

Article

Influence of Bubble Shape on Mass Transfer in Multiphase Media: CFD Analysis of Concentration Gradients

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Abstract

Our study investigates how non-spherical bubble shapes influence gas–liquid mass transfer across the bubble interface. An analytical shape descriptor, namely Superformula, is used to parametrically define the bubble interface, enabling efficient CFD simulations over a range of Reynolds (Re) and Eötvös (Eu) numbers. By prescribing the bubble geometry analytically, we avoid expensive interface-capturing simulations and directly compute the concentration field without transient boundary shape pre-equilibration. The represented approach is computationally efficient and captures the impact of bubble shape and flow parameters on the dissolved gas concentration gradients in the surrounding liquid. Results show that bubble deformation alters the distribution of dissolved gas around the bubble and the overall mass transfer rate, with higher Re enhancing convective transport and higher Eu (more deformed bubbles), leading to anisotropic concentration boundary layers. The developed framework not only advances a fundamental understanding of bubble-driven mass transfer mechanisms but also directly addresses industrial needs, particularly in optimizing oxygen delivery within bioreactors contour and similar aerated processes. The proposed efficient modeling strategy provides a basis for developing fast surrogate tools in hybrid modeling frameworks, where high-fidelity CFD insights are incorporated into larger-scale multiphase process simulations.

Keywords: mathematical modeling; mass transfer; CFD simulation; fluid dynamics; bubbles; phase interface; superformula regression; Reynolds number; Eötvös number; bioreactor



Academic Editors: Tomoaki Kunugi and Yukihiro Yonemoto

Received: 17 September 2025

Revised: 12 October 2025

Accepted: 13 October 2025

Published: 16 October 2025

Citation: Nizovtseva, I.; Mikushin, P.; Starodumov, I.; Makhaeva, K.; Nikishina, M.; Vikharev, S.; Averkova, O.; Alexandrov, D.; Chernushkin, D.; Lezhnin, S. Influence of Bubble Shape on Mass Transfer in Multiphase Media: CFD Analysis of Concentration Gradients. *Fluids* **2025**, *10*, 269.

<https://doi.org/10.3390/fluids10100269>

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1. Introduction

Bubbles in gas–liquid flows are central to the performance of various research and applied industrial systems—from experimental bubble column to jet-stream bioreactors—where the efficient mass transfer of gases (e.g., oxygen and methane) into the liquid is required for chemical or biochemical processes [1–8]. A detailed understanding of dissolved gas concentration gradients around bubbles is crucial since these gradients drive the gas uptake by the liquid: near a rising bubble, a high concentration forms at the gas–liquid interface and decays into the bulk, and the steeper and more extensive

this gradient, the faster the overall mass transfer [9–11]. Accurate prediction of these concentration profiles and mass transfer rates is particularly critical for reactor design and scale-up [3,12,13].

Bubble shape is known to strongly affect gas–liquid mass transfer: while small bubbles remain nearly spherical, larger or faster-moving bubbles deform into ellipsoidal or cap shapes under the influence of inertia and buoyancy [14,15]. Two dimensionless numbers characterize this behavior: the Eötvös number (Eo), which compares buoyancy to surface tension, and the Reynolds number (Re), which compares inertia to viscosity. As Eo increases, bubbles tend to flatten or elongate, deviating from the ideal sphere [1,16]. Such deformation changes the interfacial area and the flow pattern around the bubble (e.g., wake size and vortex shedding), which in turn influences local mass transfer coefficients [17]. Non-spherical bubbles often exhibit anisotropic mass transfer: for instance, a bubble’s front (upstream side) may have a thinner boundary layer and higher local transfer, while the rear (wake side) has a thicker diffusion layer and lower transfer. Studies have shown that changes in bubble size, shape, and rise velocity can significantly affect overall mass transfer rates [18,19]. Thus, Figueroa-Espinoza and Legendre [18] found that an oblate (flattened) bubble achieves a different Sherwood number distribution compared to a sphere, underscoring the need to account for shape in mass transfer models.

From a computational standpoint, modeling fluid flow and mass transfer around deformable bubbles is challenging: direct numerical simulation of a moving and deforming bubble—using interface-tracking methods like Volume of Fluid (VOF) or Level Set—requires resolving the time-dependent shape evolution and the coupling between flow and interface deformation [20–23]. This is computationally expensive, for instance high-fidelity VOF simulations of a single rising bubble can take tens to hundreds of hours of CPU/GPU time for a few seconds of physical time [24,25]. These methods demand fine grids (often refining the interface region below millimeter-scale cells) and small time steps to capture interfacial dynamics accurately [24]. While these simulations provide detailed insight, they are impractical for broad parametric studies or routine engineering calculations, especially when one needs steady-state information or to explore many combinations of Re , Eo , and shapes [24,26,27].

In this work, we pursue an alternative computational strategy to examine bubble mass transfer that avoids explicit interface tracking. We assume a steady-state boundary shape scenario where the bubble shape is prescribed a priori by an analytical formula, and the flow and concentration fields are solved in a fixed domain around this shape. By using analytical expressions to define the bubble surface, we can systematically vary the bubble geometry without simulating the deformation process itself. This approach drastically reduces computational cost and complexity, allowing rapid analysis of different shapes and flow conditions. Crucially, by focusing on the dissolved gas concentration gradients (rather than time-evolving interface motion), we obtain the solution directly, without the need to numerically “pre-equilibrate” the system geometry via transient simulation.

Our approach leverages a parametric shape descriptor known as the Superformula [28,29] to represent bubble interfaces. We integrate this with CFD simulations of flow and species transport to evaluate how Re and Eo influence mass transfer for various bubble shapes. The long-term motivation is to incorporate these high-accurate results into hybrid modeling frameworks—as an option when using the computed mass transfer rates as inputs to larger-scale reactor models or as training data for data-driven surrogate models. By doing so, one can achieve accurate gas–liquid mass transfer predictions in complex systems (like aeration tanks or bioreactors) without incurring the full cost of interface-resolved CFD each time. Thus, the introduction of an analytical bubble shape model enables an efficient

exploration of bubble-driven mass transfer phenomena, providing physical insights and data that bridge the gap between detailed CFD and practical engineering models [30].

