Helmholtz-Zentrum Dresden-Rossendorf (HZDR)



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Originally published:

September 2022

Chemical Engineering Science 264(2022), 118147

DOI: https://doi.org/10.1016/j.ces.2022.118147

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1 2	Investigation of Fluid-dynamics and Mass-transfer in a Bubbly Mixing Layer by Euler-Euler Simulation
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10	Abstract
11 12 13 14 15 16 17 18 19 20 21 22 23	Mass transfer in bubbly flows is a field of obvious technological importance. On industrially relevant scales it may be studied by simulations based on the Euler-Euler two-fluid model, which however requires closure models for the interfacial exchange processes. Despite recently increased efforts, modelling of the exchange of mass between the phases is still much less developed than the corresponding exchange of momentum. The present study compares several proposed models for the mass transfer coefficient using a previously established set of closure relations for the purely fluid dynamical part of the problem. A set of experimental data for the absorption of O_2 into water in a bubbly mixing layer from the literature is used to assess their relative merits. A model for the pertinent material properties of this system has been assembled from available measurements. A rather sensitive dependence of the amount of absorbed O_2 is found on the pressure, which varies with the hydrostatic head above the test section.
24 25 26	Keywords: mass-transfer, dispersed gas-liquid multiphase flow, Euler-Euler two-fluid model, closure relations, CFD simulation, model validation

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28 1 INTRODUCTION

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29 Mass-transfer between gas bubbles and the liquid surrounding them is an important 30 phenomenon in chemical engineering and biotechnology as well as cleaning and purification 31 processes in diverse fields of application. In comparison to merely fluid dynamical problems, 32 the modeling of mass transfer phenomena in bubbly flows is developed much less. On the 33 scale of technical equipment, simulations are feasible by means of the Eulerian framework of 34 multiphase flow. For practical application this requires a closure relation for the mass transfer 35 coefficient, the suitability of which has to be validated by comparing the simulations results 36 to experimental data.

37 A review of earlier work in this field has been given in Rzehak and Krepper (2016) for purely 38 physical mass transfer and in Krauß and Rzehak (2018, 2017) for the case with an 39 accompanying chemical reaction. The topic has received continued high interest since then, 40 especially with a focus on reactive systems such as CO₂ in aqueous NaOH (Hori et al. 2020) or 41 NO in aqueous Fe^{II} complexes (Hlawitschka et al. 2017a), comprising both experiments 42 (Kipping et al. 2020, Kovats et al. 2018) and simulations by the Euler-Euler and Euler-Lagrange 43 methods (Taborda and Sommerfeld 2021, Hlawitschka et al. 2017b). Despite these recent 44 advances, the quest for a well-validated and broadly applicable model for the bubbles' mass 45 transfer coefficient remains an ongoing venture (Solsvik 2018).

46 For data serving the purpose of model validation it is essential that the concentration, phase 47 fraction, and velocity fields are available with a decent resolution over the flow domain. In 48 addition, measurements of the bubble size are required as well, since this quantity appears 49 in virtually all of the closure models used in Euler-Euler simulations. Furthermore, it would be 50 highly desirable that the data also contain some variation of this parameter so that a 51 meaningful comparison between different models can be made. Sources of such data for 52 cases involving mass transfer are much scarcer than for purely fluid dynamical problems. For 53 the present investigation, the work of Ayed et al. (2007) is considered.

54 The fluid dynamic modeling used in the present work employs a baseline model established 55 in Rzehak and Krepper (2013) and thoroughly validated in a number of studies since then for 56 simple bubbly pipe flows and bubble columns (e.g. Rzehak et al. 2017, 2017a, 2015, Fleck and 57 Rzehak 2019, Rzehak and Kriebitzsch 2015, Rzehak and Krepper 2015, 2013a, Ziegenhein et 58 al. 2017, 2015, 2013), but also for more complex applications such as an airlift-column (Liao 59 et al. 2016), a helical static mixer (Zidouni et al. 2015) and a stirred tank (Shi and Rzehak 60 2018). Since this model was shown to give consistently good agreement with experimental 61 data over a significant range of conditions, it provides a reliable basis to describe the fluid 62 dynamics of bubbly flows. For the present investigation, two correlations for the drag force 63 are compared corresponding to different water quality. The general description of mass 64 transfer follows Rzehak and Krepper (2016). For the mass transfer coefficient several 65 correlations applied in previous works are evaluated. In the experiments of (Ayed et al. 2007) 66 the transferred species was oxygen, O₂, and a model for the pertinent material properties is assembled from literature sources. 67

Detailed local information is available in the work of Ayed et al. (2007) in the form of lateral profiles taken at several axial locations, but only a single test condition has been considered. In addition to the concentration of dissolved O_2 in the liquid phase, also fluid dynamical observables have been measured. This provides in addition to the investigation of mass

- transfer models also a further qualification of the fluid dynamical part of the model for a
- 73 configuration that is more complex than simple pipe flows or bubble columns.

74 In addition to the experiments, also Euler-Euler simulations have been presented by Ayed et 75 al. (2007). As will be discussed, the closure models used for the fluid dynamical part are 76 comparable to the present ones. However, upon careful inspection the source of the assumed 77 correlation for the mass transfer coefficient and its applicability to the present case is unclear. 78 Moreover, it is found that pressure has a significant effect on the amount of absorbed O₂. This 79 makes the actual water level in the reservoir at the top of the column an important variable, 80 which highlights the importance of complete specifications for test cases to be used in model 81 validation. 82 The paper is organized as follows: A summary of the experiments is given in section 2. The 83 applied models are described in section 3. Emphasis is put on the mass transfer part in section

3.1. For the fluid dynamical part a brief summary and a guide to previous work is given insection 3.2. The material model is furnished in section 3.3. In section 4, the simulation results

- 86 are presented and comparison is made to the measurements. Finally, discussion is offered in
- 87 section 5.
- 88

89 2 SUMMARY OF EXPERIMENTAL DATA

90 Ayed et al. (2007) considered bubbly flow in a mixing layer as sketched in

91 Figure 1. The test section was a vertically oriented rectangular flow channel. The inlet at the 92 bottom was composed of two square regions separated by a splitter plate. Inlet 1 was 93 supplied with pure liquid while at inlet 2 a sparger consisting of 576 needles distributed evenly 94 over the inlet area injected gas into the flowing liquid. The set values of liquid volume flux and 95 gas fraction are summarized in Table 1. Materials used were pure oxygen (O₂) for the gas and water for the liquid. A small amount of oxygen corresponding to a mass fraction of $Y_L^{O_2}$ = 96 9.96e-6 was initially dissolved in the water. No statement concerning the water quality (clean 97 98 or contaminated) is available. Temperature and pressure were at ambient values. However 99 closer inspection of the setup revealed that there is a 0.6 m deep reservoir on top of the test section which is filled to an unknown level (Roig and Larue de Tournemine 2007, Figure 2). 100 101 This leaves some uncertainty at which height precisely the system is actually open to the 102 atmosphere.

