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Multiphase Computational Fluid Dynamics Simulations of an UASB Reactor, A review

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Abstract

Extensive research efforts have concentrated on developing and validating computational fluid dynamics (CFD) models for Up-flow Anaerobic Sludge Blanket (UASB) reactors, a key technology in anaerobic wastewater treatment. This study evaluates the effectiveness of different CFD modelling approaches, single-phase, two-phase, and three-phase, in simulating UASB reactors used in wastewater treatment. By conducting a thorough literature review, the research compares how each modelling approach addresses key factors such as reactor geometry, meshing techniques, governing equations (continuity, momentum, and turbulence models), and their validation against experimental data. The study emphasizes how well each phase model captures the interactions among solid, liquid, and gas phases within UASB reactors. The findings aim to identify which modelling approach provides the most accurate predictions of velocity distribution, volume fraction, and turbulence. This analysis will help pinpoint gaps in current research and suggest improvements in CFD modelling, ultimately contributing to better water quality management and enhanced bioenergy production through optimized UASB reactor designs.

Keywords: *“Upflow Anaerobic Sludge Blanket (UASB) reactor”, “Computational Fluid Dynamics (CFD) simulation”, “Multiphase flow modelling”*

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List of abbreviations

2D	Two-dimensional
3D	Three-dimensional
CFD	Computational fluid dynamics
CFX	Chartered Financial Expert
HRT	Hydraulic retention time
AD	Anaerobic digestion
AGSR	Anaerobic granular sludge reactor
PIV	Particle image velocimetry
SST	Shear-stress transport
UASB	Up-flow anaerobic sludge blanket
MF	Multiple flows
VF	Volumetric fraction

2. Introduction

Anaerobic treatment processes are preferred for municipal wastewater management due to their advantages over conventional methods [1],[2]. Waste stabilization ponds are a great asset to any wastewater treatment system because they can withstand sudden changes in flow rate, biochemical oxygen demand, total suspended solids, inflow and ambient temperatures, and other important wastewater parameters [3]. Since the 1980s, the up-flow anaerobic sludge blanket (UASB) reactor has been a widely adopted technology for wastewater treatment. Its effectiveness depends on the amount of active biomass present and the interaction time between the biomass and the wastewater. The performance of UASB reactors is largely influenced by hydrodynamics and microbiological processes, which are crucial for energy generation and reducing chemical oxygen demand (COD). Due to the phenomenon's complexity, there is a lack of documentation on the local hydrodynamic behaviour of UASB reactors. A thorough study of flow patterns in UASB reactors would enhance our understanding of these systems [4].

Computational fluid dynamics (CFD) modelling can be a powerful tool for this purpose, aiding in control, monitoring, and optimization by visualizing flow patterns and phase distribution. Integrating a CFD model with an existing hydrodynamic model can provide insights into dispersion and improve wastewater treatment processes [5]. As a result, Computational Fluid Dynamics (CFD) has been successfully utilized in various industrial and non-industrial sectors, including the study of aircraft and vehicle aerodynamics, power plants, and chemical process engineering[6]. CFD models facilitate the assessment of design safety and risk prediction, allowing for proactive risk mitigation. The validation of CFD models, which involves comparing simulation results with theoretical or experimental data, is crucial for ensuring model accuracy. This is distinct from verification, which checks that the model's computations are correct.

Solving CFD problems typically involves three steps: pre-processing (defining geometric boundaries and creating a mesh), solving (applying constitutive equations and boundary conditions), and post-processing (analyzing results) [7]. Recent studies have applied CFD to simulate anaerobic reactors using a 3D steady-state model to analyze flow patterns and hydrodynamic parameters [8]. Wu and Chen [9] refined CFD models by incorporating non-Newtonian fluid theory. Pereira [10] used single-phase flow dynamics in CFD with COMSOL, addressing continuity, momentum conservation, and turbulence through the k-ε model. Rocha [11] used two-phase flow dynamics in CFD, and the experimental work was performed by considering two different flow rates: 26.68 (C1) and 4.0 L/D (C2). This work [12]aims to develop and validate a two-phase CFD model through Particle Image Velocimetry (PIV) techniques using a small-scale UASB reactor.