2. Materials and Methods

2.1. Modeling Approach

In order to represent non-spherical bubble shapes, we employ the Superformula proposed by Gielis [28]. The Superformula is a generalized mathematical curve capable of describing a wide variety of closed shapes with only a few parameters. In this work, the bubble surface is parameterized using the axisymmetric approximation, which enables the representation of a wide variety of bubble shapes observed in gas–liquid systems, ranging from nearly spherical to highly deformed (elongated, flattened, or cap-shaped) geometries.

The position vector of a point on the bubble surface in is given by

$$\vec{r}_0(\theta, \varphi) = f(\theta) \begin{bmatrix} \sin \theta \cos \varphi \\ \sin \theta \sin \varphi \\ \cos \theta \end{bmatrix} \quad (1)$$

where $\theta \in [0, \pi]$ is the polar angle, $\varphi \in [0, 2\pi]$ is the azimuthal angle, and $f(\theta)$ is a radial function defining the distance from the bubble center to its surface as a function of θ .

The radial function $f(\theta)$ is defined by the Superformula:

$$f(\theta) = \left(\left| \frac{\cos\left(\frac{m\theta}{4}\right)}{a} \right|^{n_c} + \left| \frac{\sin\left(\frac{m\theta}{4}\right)}{b} \right|^{n_s} \right)^{-\frac{1}{n}} \quad (2)$$

where variations of parameters a, b, m, n_c, n_s, n allow to obtain any morphology shape including different types of bubbles with the following physical and geometrical interpretations:

- a, b —scaling coefficients that control the stretching of the surface along the principal axes, analogous to the semi-axes of an ellipsoid;
- m —angular symmetry parameter, determining the number of symmetry axes (or “lobes”) in the cross-section;
- n_c, n_s —shape exponents that regulate the sharpness or smoothness of the transitions between principal directions; higher values yield more angular shapes, while lower values produce smoother contours;
- n —global exponent controlling the overall roundness or pointedness of the shape.

This parameterization is highly versatile and can be fitted to experimental bubble contours extracted from high-speed imaging or computer vision techniques. For example, the spherical bubble is recovered for $a = b = R$, $m = 4$, $n_c = n_s = n = 2$, yielding $f(\theta) = R$.

By using the Superformula, one can encode physical influences like Eötvös number into the shape: a larger Eo (stronger buoyancy relative to surface tension) tends to flatten the bubble, which we emulate by selecting parameters that increase the horizontal span relative to vertical. Similarly, we can mimic smaller surface tension (or higher capillary number) by shapes with sharper curvature at the edges. This parametric shape description is analytical and explicit, allowing us to generate mesh geometries for CFD calculations fast and reproducibly for any desired shape instance [29]. The analytical generation of complex shapes is an important step in modeling mass transfer, replacing the procedure for determining the shape through modeling with a computationally simpler procedure for selecting the parameters of a geometric model. Examples of geometries are shown on

Figure 1. Traditional methods of generating bubble shapes do not allow creating complex shapes such as drop and cap shaped.

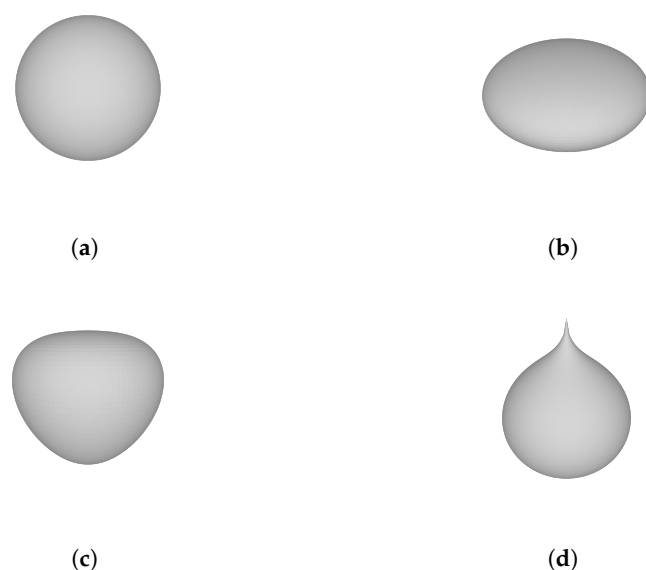


Figure 1. Various bubble geometries generated using the Superformula approach: (a) spherical: ($a = 1, b = 1, m = 4, n_c = 2, n_s = 2, n = 2$); (b) ellipsoidal: ($a = 1, b = 2, m = 4, n_c = 2, n_s = 2, n = 2$); (c) cap-shaped: ($a = 1, b = 0.5, m = 2, n_c = 2, n_s = 4, n = 1$); and (d) drop-shaped: ($a = 1.2, b = 1, m = 2, n_c = 4, n_s = 0.5, n = 1$).

With the bubble surface defined analytically, we set up a CFD model to solve the flow and mass transfer equations around the bubble in COMSOL Multiphysics 6.2. By avoiding transient interface deformation and directly solving the equations in steady-shaped approximation, computational time is drastically reduced. In practice, the computational cost for a single steady solution is on the order of minutes to an hour on a modern workstation—several orders of magnitude faster than equivalent transient bubble surface simulations that track interface motion for physical time to steady state [24]. Moreover, because the bubble shape is defined analytically rather than via a deformable mesh, mesh generation is straightforward and does not require interface reconstruction algorithms. This makes it feasible to run multiple simulations across a range of Re and Eo to systematically probe their effects. We treat Re and shape Eo as independent parameters: for instance, we can simulate a nearly spherical bubble (low Eo shape) at various Re to see purely Reynolds number effects, and separately simulate highly deformed shapes (high Eo at a fixed Re to isolate shape-induced effects on mass transfer. The results can be summarized in terms of dimensionless metrics like the Sherwood number, the ratio of convective mass transfer to diffusion, as functions of Re and shape parameters. In summary, the bubble surface modeling approach combines an analytical interface representation (Superformula-driven) with the steady-shaped CFD simulation of flow and mass transfer. This yields a computationally light framework ideal for parametric studies and integration into larger-scale models. Next, we describe the specific simulation cases examined to illustrate the method's application and the insights gained.