103



test case	$J_L(in1)$	$J_L(in2)$	$\alpha_G(in1)$	$\alpha_G(in2)$	$Y_L^{O_2}(in1)$	$Y_L^{O_2}(in2)$	$\langle d_B \rangle$
Ayed et al. (2007)	m/s	m/s	%	%	-	-	mm
-	0.57	0.29	0.0	2.0	9.96e-6	9.96e-6	1.8

128 Table 1: Summary of parameters for the test of Ayed et al. (2007).

129

Measurements were taken along lateral profiles in the mid-plane of the channel at five axiallocations above the inlet as indicated in

132 Figure 1. Measured quantities were gas fraction, bubble size, mean axial liquid velocity, axial 133 liquid velocity fluctuations, relative velocity between gas and liquid, and oxygen 134 concentration in the liquid. Oxygen concentration was measured by a Clark electrode probe. 135 For the observables pertaining to the gas phase a two-point optical-fiber probe was used, 136 while the liquid phase velocity was determined by a hot-film probe. Concerning the bubble size only minor variation with height was found, which indicates that processes of bubble-137 138 coalescence and -breakup are at most of minor importance. Averaging over all levels gave an 139 average value of $d_B = 1.8$ mm with a standard deviation of 0.3 mm. 140

141 3 DESCRIPTION OF PHYSICAL MODELS

The main focus here is on the mass transfer part of the model, which is covered in section 3.1. A concise summary of the fluid dynamical part of the model is given in section 3.2, because this part was chosen to exactly match a baseline model that was validated in a number of previous studies. Full details of this model have been given e.g. in Rzehak and Krepper (2013) or Rzehak et al. (2017). A material model for the system of O₂ and water is finally presented in section 3.3.

148 3.1 Mass Transfer

To describe mass transfer phenomena, equations for the concentration of the transferred species, which appears as a solute in both phases, are required. These are summarized as

$$\frac{\partial}{\partial t}(\alpha_G \rho_G Y_G^A) + \nabla \cdot (\alpha_G \rho_G \boldsymbol{u}_G Y_G^A) = \nabla \cdot (\alpha_G \rho_G D_G^{eff,A} \nabla Y_G^A) + \Gamma_G^A$$
(1)

$$\frac{\partial}{\partial t}(\alpha_L \rho_L Y_L^A) + \nabla \cdot (\alpha_L \rho_L \boldsymbol{u}_L Y_L^A) = \nabla \cdot (\alpha_L \rho_L D_L^{eff,A} \nabla Y_L^A) + \Gamma_L^A .$$
⁽²⁾

Here, A denotes the transferred species, $Y^A = \rho^A / \rho$ is its mass fraction and $\rho = \sum_X \rho^X$ is the 151 density of the multi-component mixture of which each phase consists. No separate equations 152 are needed for the solute, since its mass fraction can be calculated from the constraint 153 $\sum_{X} Y^{X} = 1$. Care should be taken not to confuse the mass concentration of a species in a 154 mixture with the thermodynamic density of the pure substance although unfortunately the 155 156 same letter ρ is conventionally used to denote both. The phase fraction α and phasic velocity 157 u are obtained from the fluid dynamical part of the model (see section 3.2). The mass transfer sources for both phases are related as $\Gamma_G^A = -\Gamma_L^A$ to satisfy mass conservation and their sign 158 is such that for absorption $\Gamma_L^A > 0$. Further models are needed for the effective diffusion 159 coefficient $D^{eff,A}$ and the source terms due to transport across the phase interface Γ^A , which 160 161 are described in the following.

162 Mass transfer through an element of the interface between gas and liquid is driven by the 163 difference between the concentration Y^{A*} right at the interface, where both phases are 164 assumed to be in equilibrium, and the concentration Y^A in the bulk of each phase. Frequently, 165 the difference is small in the gas phase resulting in the one-sided model sketched in Figure 2. 166 The mass transfer coefficient k_L is defined as the constant of proportionality between the 167 mass flux G_L^A into the liquid and this concentration difference within the liquid, i.e.

$$G_L^A = k_L \rho_L (Y_L^{A*} - Y_L^A) \,. \tag{3}$$

 k_L depends on details of the mass transport from the interface through the liquid boundary 168 layer to the bulk within the liquid phase, which generally may comprise diffusive and 169 170 convective contributions as well as turbulence effects. For a bubble, the overall mas transfer 171 coefficient is obtained by summing the contributions from each interface element to give the 172 mass flux through the entire bubble surface. It thus becomes a function of the bubble shape 173 and the flow around it, both of which are determined by the bubble size, its velocity relative 174 to the liquid and material parameters. Among the latter, the diffusivity appears directly in the 175 mass transport problem, while viscosity and surface tension come into play indirectly by 176 affecting the flow field.



178 Figure 2: Simplified sketch of concentrations driving mass transfer across an interface.

177

180 The volumetric source term Γ_L^A is obtained from the mass flux G_L^A by multiplying with the 181 interfacial area concentration a_I . Furthermore, concentrations in the gas and liquid at the

interface are related by Henry's law with the constant denoted as
$$He^{A}$$
. Thus one obtains

$$\Gamma_L^A = k_L a_I \rho_L \left(H e^A Y_G^A \frac{\rho_G}{\rho_L} - Y_L^A \right).$$
(4)

For the liquid side mass transfer coefficient k_L three correlations are considered which are expressed in terms of dimensionless variables, namely Sherwood number $Sh = k_L d_B/D_L^A$, Reynolds number $Re = |\mathbf{u}_G - \mathbf{u}_L| d_B \rho_L / \mu_L$, and Schmidt number $Sc = \mu_L / (\rho_L D_L^A)$. A comparison of all three correlations as function of Re is shown in the bottom part of Figure 3 below.

