments from Garthe17 in Figure 6 for the stirrer speed of 150 rpm and in Figure 7 for the stirrer speed of 200 rpm. On the x-axis the column height is given and on the y-axis the holdup or the sauter drop-diameter. Garthe17 measured both values on three positions. The symbols represent this experimental data. The lines connect the simulated values, which were evaluated at the same positions as in the experiments. The standard deviation at the experimental data points results from two column experiments per operation point. The SD at the simulated data points represents the fluctuation of the holdup or drop size over the last simulated 250 s.

The simulated and experimental holdup profiles agree quite well. The holdup increases with the load in the experiments as well as in the simulations. At a stirrer speed of 200 rpm, the simulations agree well with the experimentally measured holdup. Only for 69% of the flooding load the holdup is underestimated by 36% at the bottom of the column. Garthe17 only reported one inlet drop size distribution for all operation points. However, the drop size usually depends on the
volume flow through the disperser. Therefore, the deviation in the simulations could be caused by an inappropriate inlet drop size distribution. At a stirrer speed of 150 rpm, the holdup is underestimated for a load of 57%F in the domain of 15–30% and for 100%F in the domain of 9–24%. However, the operation point at 86%F is predicted well. All calculated and experimental holdup values are compared in Figure 8.

In sum, the simulated and experimental holdup have an averaged deviation of 13% for different loads and stirrer speeds.

The calculated sauter drop-diameter is in the domain of the experimental drop-diameters. Only at the operation point at 57% and 150 rpm the drop-diameter is ~25% to low. At all other operation points, the drop size at the top of the column is comparable between the simulations and experiments. However, in the simulations the drop size increases slightly over the column height. During the experiments a contrary behavior was observed. The drop size decreases over the column height. As a result, the simulated drop size at the bottom of the column is noticeably underestimated.

The contrary tendency of the drop-diameter results from the calculation of the breakage rate. The model of Han et al. allows for the calculation of up to four daughter drops. However, the model is very computational expensive, since a fourfold integral has to be solved for each daughter drop at each time step. Therefore, the breakage rate and daughter size distribution is calculated in advance to the simulation for a fixed set of physical properties. As a result a concentration dependent interfacial tension is neglected even though the interfacial tension decreases in the experiments due to the concentration profile from the bottom to the top of the column. This effect is neglected in the compartment-model causing the difference in the calculated drop size.
After having discussed the simulated fluid dynamic behavior, the concentration profiles are exemplarily compared to the measured profiles in Figure 9 for two operation points. The simulated concentration profiles are shown by the lines and the measured concentrations are represented by the symbols. When comparing the concentration profiles of all operation points, the simulated profiles have an averaged deviation of 8%. The concentration profiles agree very well with the experiments. Only at a column height of 0.6 m, simulations and experiments differ noticeably. However, for the one case the concentration is overestimated and for the other underrated, suggesting that the measured values have a higher error in this domain.

### 4.1 Comparison to one-dimensional models

The compartment-model was applied for Kühni extraction columns with standard geometries. Therefore, a comparison of the simulation results with one-dimensional extraction column models is possible. Weber et al. simulated the column experiments of Garthe for the extraction system toluene/water/acetone with an one-dimensional PBE model, also using a Monte-Carlo method. Both simulation models have a similar accuracy comparing fluid dynamic and concentration profiles. However, the one-dimensional model is much faster and does not require a CFD simulation, since appropriate correlations for the fluid dynamics are available. Consequently, for standard geometries one-dimensional models are recommended. However, when columns with modified or novel internals have to be evaluated, CFD can substitute not yet available experimental data. In this case, either CFD-PBE models or the proposed compartment model with a simplified CFD model are advantageous. A third approach was proposed by Hlawitschka et al. Instead of calculating all effects in CFD, the main fluid dynamic correlations for axial dispersion, slowing factor and energy dissipation are derived from CFD simulations. These correlations can then be applied in 1D models, reducing the computational time for mass transfer simulations even in comparison to the proposed compartment-model. The advantage of the proposed compartment model is, that the 3D drop path is calculated and an accumulation of the dispersed phase under the stators is modeled, which is typically not the case in 1D models.

### 5 CONCLUSION

We developed a CFD based compartment-model, including PBE (Monte-Carlo approach) and sub-models for the drop movement, coalescence, breakage and mass transfer. The compartment-model requires the velocity profile of the continuous phase, which is calculated in CFD. The dispersed phase is neglected in the CFD-simulation. However, the
influence of the dispersed phase on the continuous phase velocity is
approximated in the developed compartment-model.

The compartment-model was applied for the simulation of a
DN80 Künni-extractor and the extraction system toluene/water/ace-
tone. The model was used to simulate all operation points, which were
investigated by Garthe^{17} for the toluene extraction system. The
holdup is simulated well with an averaged deviation of 13% and the
sauter drop-diameter is in the domain of the experiments. However,
the effect of concentration dependent properties was neglected in
the breakage model leading to higher errors in the simulated sauter
drop-diameters. The concentration profile is calculated very well.

Summing up, in this study the applicability of the compartment-
model to calculate extraction columns type Künni is shown. With the
developed model potential novel designs of column internals can be
evaluated.

NOTATION

\[
\begin{align*}
\alpha & \quad \text{volume fraction} \\
\beta & \quad \text{mass transfer coefficient} \\
\gamma & \quad \text{interfacial tension} \\
\Delta m & \quad \text{transferred mass} \\
\Delta t & \quad \text{time step} \\
\rho & \quad \text{density} \\
\mu & \quad \text{viscosity} \\
\xi & \quad \text{coalescence parameter} \\
\tau_c & \quad \text{drop statistic lifespan} \\
A & \quad \text{free area} \\
a_{15} & \quad \text{parameter for rise velocity of single drop} \\
a_{16} & \quad \text{parameter for rise velocity of single drop} \\
C_{IP} & \quad \text{instability parameter} \\
d & \quad \text{drop-diameter} \\
d_{\text{DLT}} & \quad \text{transition parameter of a rigid drop interface to a mobile}
\text{interface} \\
D & \quad \text{diffusion coefficient} \\
g & \quad \text{gravitation} \\
H_{\text{col}} & \quad \text{Hamaker coefficient} \\
K & \quad \text{distribution coefficient} \\
t & \quad \text{drop age} \\
\Delta t & \quad \text{time step size} \\
\bar{v} & \quad \text{velocity} \\
\dot{V} & \quad \text{volume flow} \\
x & \quad \text{concentration in continuous phase} \\
y & \quad \text{concentration in dispersed phase} \\
Z & \quad \text{coalescence or breakage probability}
\end{align*}
\]

\text{SUB- AND SUPERSCRIPT}

\begin{align*}
\text{bre} & \quad \text{breakage} \\
c & \quad \text{continuous phase}
\end{align*}

ABBREVIATIONS

CFD \quad \text{computational fluid dynamics}

PBE \quad \text{population balance equation}

RDC \quad \text{rotating disc contactor}

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