2.2. Simulation Cases Description

In order to demonstrate the methodology, we consider two representative simulation cases, which highlight together the differences between spherical and deformed air bubbles in terms of flow patterns and dissolved gas concentration fields, serving as a basis for discussion of mass transfer behavior. We investigate the variation of the concentration field around single bubbles of characteristic shapes determined by the values of Eötvös and

Reynolds numbers at different regimes of laminar flow velocities. The laminar fluid flow field is described by incompressible Navier–Stokes equations and continuity equations:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot \left[-p\mathbf{I} + \mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right] \quad (3)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (4)$$

where ρ is the density of the liquid phase, $\mathbf{u}$ is the velocity vector, t is time, p is pressure, μ is dynamic viscosity, and $\mathbf{I}$ is the identity matrix.

Oxygen transfer from the bubble surface occurs by diffusion and convection. For this purpose, the following mass conservation equation is solved:

$$\frac{\partial c_i}{\partial t} + \mathbf{u} \cdot \nabla c_i = \nabla \cdot (D_i \nabla c_i) \quad (5)$$

where c_i is the concentration of the species, and D_i denotes the diffusion coefficient. In pure water, the bubble surface cannot resist any tangential shear, which means that the tangential velocity at the interface should equal the velocity of liquid flow right next to it. This boundary condition is defined as the free-slip boundary condition [31]. In order to solve the problem, an air-filled bubble is placed in a cubic domain $40 \times 40 \times 40$ mm with water. To simulate continuous flow, periodic boundary conditions are defined on the walls of the cube, and a slip boundary condition is used on the bubble boundary. The relationship between pressure and velocity is constructed using the P1 + P1 scheme. GMRES is chosen as the solver. A set of bubbles of various shapes in a water–air bubble stream is captured by a high-speed camera and processed by a computer vision algorithm as shown in the article [29]. Artificial geometric images (Superformula approximation) of two spherical and two non-spherical bubbles are obtained (see Figure 2).

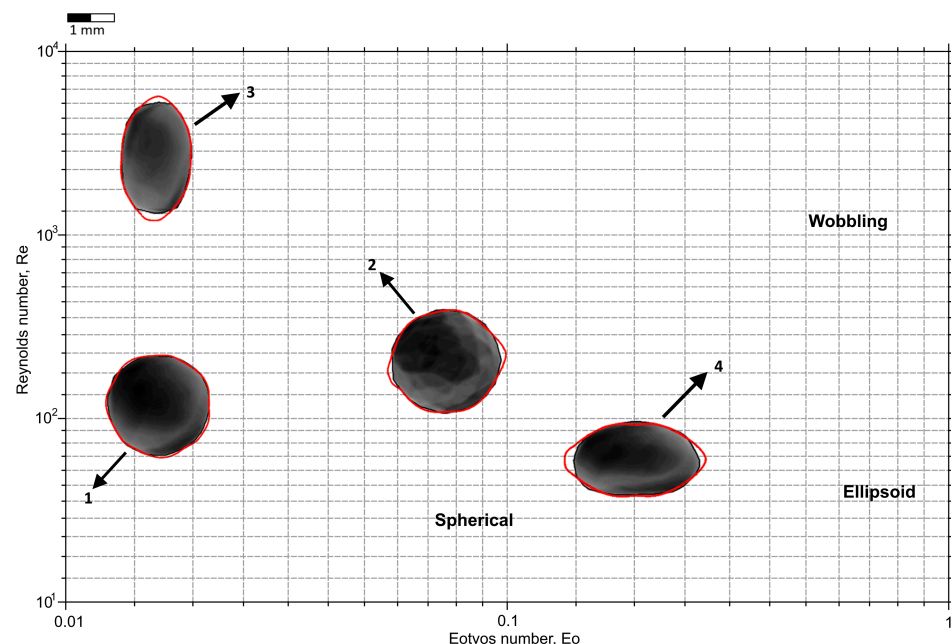


Figure 2. Diagram with bubbles obtained by CFD modeling for different regimes of Reynolds and Eötvös numbers. Red lines show the contours of artificial bubbles generated using the presented framework in [29]. Superformula parameters used to generate these bubbles (see Table 1).

In the first case, a bubble with a spherical shape is simulated. The bubble diameter $D = 1.7$ mm is chosen as the characteristic length for defining $Re = 193$ and $Re = 966$, where Eötvös numbers are 0.01 and 0.046, respectively (1 and 2 bubbles in the diagram

Figure 2). In the second case, we simulate a non-spherical bubble (3 and 4 bubbles in the diagram Figure 2) that has $Re = 991$, $Eo = 0.01$ and $Re = 205$, $Eo = 0.3$, respectively.

Table 1. Superformula parameters for generating bubble shapes.

Bubble Number	a	b	m	n_c	n_s	n	Re	Eo
1	1.74	1.65	4.78	1.91	2.12	0.24	193	0.01
2	1.7	1.82	3.77	2.14	1.8	0.24	966	0.046
3	1.7	1.69	4.01	2.1	1.86	0.26	991	0.01
4	1.73	1.77	4.01	2.15	1.79	0.25	205	0.3

The mass transfer characteristics are calculated assuming that one bubble has a gas (air) content of 10% or 15%. To achieve the required gas content, it is assumed that the bubble fits into a liquid cube with a volume of V_L (see Table 2). The gas content is calculated using the following formula:

$$\varepsilon = \frac{V_b}{V_L + V_b} \quad (6)$$

where V_b is the bubble volume.