188 The first one,

$$Sh = \left(2 + \frac{0.651 \, (Re \, Sc)^{1.72}}{1 + (Re \, Sc)^{1.22}}\right) \, ((1 + 0.433 \, Re^2)^{-1} + 4.23)^{-0.055} \,, \tag{5}$$

was used in the simulations of Ayed et al. (2007) with reference to Mewes and Wiemann 189 190 (2003), who in turn quote it as a result for spherical bubbles from Brauer (1981). This latter 191 reference is obviously erroneous and should likely have been Brauer (1979) as also given by Ayed et al. (2007). Upon close inspection however, the expression for the last factor in Eq. 192 (5) does not appear in Brauer (1979). Instead, a graphical result is displayed, from which a 193 number of data points are shown in the top part of Figure 3 (crosses). As may be seen, these 194 are very different from the expression given by Mewes and Wiemann (2003) (dotted line). 195 196 Hence, the origin and meaning of Eq. (5) is somewhat unclear.

197 Therefore, a fit formula to the graphical result from Brauer (1979) was developed (solid line 198 in the top part of in Figure 3) and is used in a second correlation for the mass transfer 199 coefficient, namely

$$Sh = \left(2 + \frac{0.651 \, (Re \, Sc)^{1.72}}{1 + (Re \, Sc)^{1.22}}\right) \, \left(1 + \frac{0.037 \, Re^{0.9}}{1 + 0.05 \, Re^{0.9}}\right). \tag{6}$$

200 The results for spherical bubbles from Brauer (1979) on which Eq. (6) is is based were 201 obtained by direct numerical simulations of the coupled equations for fluid dynamics and 202 mass transfer. Surfactants were not included in the simulations, hence it corresponds to an 203 absolutely clean bubble with a fully mobile interface. Conditions imposed at the bubble 204 surface were a free slip condition for the fluid dynamical part and a fixed concentration for 205 the mass transfer part. Accordingly, the internal circulation and the gas side resistance to 206 mass transfer are neglected. Both of these assumptions are typically made for gas bubbles 207 since the viscosity and diffusivity in the gas are much smaller than those in the liquid. The 208 motion of the interface relative to the liquid is of course determined by the imposition of the 209 spherical bubble shape, but within this assumption the development of the boundary layer from the stagnation point at the bubble front to detachment and wake formation and the 210 211 rear end of the bubble are captured by the simulations.

212 Finally, a third correlation is considered that applies for deformed bubbles, i.e.

$$Sh = (2 + 0.015 \, Re^{0.89} Sc^{0.7}) \,. \tag{7}$$

This also appeared in Brauer (1979) and was quoted by Mewes and Wiemann (2003). In 213 214 addition it was compared with recent measurements on single bubbles (Merker et al. 2017) 215 and applied in a number of other simulations including mass transfer (e.g. Krauß and Rzehak, 216 2018 and references therein). The correlation Eq. 7 was proposed by Brauer (1979) based on 217 a review of experimental studies at varying Re and Sc. Unfortunately the water quality was 218 not reported, so the interface mobility is not known with certainty. While the internal 219 circulation and gas side resistance to mass transfer are included in principle, they are still 220 small effects for the reasons mentioned above. The dominant effect distinguishing this model 221 from the previous one is that the bubble shape and wobbling and their influence on the 222 boundary layer development and wake formation are captured.





Figure 3: Comparison of mass transfer correlations. Top part: the last factor in the correlation from Mewes and Wiemann (2003), Eq. (5), (dotted line) is compared to the second factor in the correlation from Brauer (1979), Eq. (6), (crosses: scanned from the graphical result in the original work; solid line: fit formula used herein). Bottom part: the dependence of *Sh* on *Re* for *Sc* = 371 corresponding to O_2 in water at 25°C according to the correlations discussed in section 3.3 is compared for the correlations from Eqs. (5) to (7). Also indicated are the values of *Re* obtained for the terminal velocities for the two drag laws considered (see section 3.2).

231 The interfacial area concentration a_I in Eq. (4) is expressed as

$$a_I = \frac{6\alpha_G}{d_B} \tag{8}$$

by assuming spherical bubbles.

The Henry constant He^A , the molecular diffusion coefficient D_L^A , liquid density ρ_L and viscosity μ_L as well as the gas density ρ_G are obtained from the material model (see section 3.3) by inserting the appropriate values for the local temperature and pressure. The bubble size d_B is taken as a constant in accordance with the experiments as discussed in section 2.

237

The effective diffusion coefficients $D^{eff,A}$ consist of two contributions, a molecular one D^A and a turbulent one $D^{turb,A}$. The latter is typically dominant in the continuous liquid phase and calculated from the simple but frequently used assumption of unity Schmidt number (e.g. Cockx et al. 2001), i.e. from

$$Sc_L^{turb} = \frac{\nu_L^{turb}}{D_L^{turb,A}} = 1.$$
(9)

Herein, the turbulent kinematic viscosity v_L^{turb} is obtained from the turbulence model (see section 3.2). No diffusive transport occurs between bubbles in the dispersed gas phase, i.e. $D_G^{eff A} = 0.$

- Boundary conditions required to obtain a unique solution of Eqs. (1) and (2) are a specified value of the mass fraction at an inlet, a vanishing normal derivative at an outlet, and $Y_G^A = Y_L^A = 0$ on impermeable walls.