The use of more inlet pipes at [13], directed upward, provided a more uniform flow but also resulted in a less turbulent flow field, which can cause a poor mixture inside the reactor. Research on two-phase flow dynamics in UASB systems has also been conducted [14], and three-phase flow dynamics have been applied to both UASB and Modified UASB (MUASB) reactors[15]. Despite these advancements, there is still limited research on modelling the intricate interactions of gas, liquid, and solid phases in UASB reactors.

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This paper evaluates and compares single-phase, two-phase, and three-phase CFD modelling approaches for UASB reactors. It seeks to assess the effectiveness of each model in capturing interactions between solid, liquid, and gas phases, identify their strengths and limitations in predicting key parameters like velocity distribution and turbulence, and suggest improvements. By addressing these gaps, the study aims to enhance the accuracy and reliability of CFD simulations, thereby optimizing UASB reactor designs and improving wastewater treatment and bioenergy production.

3. Methodology

The methodology for this study involves a comparative analysis of various CFD modelling approaches applied to UASB systems, focusing on single-phase, two-phase, and three-phase models. A comprehensive review of existing literature is conducted to assess how each modelling approach handles critical aspects such as reactor geometry, meshing techniques, and the governing equations for continuity, momentum, and turbulence. Special attention is given to the validation and calibration of these models against experimental data to determine their accuracy.

- **3.1. Single-Phase Modeling:** Studies focusing on single-phase models are examined for their use of geometry and mesh design and their application of the k-ε turbulence model. These studies typically analyze hydrodynamic behaviour and velocity fields, providing baseline data for comparison.
- **3.2. Two-Phase Modeling:** The review includes investigations using two-phase models to simulate interactions between liquid and gas phases in UASB reactors. These studies are evaluated for their approach to modelling phase interactions, turbulence, and flow distribution using tools like Ansys and Fluent.
- **3.3. Three-Phase Modeling:** Research utilizing three-phase models, which incorporate solid, liquid, and gas phases, is analyzed for its complexity and accuracy. This includes studies employing Eulerian-Eulerian approaches and mixture models to capture the dynamics of biogas, sludge, and wastewater dynamics.

Each modelling approach is assessed for its ability to accurately predict key parameters such as velocity distribution, volume fraction, and turbulence within the reactor. The study also highlights gaps between simulated and experimental results, providing insights into potential areas for improvement. The comparative analysis aims to determine which modelling approach offers the most reliable predictions and to suggest enhancements for CFD modelling practices.

4. Multiphase Flow Dynamics in CFD Modeling of UASB Systems

4.1. Single-Phase Flow Dynamics in CFD Modeling of UASB Systems

Pereira's study [10] employed a three-dimensional grid comprising 80,347 tetrahedral elements to simulate the hydrodynamics of the liquid phase within a system, as shown in **Figure 1**. CFD tools from COMSOL Multiphysics have been widely recognized for their effectiveness in solving complex numerical challenges. Specifically, the equations governing continuity, momentum conservation, and turbulence were addressed using the k-ε turbulent flow model. The model assumed a flow rate of 0.66 litres per second. However, the simulation did not specify the time frame, introducing an element of uncertainty in the results. **Figure 2** illustrates the velocity distribution and water flow direction. This research primarily focused on analyzing the hydrodynamic behaviour within a UASB reactor. The numerical solution effectively captures the fluid dynamics of the reactor, particularly in terms of velocity fields. In the sedimentation zone, the vertical velocity components remained relatively constant with low-velocity gradients (<1 m/h). However, changes in velocity components were observed within the sludge blanket region, with higher intensities near the walls, where a preferential flow pathway and a recirculation zone formed. While the up-flow velocities at the top of the sludge blanket and within the sedimentation zone were consistent with the recommended range (0.8-1.0 h), several areas near the walls exhibited significantly higher velocities (>10 m/h).