The calculated total dissolved oxygen flux through the bubble surface can be expressed as

$$J = V_L k_L a_b \Delta C \quad (7)$$

where V_L is the volume of the liquid cube that satisfies a certain gas content, a_b is the specific interfacial area, which is the ratio of the total interfacial surface area A to the volume of liquid V_L , ΔC is the driving force, calculated as $\Delta C = C^* - C$, where C^* is the oxygen saturation concentration at the surface of the bubble, and C is the concentration of dissolved oxygen in the liquid. The calculations are performed under conditions where $C = 0$ and the saturation concentration at the bubble surface is $C^* = 0.22 \text{ mol/m}^3$, which corresponds to the equilibrium oxygen concentration in liquid at 40 °C. Thus, the volumetric mass transfer coefficient is

$$k_L a_b = \frac{J}{V_L} \cdot \frac{1}{\Delta C} \quad (8)$$

Table 2. Simulation modes of a mass transfer unit.

Bubble Type	ε , %	$V_L \cdot 10^{-9}$, m ³	a_b , m ⁻¹
spherical	10	22	399
	15	14	634
non-spherical	10	16	454
	15	9	767

3. Results

Further, for a spherical bubble, we will analyze the results of computer simulations that will be presented for the first seconds of the calculation (0.01 s), when the velocity and concentration field around the bubble is just beginning to form, and for the regime when the flow pattern around the bubble has stabilized.

In the first seconds of the calculation, virtually no tail zones (recirculation zones) form behind the bubble, and therefore their contribution to the mass transfer characteristics tends to zero. In this case, the solution in the first seconds can be compared with the analytical solution for the problem of laminar flow around a spherical bubble.

Figures 3 and 4 show the distribution of the velocity field around a spherical bubble under different flow regimes. In the first few seconds, at low flow velocity (see Figure 3), a low-velocity low-pressure zone forms near the bubble surface, but there is no vortex formation behind the bubble. When the flow pattern stabilizes, a stable tail zone forms behind the bubble.

At high speeds, as a result, the low-pressure zone behind the bubble is much larger (see Figure 4, on the left), and even in the first 0.01 s, small vortex structures are observed. With a steady flow, the tail region behind the bubble is not stationary but oscillates, causing its sizes to change.

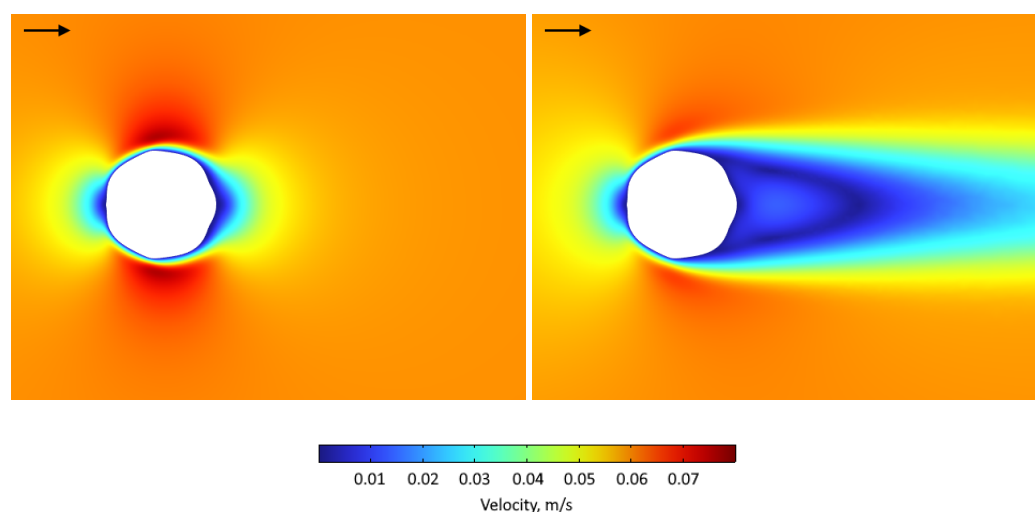


Figure 3. Distribution of velocity near a spherical bubble. The direction of fluid flow is shown by the arrow. The distribution is presented for the first 0.01 s (on the **left**) and final-state flow (on the **right**). The results are presented for a mode with the following characteristics: $Re = 193$, $Eo = 0.01$, $u = 0.06$ m/s.

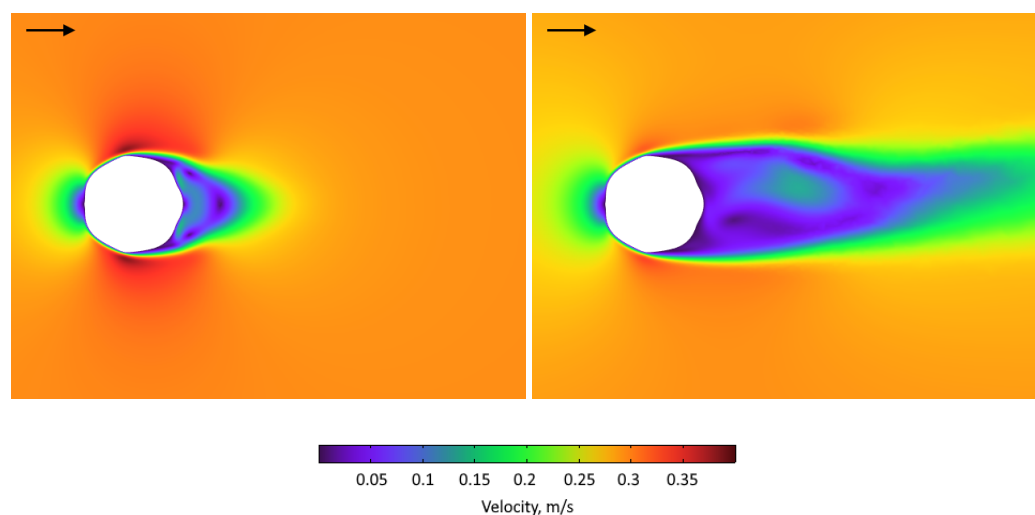


Figure 4. Distribution of velocity near a spherical bubble. The direction of fluid flow is shown by the arrow. The distribution is presented for the first 0.01 s (on the **left**) and final-state flow (on the **right**). The results are presented for a mode with the following characteristics: $Re = 966$, $Eo = 0.046$, and $u = 0.3$ m/s.