249 3.2 Fluid Dynamics

Fluid dynamic phenomena are described by balance equations for mass and momentum in each phase, which are summarized as follows. The continuity equations for both phases are

$$\frac{\partial}{\partial t}(\alpha_G \rho_G) + \nabla \cdot (\alpha_G \rho_G \boldsymbol{u}_G) = \Gamma_G^A$$
(10)

$$\frac{\partial}{\partial t}(\alpha_L \rho_L) + \nabla \cdot (\alpha_L \rho_L \boldsymbol{u}_L) = \Gamma_L^A , \qquad (11)$$

and the momentum equations read

$$\frac{\partial}{\partial t} (\alpha_G \rho_G \boldsymbol{u}_G) + \nabla \cdot (\alpha_G \rho_G \boldsymbol{u}_G \otimes \boldsymbol{u}_G)
= -\alpha_G \nabla p_G + \nabla \cdot (\alpha_G \mathbf{T}_G) + \alpha_G \rho_G \boldsymbol{g} + \boldsymbol{F}_G^{inter} + \boldsymbol{\Phi}_G^A$$
(12)

$$\frac{\partial}{\partial t} (\alpha_L \rho_L \boldsymbol{u}_L) + \nabla \cdot (\alpha_L \rho_L \boldsymbol{u}_L \otimes \boldsymbol{u}_L)
= -\alpha_L \nabla p_L + \nabla \cdot (\alpha_L \mathbf{T}_L) + \alpha_L \rho_L \boldsymbol{g} + \boldsymbol{F}_L^{inter} + \boldsymbol{\Phi}_L^A.$$
(13)

Details on the derivation of these equations are available in several monographs (e.g. Drew
and Passman 1998, Yeoh and Tu 2010, Ishii and Hibiki 2011).

The last terms on the right in in Eqs. (12) and (13) represent sources due to the mass transfer. The mass sources Γ^A are the same as already discussed in section 3.1. The so-called secondary momentum sources Φ^A represent the momentum carried along by the transferred mass. A physical model for these sources consistent with all other aspects of the overall model is given by

$$\boldsymbol{\Phi}_{G}^{A} = -max(0, \Gamma_{L}^{A}) \boldsymbol{u}_{G} - min(0, \Gamma_{L}^{A}) \boldsymbol{u}_{L}$$
(14)

$$\boldsymbol{\Phi}_{L}^{A} = max(0, \Gamma_{L}^{A}) \boldsymbol{u}_{G} + min(0, \Gamma_{L}^{A}) \boldsymbol{u}_{L} .$$
(15)

Since for the present application only a small amount of mass is transferred between the phases, their magnitude is likewise small, but they are nonetheless included for the sake of completeness.

263 The stress tensor is given by

$$\mathbf{T} = \mu^{eff} (\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T), \qquad (16)$$

where the effective dynamic viscosity μ^{eff} comprises a viscous and a turbulent contribution. For the liquid phase, the latter is calculated based on a k- ω SST model (Menter 2009). According to the baseline model applied here, source terms are added to the base model, which account for the bubble- induced turbulence (e.g. Rzehak and Krepper 2013a, Rzehak and Kriebitzsch 2015, Ziegenhein et al. 2017, Parekh and Rzehak 2018). For the gas phase, turbulence may be neglected because of the low gas density and the small spatial scales imposed by the bubble size, i.e. $\mu_G^{eff} = 0$.

The primary momentum sources F_{G}^{inter} represent the direct transfer of momentum across the interface and are related as $F_{G}^{inter} = -F_{L}^{inter}$ to satisfy momentum conservation. They comprise several different contributions and the closure relation used for each of these according to the applied baseline model is shown in Table 2 (e.g. Ziegenhein et al. 2013, Rzehak et al. 2015, Rzehak and Krepper 2015, or Rzehak et al. 2017a). The drag force

- correlation of Ishii and Zuber (1979) used in the original baseline model corresponds to a
- 277 contaminated water quality. In addition, a correlation proposed by Tomiyama et al. (1998) for
- 278 clean water is considered. To be definite, the correlation of Ishii and Zuber (1979) reads

$$C_D = \max\left(\frac{24}{Re}\left(1 + 0.1\,Re^{0.75}\right), \min\left(\frac{2}{3}\sqrt{Eo},\frac{8}{3}\right)\right)\,,\tag{17}$$

while that of Tomiyama et al. (1998) is given by

$$C_D = \max\left(\min\left(\frac{16}{Re}(1+0.15\ Re^{0.687}), \frac{48}{Re}\right), \frac{8}{3}\frac{Eo}{Eo+4}\right).$$
 (18)

Two further relations are required to complete the above system of equations. With the assumption that each phase is incompressible, these are provided by conservation of volume, expressed as $\alpha_G + \alpha_L = 1$, and equilibrium of pressures, expressed as $p_G = p_L = p$.

Boundary conditions on solid walls are no-slip for the liquid and free slip for gas phase. The latter assumes that direct contacts between the bubbles and the walls can be neglected. The need to resolve the viscous boundary layer is avoided by applying a single phase turbulent wall function. At an inlet, profiles for the gas fraction and gas and liquid velocities are prescribed. Pressure is imposed as an outlet condition together with vanishing tangential velocity components and a vanishing normal derivative of gas fraction.

289 Table 2: Summary of bubble force correlations.

force	reference
drag (contaminated condition)	Ishii and Zuber (1979)
drag (clean condition)	Tomiyama et al. (1998)
shear lift	Tomiyama et al. (2002)
wall lift	Hosokawa et al. (2002)
turbulent dispersion	Burns et al. (2004)
virtual mass	constant coefficient C_{VM} = $\frac{1}{2}$

290

291

293 3.3 Material Properties

The present section summarizes correlations assembled from the literature to model the temperature dependence of solubility and diffusivity of O_2 in water, surface tension between O_2 and water as well as viscosity and density of water and gaseous O_2 . All correlations are valid at atmospheric pressure.

298 3.3.1 Solubility

299 The solubility of O₂ in water is quite well studied. A rather recent compilation of data and 300 assessment of correlations for the Henry constant is given in Clever et al. (2014). In this 301 review, the most precise measurements are attributed to Rettich et al. (2000). These are 302 shown in Figure 4 together with a correlation based on the recommended one from Clever et al. (2014). Since the results of Clever et al. (2014) and Rettich et al. (2000) were expressed in 303 304 units of 1/Pa rather than mol/mol as desired here, these results were multiplied by $\rho^{H_2 0} / M^{H_2 0}$ where $\rho^{H_2 0}$ was determined in accordance with Rettich et al. (2000) from a 305 correlation due to Kell (1975) and $M^{H_2O} = 0.018 kg/mol$. Then the fit coefficients were 306 307 adjusted to get the desired result in a single pass as

He =
$$R T \exp\left(-4.072752 - \frac{5756.888 [K]}{T} + \frac{1075294 [K^2]}{T^2}\right) \cdot \left[\frac{mol}{J}\right]$$
. (19)

308 It may be noted that a three-parameter fit formula of different form proposed in the earlier

review of Battino et al. (1983) yields numerically the same results. A simpler two-parameter

310 fit due to Sander (2015) applies only to a more limited range around room temperature.