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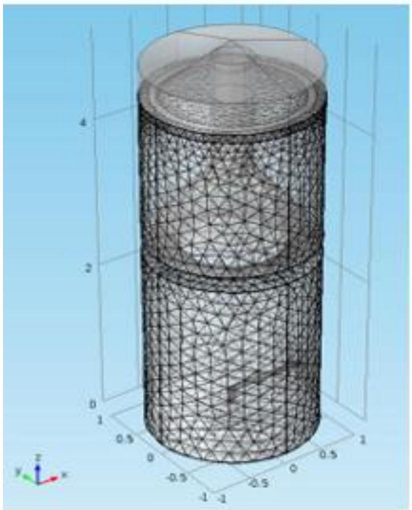


Figure 1. UASB reactor geometry and mesh [10].

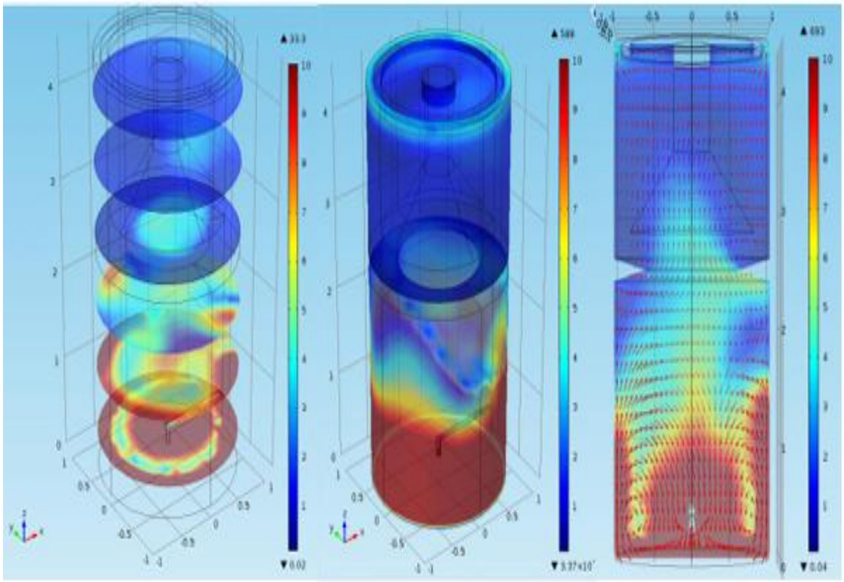


Figure 2. Velocity intensity (m/h) and vector direction [10].

Cisneros, as detailed in[14], Features a height of 8.1 meters and a diameter of 2.5 meters, providing an effective volume of approximately 41 m^3. The conical gas-liquid-solid separator (GLSS) within the reactor, in conjunction with the gas baffle, efficiently channels treated water into an external gutter. Classified as a transient laminar system, this reactor was analyzed through isothermal simulations using the Fluent 19.5 CFD software. Various configurations tested in the study are as follows: a solitary radial flow (C1), an ascending axial flow (C2), a scattered downward axial flow (C3), an inflow that is both radial and counter-radial (C4), and an inflow that is tangential and downward (C5). The physical properties of the liquid are 998.8 kg/m^3 density and dynamics viscosity of 1.08x10^{-3} kg/m.s. CFD boundary conditions are velocity inlet for water inlet, pressure outlet for water outlet, no-slip wall for reactor and GLSS walls, and zero-shear wall for water surface. The application of the realizable k-epsilon model was a key aspect of the simulation, which indicated low-pressure conditions. **Figure 3** detailed the velocity magnitude contours under different settings, particularly noting the maximum velocity at the inlet. This research mainly aimed to simulate the impact of five different influent distribution system configurations on the reactor's hydrodynamics and, subsequently, on the development of granular sludge. The validation process yielded an NSE of 0.98, demonstrating the high accuracy of the CFD model. The results suggest that the least favourable IDS configurations for granulation are IDS C2 and C5, which have relative granulation volumes of 13.07% and 14.12%, respectively. Conversely, the most favourable IDS configurations are C3 and C4, with relative granulation volumes of 31.23% and 22.88%, respectively.