Figures 5 and 6 show the distribution of dissolved gas concentration near the surface of a spherical bubble. We note that a non-uniform concentration field is characteristic of all laminar flow velocities studied.

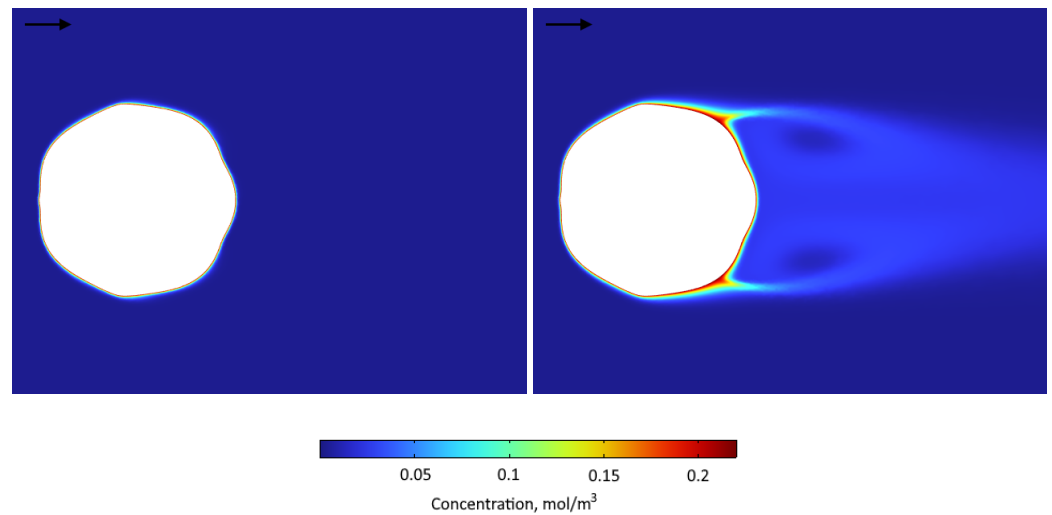


Figure 5. Distribution of dissolved gas concentration near a spherical bubble. The direction of fluid flow is shown by the arrow. The distribution is presented for the first 0.01 s (on the **left**) and final-state flow (on the **right**). The results are presented for a mode with the following characteristics: $Re = 193$, $Eo = 0.01$, $u = 0.06$ m/s.

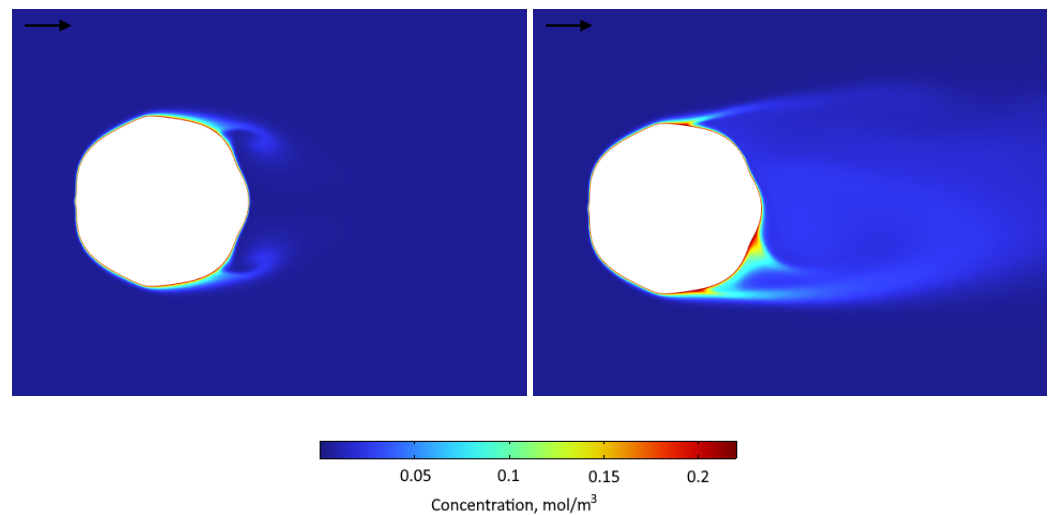


Figure 6. Distribution of dissolved gas concentration near a spherical bubble. The direction of fluid flow is shown by the arrow. The distribution is presented for the first 0.01 s (on the **left**) and final-state flow (on the **right**). The results are presented for a mode with the following characteristics: $Re = 966$, $Eo = 0.046$, $u = 0.3$ m/s.

At low velocities (see Figure 5, on the left), the concentration profile near the bubble changes very slowly, so there are practically no changes in the first few seconds. At velocities an order of magnitude higher (Figure 6, on the left), gas from the bubble surface is transferred faster due to higher convection. Therefore, a stable concentration profile is formed in the first few seconds.

At $u = 0.06$ m/s, zones of stationary low-speed vortex (Figure 5, on the right) are observed behind the spherical bubble. As a result, the concentration gradient in this region is low and insignificant. At higher velocities, the concentration gradient is determined to a greater extent by convection (Figure 6, on the right). This manifests itself in a more non-uniform distribution of concentration in the boundary layer around the bubble and a more pronounced trail forming behind it.

Figures 7 and 8 demonstrate the results for a non-spherical bubble. Depending on the hydrodynamic conditions, a non-spherical bubble takes on different shapes, but it is generally close to ellipsoidal.

In the first case, when the flow velocity is not high and the Eötvös number is large (see Figure 7, upper panel), the bubble is located perpendicular to the flow direction, and a stable trail with two practically symmetrical tail zones forms behind it.

On the other hand, when the flow velocity is high and the Eötvös number is not large (Figure 7, lower panel), the bubble deforms under the force of the flow and again takes on a shape close to ellipsoidal but is located along the direction of the flow. As a result, although a trailing zone is formed, it becomes unstable and begins to oscillate as in the case of a spherical bubble.