313 Figure 4: Henry constant for O₂ in water.

314 3.3.2 Diffusivity

As shown in Figure 5, data on the diffusivity of O₂ in water found in the literature (Akgerman and Gainer 1972, Verhallen et al. 1984, Han and Bartels 1996) exhibit a rather large spread in particular at elevated temperatures. Since a detailed assessment of the accuracy of the different measurements is not possible here, we have chosen the older but more frequently relied on data compiled by Akgerman and Gainer (1972) which comprise results from the earlier works of Himmelblau (1964), Ferrell and Himmelblau (1967), Wise and Houghton (1966) and a few smaller studies. These data are fitted by correlation

$$D_L^{O_2} = \exp\left(1.228 + \frac{2100 \, [K]}{T} - \frac{657600 \, [K12]}{T^2}\right) \cdot 10^{-9} \left[\frac{m^2}{s}\right].$$
(20)



322

323

324 Figure 5: Diffusivity of O₂ in water.

325 3.3.3 Surface Tension

Data on the surface tension between mutually saturated mixtures of O₂ and water could not be found in the literature. However, for non-adsorbing gases the surface tension to the same liquid is typically the same. Therefore, we here substitute the surface tension for water with its own vapor which is quite well characterized (Vargaftik et al. 1983). From Figure 6, it is seen that these data are undistinguishable from data on air in contact with water (Gray, 1957, sect. 2p-2). In a range of temperatures around ambient conditions these data are well represented by a linear temperature dependence

$$\sigma = \left(122.37 - 0.1691 \, \frac{T}{[K]}\right) \cdot 10^{-3} \left[\frac{N}{m}\right],\tag{21}$$

which is also shown in Figure 6.



335 Figure 6: Surface tension of gases in water.

336 3.3.4 Viscosity

In the dilute limit, the presence of O₂ in the liquid phase may be neglected. For the viscosity of pure water a highly accurate description valid over a very large range of conditions is available (Huber et al. 2009) which is adopted by the IAPWS. However, sometimes a simpler correlation with a smaller range of applicability is advantageous to work with. To this end the Vogel-Fulcher-Tammann type formula

$$\mu_L^{H_2 0} = \exp\left(3.184 + \frac{570.6[K]}{T - 140[K]}\right) \cdot 10^{-6}[Pa s]$$
(22)

has been shown to provide a good description in the range from 5 ... 95 °C (Rzehak andKrepper 2016).

For the gas phase Sutherland's formula is applied (e.g. Chapman and Cowling 1970, sect. 12.32), i.e.

$$\mu_{G} = \mu_{ref} \left(\frac{T}{T_{ref}}\right)^{3/2} \frac{T_{ref} + T_{S}}{T + T_{S}},$$
(23)

where μ_{ref} is the viscosity at the reference temperature T_{ref} and T_s is a material dependent constant. The parameters for O₂ and air are summarized in Table 3.

348

gas	$T_{S}[K]$	$T_0[K]$	$\mu_0 [10^{-6} Pa s]$
O ₂	127	292.25	20.18

349

350 Table 3: Parameters for Sutherland correlation Eq. (23).

- 352 3.3.5 Density
- 353 Similarly, for the density of pure water the most accurate and complete description adopted
- by the IAPWS is given in Wagner and Pruß (2002). A simpler and more easily applicable quadratic fit formula

$$\rho_L^{H_2 0} = \left(-0.0035 \left(\frac{\mathrm{T}}{\mathrm{[K]}}\right)^2 + 1.824 \frac{\mathrm{T}}{\mathrm{[K]}} + 763.42\right) \cdot \left[\frac{kg}{m^3}\right],\tag{24}$$

- can be applied in the range from 5 ... 95 °C (Rzehak and Krepper 2016).
- The gas phase is modeled as an ideal gas or an ideal mixture thereof, i.e. the gas density givenby

$$\rho_G = \frac{p \, M_G}{R \, T},\tag{25}$$

where $M^{o_2} = 32.0 \text{ kg} / \text{ kmol}$ is the molar mass of O₂ and **R** is the universal gas constant. The pressure in Eq. (25) is the local fluid pressure, which varies over the height of the fluid domain mainly due to hydrostatics. As it will turn out this variation has a significant influence on the equilibrium at the interface. In principle a Laplace pressure of $4 \sigma/d_B$ should also be included, but this term is negligibly small for the present applications.

365 4 SIMULATION RESULTS

366 To perform the simulations the commercial software ANSYS CFX 17.2 is used. Due to a lack of 367 symmetry in the geometry and boundary conditions, a fully three-dimensional simulation is run. A grid spacing of 5 mm in the lateral directions and stretched by a factor of 6 in the axial 368 369 direction was determined to provide a reasonably well converged solution in a grid 370 independency study. Concentrations, phase fractions, and phasic velocities at the two inlets 371 are set according to the experimental description given in Section 2. For the turbulence, 372 generic values of intensity (5%) and viscosity ratio (10) are imposed. Uniform distributions of 373 all of these quantities over each inlet are assumed. Pressure at the outlet is set to atmospheric 374 pressure unless stated otherwise. This corresponds to neglecting the hydrostatic head of the water in the reservoir above the test section. Based on the measurements dicussed in Section 375 2, the bubble size distribution may be taken as monodisperse with a constant bubble size. The 376 377 experimentally determined mean value of $d_B = 1.8$ mm is used. Material properties according to the correlations of section 3.3 are evaluated at a temperature of 25 °C and the local 378 379 pressure. In the course of the investigation, several model variants are considered, which are 380 summarized in Table 4 for convenience. More detailed explanations are provided in the text.