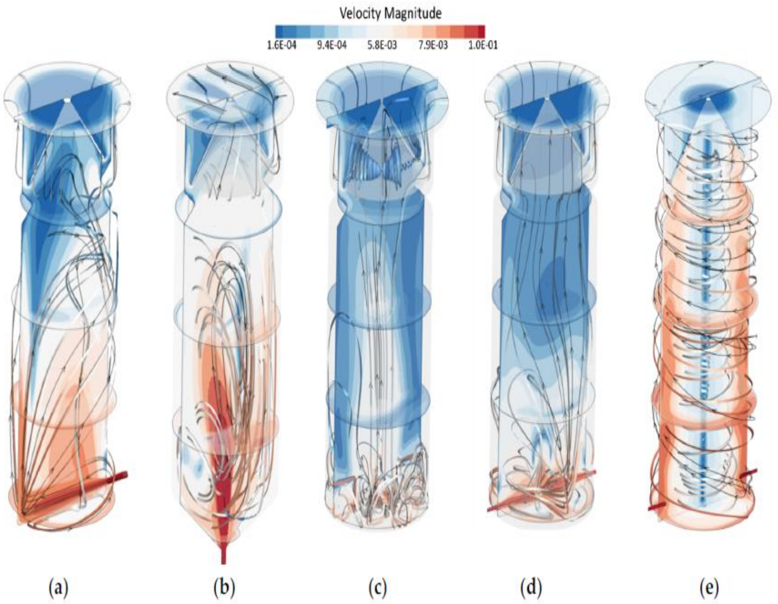
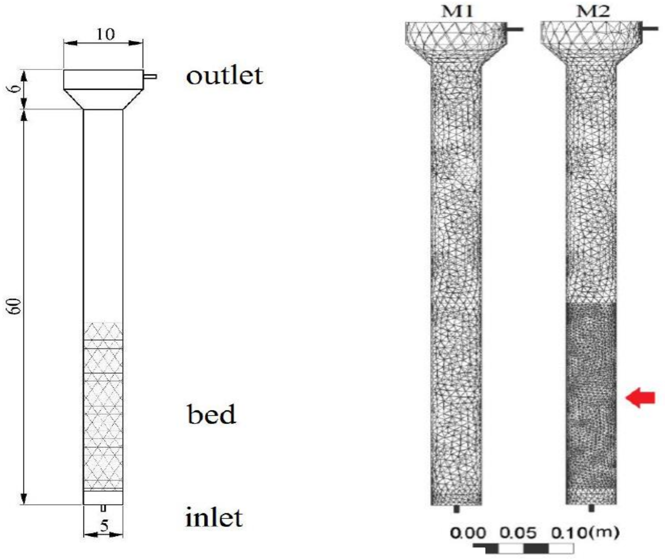


Figure 3. Curves of velocities and CFD flow paths for a variety of IDS setups. (**a**) (C1); (**b**) (C2); (**c**) (C3); (**d**) (C4); (**e**) (C5) [14].