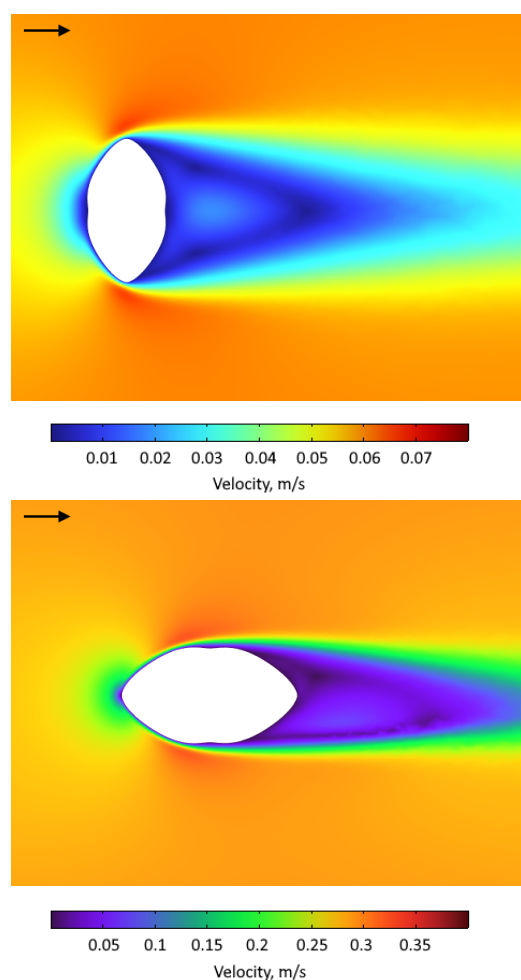


Figure 7. Distribution of velocity near a non-spherical bubble. The direction of fluid flow is shown by the arrow. The distribution is presented for the final-state flow. The results are resented for different mode with following characteristics: $Re = 205$, $Eo = 0.3$, $u = 0.06$ m/s (**upper** panel); $Re = 991$, $Eo = 0.01$, $u = 0.3$ m/s (**lower** panel).

Figure 8 shows the concentration field of dissolved gas near of the bubble. When flowing around a deformed bubble that takes the shape of an ellipsoid, vortex regions continue to form behind the bubble, just as when flowing around a spherical bubble (Figure 8, on the left). Since the surface of the deformed bubble is more flattened and elongated, and the bubble is positioned relative to the flow in such a way as to create maximum resistance, larger tail zones form behind it, which leads to a decrease in mass transfer. When the deformed bubble is located along the flow direction, the tail zone behind the bubble begins to oscillate (Figure 8, on the right).

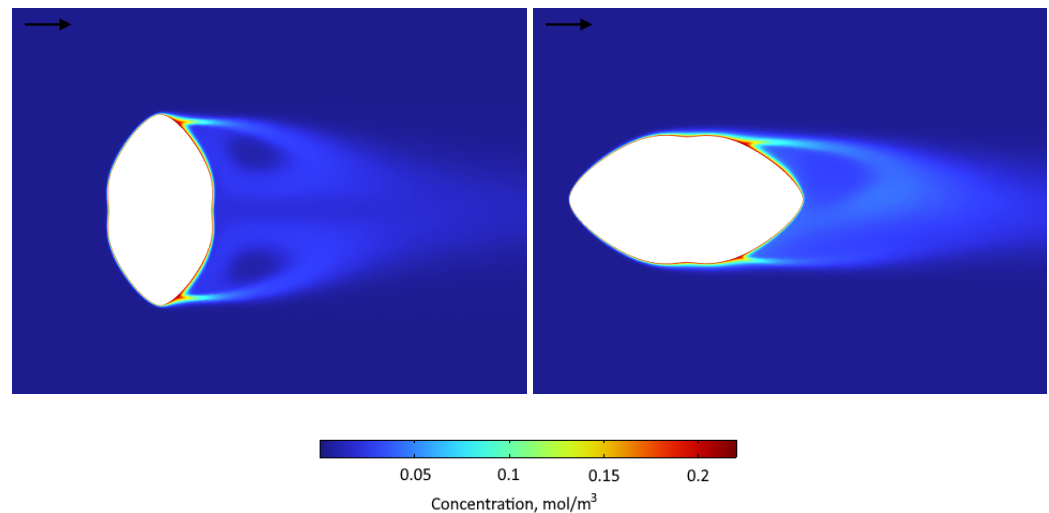


Figure 8. Distribution of dissolved gas concentration near a non-spherical bubble. The direction of fluid flow is shown by the arrow. The distribution is presented for different modes of laminar flow: $Re = 205$, $Eo = 0.3$, $u = 0.06$ m/s (on the **left**); $Re = 991$, $Eo = 0.01$, $u = 0.3$ m/s (on the **right**).

The results of mass transfer characteristics for bubbles under different flow conditions are shown in Tables 3–5.

Tables 3 and 4 present the results of mass transfer characteristics for a spherical bubble after 0.01 s and 1 s. It should be noted that in the first few seconds, the flow of dissolved gas through the bubble surface is much higher. This is due to the high driving force (concentration gradient) and the absence of tail zones. The presence of a tail zone behind the bubble over time leads to a decrease in the concentration gradient and, consequently, to mass transfer. This occurs because the tail zone is low speed, and significant vortex formation creates a stagnant area. In a final state at higher speeds, dissolved gas from the bubble surface is transferred more efficiently due to intense convection.