381

designation	drag force model	mass transfer coefficient model	pressure
ShConst-CdTomi	Eq. (18)	Sh = 400	reservoir empty
ShConst-CdIshii	Eq. (17)	Sh = 330	reservoir empty
ShZero-CdTomi	Eq. (18)	Sh = 0	reservoir empty
ShZero-CdIshii	Eq. (17)	Sh = 0	reservoir empty
ShDef-CdTomi	Eq. (18)	Eq. (7)	reservoir empty
ShSph-CdIshii	Eq. (17)	Eq. (5)	reservoir empty
ShXxx-CdIshii	Eq. (17)	Eq. (6)	reservoir empty
ShDef-CdTomi-pressure	Eq. (18)	Eq. (7)	reservoir full
ShXxx-CdIshii-pressure	Eq. (17)	Eq. (6)	reservoir full

- 382
- 383 Table 4: Summary of investigated model variants.
- 384
- 385

386 4.1 Fluid Dynamics

Turning first to the fluid dynamics, results from experiment (symbols) and simulations (lines) 387 388 are displayed in Figure 7 and Figure 8. Lateral profiles of gas fraction, liquid velocity and 389 turbulent kinetic energy, as well as relative velocity between liquid and gas are shown at 390 different locations along the test section. Since in the experiments only liquid velocity 391 fluctuations in the axial direction have been recorded, isotropy is assumed like in Ayed et al. 392 (2007) to express the turbulent kinetic energy as $\kappa_L = 3u_L^{\prime 2}/2$. In the simulations, the two 393 models for the drag force described in section 3.2 are compared, one being valid for 394 contaminated interfaces (thick lines, labeled "Ishii") while the other one was proposed for 395 clean interfaces (thin lines, labeled "Tomi"). Each of these models is combined with two prescriptions for the mass transfer, which has either been negelcted (solid lines labeled 396

397 "ShZero") or set to an adjusted value as described further below in section 4.2 (dotted lines398 labeled "ShConst").

399 From the comparison of the two mass transfer prescriptions it is seen that for the present 400 case, where the bubble size remains unaffected and the only action of the mass transfer on 401 the fluid dynamics comes from the secondary momentum sources in Eqs. (14) and (15), 402 there is only a minor effect. This influence of the mass transfer is most visible in the gas 403 fractions at the highest level, but even there it is much smaller than that of the different drag 404 forces. Otherwise, the effect is sometimes hardly discerned at all. Hence, this may be termed 405 a one-way-coupling situation, in which the fluid dynamics of course affects the mass transfer, 406 but not vice versa.

407 Looking in more detail at the flow development, it can be seen in qualitative terms that the 408 liquid velocities on both sides, left without and right with gas injection, tend to equalize up to 409 a height of around 500 mm. This would be expected also for a single phase flow due to the 410 action of viscosity. In the present multiphase flow, the liquid on the right with gas injection is 411 further accelerated due to momentum transfer from the buoyant gas. Therefore, from around 412 800 mm height on, the liquid velocity on the right exceeds that on the left side. Near the inlet, 413 the gas content is distributed almost uniformly over the cross section of the right side of the 414 channel, where the injection takes place. The left side of the channel remains free of gas over 415 the entire height where measurements are taken. In fact, with increasing height the gas is 416 continually shifted away from the channel center and towards the right wall. This can be 417 attributed to the action of the lift force. The level of turbulence is significantly higher on the 418 right side of the channel (where gas is injected) than on the left side of the channel (without 419 gas injection) at all height levels. This is a clear signature of the bubble-induced turbulence. 420 At the lower heights a peak in the turbulent kinetic energy is seen at the position of the splitter 421 plate separating the two inlet regions which is caused by the strong shear gradient at this 422 position. Also caused by shear turbulence is the peak developing with increasing height near 423 the left wall of the channel where no gas is present.

424 Quantitatively, differences between the two drag models are most pronounced for the 425 relative velocity between gas and liquid phase shown in Figure 8, hence these are discussed 426 first. As is well known, the rise velocity is higher for clean bubbles than for contaminated ones 427 which is also seen in the simulations. In comparison with the experimental data (symbols), 428 the measurements are closer to the calculations for the clean case (thin lines) at the lowest 429 level and closer to the calculations for the contaminated case (thick lines) at the highest level. 430 This suggests the possibility that the bubbles are clean when they are injected in the system 431 but collect contaminations during their rise. Taking into account the intermediate levels, this 432 picture is not so clear anymore, hence it must be left as a hypothesis. It can be stated clearly 433 however, that the calculations for clean and contaminated cases provide upper and lower 434 bounds for the observed behavior.

Results for gas fraction, liquid velocity, and turbulent kinetic energy are collected in Figure 7.
Smaller differences between the simulations based on the two drag models are seen which
can be understood as consequences of the different relative velocities. A higher relative
velocity of the bubbles tends to decrease the residence time of the bubbles which leads to a
lower observed gas content. Hence, gas fractions calculated for the clean case (thin lines) tend



Figure 7: Comparison of experimental data (symbols) and simulation results (lines) using several models as described in the text. Lateral profiles are shown at different locations in the test section as indicated on the left of each row for gas fraction α_G (left column), liquid

443 velocity v_L (middle column), and turbulent kinetic energy κ_L (right column).



Figure 8: Comparison of experimental data (symbols) and simulation results (lines) using several models as described in the text. Lateral profiles are shown at different locations along the test section as indicated on the left of each row for the relative velocity $v_G - v_L$.

448 to be lower than those calculated for the contaminated case (thick lines). Due to the higher 449 gas content, a larger amount of momentum is transferrred from the gas to the liquid phase 450 which gives a higher liquid velocity in the right part of the test sction where gas is present for 451 the contaminated case than for the clean case. Likewise a higher turbulent kinetic energy 452 might be expected since the contribution to the bubble-induced turbulence is proportional to 453 the gas fraction. However, it is also proportional to the relative velocity which is higher for 454 the clean than for the contaminated case. Of the two competing effects the latter is seen to 455 dominate.