Table 3. The results of mass transfer characteristics at 0.01 s of simulation (spherical bubbles).

u , m/s	ε , %	$J \cdot 10^{-9}$, mol/s	$k_L a_b$, h ⁻¹	$k_L \cdot 10^{-4}$, m/s	OTR, kg/m ³ · h
0.06	10	1.3	969	7	7
	15	1.3	1539	7	11
0.30	10	4.2	3158	22	22
	15	4.2	5014	22	35

Table 4. The results of mass transfer characteristics after 1 s of simulation (spherical bubbles).

u , m/s	ε , %	$J \cdot 10^{-9}$, mol/s	$k_L a_b$, h ⁻¹	$k_L \cdot 10^{-4}$, m/s	OTR, kg/m ³ · h
0.06	10	0.3	253	2	2
	15	0.3	402	2	3
0.30	10	2.3	1714	12	12
	15	2.3	2723	12	19

Table 5 shows the results for a non-spherical bubble after 1 s. As with a spherical bubble, mass transfer is higher and more intense at high flow velocities for a bubble close to ellipsoidal. However, in the case of non-spherical bubbles, their shape and position relative to the flow depend significantly on the hydrodynamic conditions. At low velocities, mass transfer is higher for a deformed bubble than for a spherical one, whereas at low velocities,

mass transfer is higher for a spherical bubble. This can be explained, for example, by the non-uniform flow around the bubble.

Table 5. The results of mass transfer characteristics after 1 s of simulation (non-spherical bubbles).

u , m/s	ε , %	$J \cdot 10^{-9}$, mol/s	$k_L a_b$, h ⁻¹	$k_L \cdot 10^{-4}$, m/s	OTR, kg/m ³ · h
0.06	10	0.3	293	2	2
	15	0.3	495	2	3
0.30	10	1.4	1466	9	10
	15	1.4	2474	9	17

4. Discussion

The simulation results from the two cases above confirm that the bubble shape has a significant impact on the distribution of dissolved gas around the bubble and the total mass transfer rate.

4.1. Case 1 (Spherical Bubble) Considerations

For the spherical bubble (Case 1), the concentration boundary layer is fairly uniform around the forward portion of the bubble, thinning near the front stagnation point where the liquid first contacts the bubble and thickening toward the rear. This corresponds to higher local Sherwood numbers at the front and lower at the back, but overall the variation around a sphere is limited due to axial symmetry. The integrated mass transfer (Sherwood number) for the sphere at $Re \approx 100$ in our simulation aligns well with the established literature values, lending credibility to our modeling approach. This agreement with the Frössling-type correlation for spheres (within a few percent) indicates that even though we used a free-slip boundary (appropriate for a clean bubble), the effective transfer is similar to that of a solid sphere at this moderate Reynolds number. The small discrepancy can be attributed to the difference in boundary condition (a fully mobile interface tends to yield slightly higher mass transfer than a rigid sphere because there is less resistance in the boundary layer) [1].

4.2. Case 2 (Non-Spherical Bubble) Considerations

Meanwhile for the non-spherical bubble (Case 2), several important observations emerge. First, the dissolved gas concentration field is highly non-uniform around the bubble. The front face of the bubble (which directly impinges on the incoming flow) experiences intense convective refreshment: the high-velocity liquid continually replaces fluid at the interface, resulting in a thin concentration boundary layer and high local mass transfer rates. In contrast, the rear of the bubble (the lee side) falls within a recirculating wake where liquid motion is much slower. Our CFD results show that this wake region becomes nearly saturated with gas (since the gas that diffuses into that zone cannot be quickly carried away), effectively forming a “mass transfer shadow” behind the bubble. Consequently, the back side of the bubble contributes very little to the overall transfer—a phenomenon noted qualitatively in experiments and simulations of rising bubbles [18]. The net effect is that the overall Sherwood number for the deformed bubble is lower than that of the sphere in the same flow conditions, even though the deformed bubble has a larger surface area. This somewhat counterintuitive result highlights that interfacial area utilization is more important than area alone: a streamlined or spherical bubble uses its entire surface more effectively for transfer, whereas a flattened bubble has “dead zones” of transfer in its wake.

Second, the influence of the Reynolds number is evident when comparing how convective transport dominates over diffusion in different regions. At the moderate Re considered, convection is strong around the front (peeling off the boundary layer), but the wake still sees significant diffusive accumulation. If Re were increased further, holding shape fixed, we would anticipate an even thinner front layer and possibly a detached wake eddy; mass transfer from the front might increase, but the wake could remain stagnant. Conversely, at very low Re (creeping flow), shape would matter less because diffusion dominates around the entire bubble (in the limit of $Re \rightarrow 0$, Sherwood tends to 2 for any shape under steady conditions because convection vanishes). Our chosen Re is in the intermediate regime where both convection and diffusion are important, making the shape effects pronounced. These considerations suggest that **the optimal bubble shape for mass transfer might depend on the flow regime**: in convective regimes, a more streamlined shape might maximize usable surface, whereas in diffusion-limited regimes, shape is less critical.

Third, the role of the Eötvös number (surface tension effects) is implicitly reflected through the bubble shape in our model. A higher Eötvös number produced the flatter bubble which, as discussed, showed reduced mass transfer efficiency in the wake. In real multiphase flows, Eo often correlates with bubble size (larger bubbles have higher Eo and deform more). Our findings imply that beyond a certain size, the advantage of larger surface area can be offset by poor flow in the wake. This could partially explain why mass transfer coefficients in bubble swarms do not scale linearly with bubble size—shape-induced flow changes play a role. Although our study looked at a single bubble in isolation, in an actual bubble column **the wakes of deformed large bubbles can affect nearby smaller bubbles and overall gas holdup** [2]. The anisotropic concentration field around non-spherical bubbles could also influence where dissolved gas is available in the liquid: for instance, the wake might carry a pocket of high-concentration fluid that eventually peels off and mixes, potentially affecting downstream mass transfer or chemical reactions locally.