456 Overall agreement between simulation results (lines) and and experimental data (symbols) is 457 quite good for both drag force models. The model of Ishii and Zuber (1979) for contaminated 458 interfaces comes a bit closer to the measurements for the gas fraction while the model of 459 Tomiyama et al. (1998) for clean interfaces matches the liquid velocity and turbulent kinetic 460 energy a bit better. The peak in turbulent kinetic energy seen in the experiment for the lowest 461 height levels at the location of the splitter plate is significantly underestimated in the 462 simulations. The same holds for the peak near the left channel wall that becomes most 463 prominent at the highest levels. Both of these are likely due to shortcomings of the shear-464 induced turbulence modeling by the k- ω SST model. In addition, the simulations show 465 pronounced peaks in gas fraction and turbulent kinetic energy near the right channel wall. 466 Since these are below the spatial resolution of the measurements, their significance remains 467 open.

468 4.2 Mass Transfer

469 Concerning mass transfer several different model variants are compared. In addition to the 470 choice of the model for the mass transfer coeffcient (see Eqs. (5) to (7)) simulation results 471 for the mass transfer also depend on the drag model, because this determines the bubble 472 Reynolds-number. To keep the number of different variants tractable, the Ishii-Zuber drag 473 model for contaminated bubbles is combined with the mass transfer coeffcient models of Eqs. 474 (5) (designated as ShXxx-CdIshii) and (6) (designated as ShSph-CdIshii) for spherical bubbles, 475 since the shape of contaminated bubbles is closer to spherical. For deformable clean bubbles 476 the Tomiyama drag model is combined with the mass transfer coeffcient models of Eqs. (7) 477 (designated as ShDef-CdTomi). A further significant dependence is found on the pressure, 478 which in the experiment depends on the water level in the reservoir above the test section. 479 This effect is caused by a corresponding change in the gas density according to the ideal gas 480 law Eq. (25), which in turn appears in the mass transfer source Eq. (4). To assess this effect, 481 in addition to the standard setting corresponding to an empty reservoir, also the case of a 482 completely filled reservoir is considered (the latter identyfied by appending -pressure to the 483 designation).

484 A comparison of the above variants is made for the concentration profiles of O_2 in the liquid 485 at the highest level in the test section, where the differences are most pronounced. From the results shown in Figure 9, it may be seen that no model variant gives an entirely satisfactory 486 487 match with the measurements. With the imposed concentration at the inlet as the reference, 488 the spherical model (ShSph-CdIshii) overpredicts the measured concentrations by ~20% while 489 the deformable model (ShDef-CdTomi) underpredicts them by a similar amount. The model 490 of somewhat unclear origin (ShXxx-CdIshii), although decribed as applying to spherical 491 bubbles by Mewes and Wiemann (2003) gives more similar results as the one for deformable 492 bubbles. Differences arising from the drag model appear small compared to differences 493 arising from the mass transfer model. The effect of an increased pressure due the condition 494 of a filled reservoir at the top of the test section (ShDef-CdTomi-pressure and ShXxx-CdIshii-495 pressure) is to increase the concentration cutting the difference to the measurement in half.



496

497 Figure 9: Comparison of experimental data (symbols) and simulation results (lines) using 498 several models as described in the text. Lateral profiles are shown at highest level of the test 499 section (y = 1200 mm) for the mass concentration of oxygen in the liquid $\rho_L^{O_2}$.

500

It is clear from the definitions in section 3.1 that the mass transfer coefficient does not vary throughout the flow domain. Thus, each mass transfer correlation only picks a constant value according to the overall flow parameters. In order to see how the development of the concentration profiles within the flow domain can be represented in the simulations, an adjusted value of the mass transfer coefficient has been determined that matches the data at the highest level (designated as ShConst). Values provding the best match are Sh = 330 for the Ishii-Zuber drag law and Sh = 400 for the Tomiyama drag law.

508 These results are shown in Figure 10. As may be expected, the concentration of oxygen in the 509 liquid phase increases with increasing height. The shape of the concentration profiles follows 510 the distribution of the gas fraction rather closely. In the left part of the channel, where no gas 511 is injected, the concentration stays at its inlet value over the entire height where 512 measurments are taken. With the adjustment at the highest level, the overall agreement 513 between simulated (lines) and measured (symbols) concentrations of O₂ at the lower levels is 514 quite good. Only at the lowest level (y = 50mm) the measured data are significantly 515 underpredicted. Concerning the shape of the concentration profiles, the step between the 516 two streams of the mxing layer is captured rather well. However, the dip at the nearest 517 measurement point to the wall is not reproduced by the simulations. Still closer to the wall the simulations results show a steep increase similar as already observed for the gas fractions. 518 519 Differences between the two drag models are found to be only small.



521 Figure 10: Comparison of experimental data (symbols) and simulation results (lines) using 522 several models as described in the text. Lateral profiles are shown at different locations along 523 the test section as indicated on the left of each row for the mass concentration of oxygen in 524 the liquid $\rho_L^{O_2}$.

525 5 DISCUSSION AND CONCLUSIONS

526 Concerning fluid dynamics, quite good agreement was found for all of the measured 527 quantities, namely gas fraction, mean liquid velocity, liquid turbulent kinetic energy, and 528 relative velocity between the phases. The biggest uncertainty comes from the unknown water 529 quality which has a significant impact on the relative velocity, that in turn affects all other 530 fluid dynamic aspects as well as the mass transfer. In the present work, two different drag 531 models from Ishii and Zuber (1979) and Tomiyama et al. (1998) corresponding to 532 contaminated and clean conditions, respectively, were applied. Simulation results from these 533 two models bracket the measured relative velocities and give approximate bounds for the 534 other observables. Since water quality is difficult to control in practical applications this 535 finding is quite useful. Comparison at different positions along the test section indicates the 536 possibility that clean conditions prevail at the inlet but contaminations are accumulated on 537 the gas-liquid interfaces during the flow. A more precise analysis is impeded by superimposed 538 statistical variations in the measured data. However, to capture such effects the commonly 539 used model frameworks would need to be substantially augmented by equations describing 540 the contaminant concentration in the bulk and at the interfaces as well as models for the 541 adsorption process.

542 Concerning mass transfer, none of the simple but frequently used correlations for the mass 543 transfer coefficient of single bubbles that were compared gave an entirely satisfactory 544 agreement with the measured concentrations. Assuming the most favorable condition for the 545 pressure, the model for deformable bubbles from Brauer (1979) and the model of somewhat 546 unclear origin used by Ayed et al. (2007) come within reach of the measurements. Which drag 547 law is used in conjunction with the mass transfer model appears to be of minor importance. 548 However, due to the uncertainties involved and the restriction of the test case to only a single 549 value of the bubble size a definite recommendation for their general use cannot yet be given. 550 Hence, to obtain a general correlation for the mass transfer coefficient of single bubbles that 551 applies in a wide range of relevant parameters including different regimes of bubble shape 552 and dynamics further investigations are necessary. A related aspect of the overall model that 553 should be considered further is a more refined model describing the turbulent diffusivity 554 depending on the local flow conditions by additional model equations for the variance of 555 concentration fluctuations and its dissipation rate, as considered e.g. by Zhang et al. (2018), 556 rather than just using a constant turbulent Schmidt number. A final minor issue in this context 557 that nonetheless deserves to be improved is a lack of precise data on the diffusivity of O₂ in 558 water.

559 Comparison may also be made with the previous simulation model by Ayed et al. (2007). The 560 main difference concerning the applied closures is that these authors use a more elaborate turbulence model that treats shear- and bubble-induced turbulence as separate fields, while 561 in the present work no such distinction is made and a single field representing the sum of 562 563 both is used. While the model of Ayed et al. (2007) is potentially more general, it also requires further assumptions to be introduced in order to model the coupling between the fields 564 565 relating to which hardly any evidence is available. As the present results show, at least for the conditions investigated no benefit results from the more complex model. 566

567 Comparing the simulation results mostly similar observations are made. In particular, the 568 peak near the right channel wall in the gas fraction, turbulent kinetic energy, and oxygen 569 concentration is also found in the simulations of Ayed et al. (2007) although for the 570 concentration it is of lower magnitude there. Likewise, the underprediction of the peak in 571 turbulent kinetic energy near the left channel wall also occurs in the simulations of Ayed et 572 al. (2007). However their simulations overpredict TKE peak at splitter plate for the second 573 height level, which is likely related to the different inlet conditions, which they took from the 574 measured profiles at the lowest lowest instead of constant generic values as used here. The 575 biggest difference is that in the simulations of Ayed et al. (2007) the transition between the 576 two streams occurs further towards the right channel wall for the turbulent kinetic energy as 577 well as for the gas fraction and oxygen concentration. In this regard the present simulations 578 are closer to the measured data. The difference can be traced to different profiles of turbulent 579 viscosity and thus ultimately to the different turbulence models that were used. On the other 580 hand, the overall concentration level in the right stream matches the measurements better 581 in their simulations than in the present ones. Both of these differences may in fact be related. 582 Overall, considering the difference in turbulence modeling which gives rise to different 583 turbulent viscosities and hence different distribution of gas, the agreement between the 584 simulations is as good as may be expected.

585 To support further model development for the mass transfer, better validation data are still 586 needed, which provide a parametric variation especially of the bubble size that figures as an 587 important parameter in the closure correlations. In this context, the present results show that 588 a precise knowledge of the pressure is required since this has a significant impact on the 589 equilibrium concentrations in gas and liquid. This is an issue that has not received due 590 attention in previous validation experiments. An accompanying measurement of pressure 591 within the test section can serve this purpose and is easily done. To the least a precise 592 specification where exactly the facility is open to the atmosphere must be provided such that 593 the hydrostatic pressure at any point in the system can be calculated. The effect of 594 temperature is relatively small since kinematic viscosity and diffusivity have a similar 595 temperature-dependence which gives only a weak influence on the Schmidt number. A 596 quantification of measurement errors would be very helpful in order to determine which part 597 of eventual deviations should be attributed to the simulation model.

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599 6 ACKNOWLEDEGEMENT

This work has been carried out in the frame of a research project (GZ: RZ 11/3-1) funded by the DFG.

602

603 7 NOMENCLATURE

Latin Formula Characters

Symbol	Description	Unit	Symbol	Description	Unit
a _i	interfacial area concentration	m ⁻¹	R	universal gas constant	J K ⁻¹ mol ⁻¹
С	molar concentration	mol m ⁻³	Re	Reynolds number	-
d_B	bubble diameter	m	Sc	Schmidt number	-
D	lateral dimension	m	Sh	Sherwood number	-
D	diffusion coefficient	m ⁻² s ⁻¹	t	time	S

F	force per unit volume	N m⁻³	Т	temperature	° C, K
g	acceleration of gravity	m s⁻²	Т	stress tensor	N m⁻²
G	mass flux	kg m ⁻² s ⁻¹	u	mean velocity	m s⁻¹
Н	axial dimension	m	u'	fluctuating velocity	m s⁻¹
Не	Henry constant	-	W	spanwise dimension	m
J	Superficial velocity = volumetric flux	m s⁻¹	x	lateral coordinate	m
k	mass transfer coefficient	m s⁻¹	Х	mole fraction	-
М	molar mass	-	у	axial coordinate	m
p	pressure	Ра	Y	mass fraction	-
r	padial coordinate	m	Ζ	spanwise coordinate	m

Greek Formula Characters

Symbol	Description	Unit	Symbol	Description	Unit
α	phase fraction	-	ν	kinematic viscosity	m ² s ⁻¹
ϵ	turbulent dissipation rate	m² s⁻³	ρ	density, mass concentration	kg m ⁻³
Г	source term due to mass transfer	kg m ⁻³ s ⁻¹	σ	surface tension	N m ⁻¹
κ	specific turbulent kinetic energy	m² s-²	φ	secondary momentum source due to mass transfer	N m ⁻³
μ	dynamic viscosity	kg m ⁻¹ s ⁻¹	ω	turbulent frequency	S ⁻¹

605

Latin Indices

Symbol	Description	Symbol	Description
A	of transferred species	L	liquid phase
eff	effective	mol	molecular
G	gas phase	02	of oxygen
H_2O	of water	turb	turbulent
in1	at inlet 1	X	of any species
in2	at inlet 2		

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