4.3. Approach Advantages

An important outcome of this work is demonstrating the viability of a steady-shaped CFD approach with the prescribed bubble geometry. By sidestepping the computational burden of interface dynamics, we achieved rapid predictions of mass transfer metrics. This opens the door for using such simulations as part of a hybrid modeling strategy. In hybrid modeling, one might combine first-principles simulations with data-driven or reduced-order models to capture system behavior efficiently. Our approach can supply high-accuracy data (e.g., Sherwood number as a function of Re and shape parameters) to build correlations or train machine learning models that run in real time within a larger process simulation. For example, a bubble column reactor model could call upon a surrogate correlation $Sh(Re, \text{shape})$ that is informed by our CFD results, rather than assuming all bubbles are perfect spheres or relying on overly simplified mass transfer coefficients. This is particularly relevant for surrogate modeling efforts in multiphase flows where one aims to optimize design or control parameters without running full CFD each time. Recent studies have shown the effectiveness of CFD-informed surrogate models for bubble column performance [3], and the present approach could enrich such models by accounting for shape effects explicitly.

Another potential application is in coupled Euler–Lagrange simulations of bubbly flows. Instead of resolving each bubble’s interface on the fly, one could track bubble parcels (as Lagrangian entities) with properties (drag, mass transfer rate, etc.) obtained from pre-computed maps. Our parametric CFD results essentially provide those maps: for a bubble of a given equivalent diameter and shape factor, at a given relative velocity, one can interpolate the Sherwood number and use it in the coarse simulation. This is a classic

multiscale coupling that significantly enhances tractability. It embodies the spirit of hybrid modeling by marrying detailed physics (captured in our CFD library of cases) with efficient coarse-grained simulation. We expect that such an approach would be especially useful for systems where many bubbles interact, like jet-stream bioreactors, and bubble columns, regimes where tracking detailed interfaces for all bubbles is currently infeasible.

4.4. Approach Limitations

While the present method is powerful, it is not without limitations. We assumed a stable bubble shape; real rising bubbles might oscillate, especially at higher Reynolds numbers, and such oscillations can enhance mixing (for instance, path instabilities or shape oscillations could increase the mass transfer intermittently).

Another limitation is that we treated the bubble surface as clean (free-slip). In practical applications, surfactants or contaminants can accumulate on bubble interfaces, effectively immobilizing them (no-slip condition) and reducing mass transfer. Our framework could incorporate this by altering the boundary condition, but the Superformula shape generation remains the same. Additionally, we focused on a single isolated bubble. In dense swarms, bubble–bubble interactions (like wake entrainment or coalescence) can modify effective mass transfer rates. Extending the method to consider multiple bubbles or periodic arrangements would be a logical next step for applicability to real reactors. Despite these caveats, the insight gained—that shape-induced flow modifications are pivotal for mass transfer—is robust and can guide more complex studies.

In summary, the discussion highlights that bubble shape should be considered a first-class parameter in multiphase mass transfer research. The combination of analytical shape modeling and CFD simulation has enabled us to dissect the role of shape in a controlled manner. The trends observed here can inform improved correlations and simulation strategies for systems where bubbles are not spherical. By integrating these findings into hybrid models, one can achieve more accurate and computationally feasible predictions for industrial gas–liquid applications.

5. Conclusions

The computational study on dissolved gas concentration gradients and mass transfer around bubbles of various shapes using a novel combination of analytical shape specification and CFD simulation is presented. Non-spherical bubbles (e.g., oblate or flattened shapes) exhibit highly non-uniform dissolved gas concentration fields, with enhanced mass transfer at the front and diminished transfer in the rear wake, while overall mass transfer rates for deformed bubbles can differ substantially from those of spherical bubbles under the same flow conditions, underscoring the importance of accounting for bubble shape in design and scale-up calculations. The use of the Superformula to prescribe bubble geometry proved to be an effective and flexible approach. It allowed us to easily generate a family of bubble shapes corresponding to different Eötvös numbers and to investigate their behavior without complex interface tracking. The proposed method preserves the essential physics of how shape influences flow and mass transfer while greatly simplifying the computational setup.

By focusing on steady-shaped solutions with a fixed interface, we achieved significant computational savings relative to traditional transient multiphase CFD. The baseline spherical bubble case validated our approach against known correlations and literature data, giving confidence in the accuracy of the simulations with free-slip interfaces. This efficient CFD framework makes it feasible to perform extensive parametric sweeps (varying Re , Eo , etc.) and to obtain results [within hours instead of weeks]. The insights and data generated in this work lay the groundwork for hybrid modeling strategies in multiphase

flows. Our results can be distilled into correlations or machine-learning models for rapid prediction of mass transfer coefficients as a function of bubble shape and flow conditions. Such surrogate models can be embedded in reactor-scale simulations or control schemes, bridging the gap between high-fidelity interface-resolved physics and real-time process modeling. The approach demonstrates a viable path to create surrogate CFD tools that retain accuracy while remaining computationally tractable.

Incorporating bubble shape effects through analytical modeling and efficient CFD is a promising avenue for advancing multiphase flow science. It enables deeper physical understanding of gas–liquid mass transfer and provides practical modeling tools for engineers. Future work will extend this approach to unsteady flows, bubble swarms, and the interaction of multiple bubbles, as well as explore integration with data-driven models. We anticipate that these developments will contribute to more accurate predictions and optimizations in gas–liquid reactors, ultimately improving the design of industrial processes involving mass transfer in bubbly flows.

Author Contributions: Conceptualization, I.N. and P.M.; methodology, P.M., K.M. and D.C.; software, P.M. and K.M.; formal analysis, I.N., S.V. and D.A.; investigation, P.M. and M.N.; resources, I.S. and S.L.; writing—original draft preparation, I.S. and I.N.; writing—review and editing, I.S., O.A. and S.L.; visualization, K.M.; project administration, I.N.; funding acquisition, S.L. All authors have read and agreed to the published version of the manuscript.

Funding: This study was supported by the Russian Science Foundation (project no. 24-11-00351).

Data Availability Statement: The original contributions presented in this study are included in the article. Further inquiries can be directed to the corresponding authors.

Conflicts of Interest: Author Dmitrii Chernushkin was employed by the company NPO Biosintez Ltd. The remaining authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as potential conflicts of interest.

Abbreviations

The following abbreviations are used in this manuscript:

CFD	Computational Fluid Dynamics
Re	Reynolds number
Eo	Eötvös number

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