4.1. Two-Phase Flow Dynamics in CFD Modeling of UASB Systems

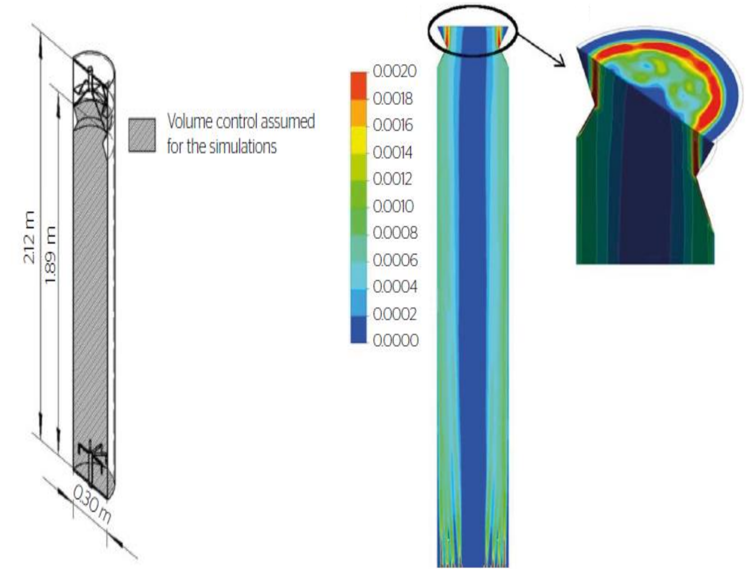
ROCHA UASB reactor in [11], constructed from acrylic, included MBBR (moving bed biofilm reactor) polymers to simulate a sludge blanket. A 2.0 cm buffer zone was positioned just above the reactor's inlet. The reactor used in the study has a height of 66 cm, a larger diameter of 10 cm, and a smaller diameter of 5 cm. The reactor has a total volume of 1.50 litres, with an effective volume of 1.38 litres for processing. It has a porosity of 0.88 and smooth internal walls with a roughness of 0.005 mm. The liquid within the reactor was maintained at 30°C, with a specific mass of 995.6 kg/m^3, a molar mass of 18.02 g/mol, a dynamic viscosity of 0.798 x 10^{-3} N·s/m^2, thermal conductivity of 0.6069 W/m·K, and a specific heat capacity of 4172.7 J/kg·K. To thoroughly understand the hydrodynamic behaviour of this small-scale UASB reactor, the study combined CFD modelling with experimental testing. The experiments were conducted at two different flow rates, 26.68 L/D (C1) and 4.0 L/D (C2), and the statistical analysis confirmed the method's validity. The research utilized the Ansys 14.0® CFD software, which includes a geometry creator (Design Modeler TM) and a Mesher (Meshing TM). The reactor's geometry is depicted in **Figure 4. a**, the standard mesh in **Figure 4. b**, and the refined mesh in **Figure 4. c**. Transient analysis and boundary conditions were defined for CFD cases, with turbulence modelled using the SST k-ω model. The CFD tool has proven to be powerful and innovative in analyzing the hydrodynamic behaviour of a UASB reactor. It was possible to establish a higher level of confidence in this tool through the experimental validation of the computationally obtained data.



(a) (b) (c)

Figure 4. (**a**) the small-scale UASB reactor, (**b**) mesh 1 (standard), (**c**) mesh 2 (refined)[11].

Numerical simulations conducted by **Bastiani** in [12] used Fluent 16.2 to study a 2.12 m high, 0.3 m diameter reactor with a 140-litre volume. The simulations applied a two-phase laminar Eulerian-Eulerian model, considering water at 293.15 K with an average upward liquid velocity of 2.525×10^{-5} m/s and a Reynolds number of 7.45 based on the reactor's tubular section with a diameter of 0.3 m. The biogas composition was set to 65% CH_4 and 35% CO_2. The reactor assumed symmetry at its centre, as shown in **Figure 5. a**, with non-slip boundary conditions on the walls. The phase-coupled SIMPLE method was used for velocity-pressure coupling, with momentum and volume fractions calculated using second-order upwind and QUICK methods. Gas and liquid mixing was enhanced with a distributor at the reactor's base. The study aimed to validate a CFD model using particle image velocity (PIV) for a small-scale UASB reactor, comparing analytical and simulated mass flow rates. Results showed minimal mass imbalance for the gas phase (0.0001 kg/hr, 0.28% error), while the liquid phase had a larger imbalance (0.31781 kg/hr, 4.95% error). The gas volume fraction peaked at the tank's top, as illustrated in **Figures 5. b** and **5. c** and higher gas velocities improved liquid circulation.

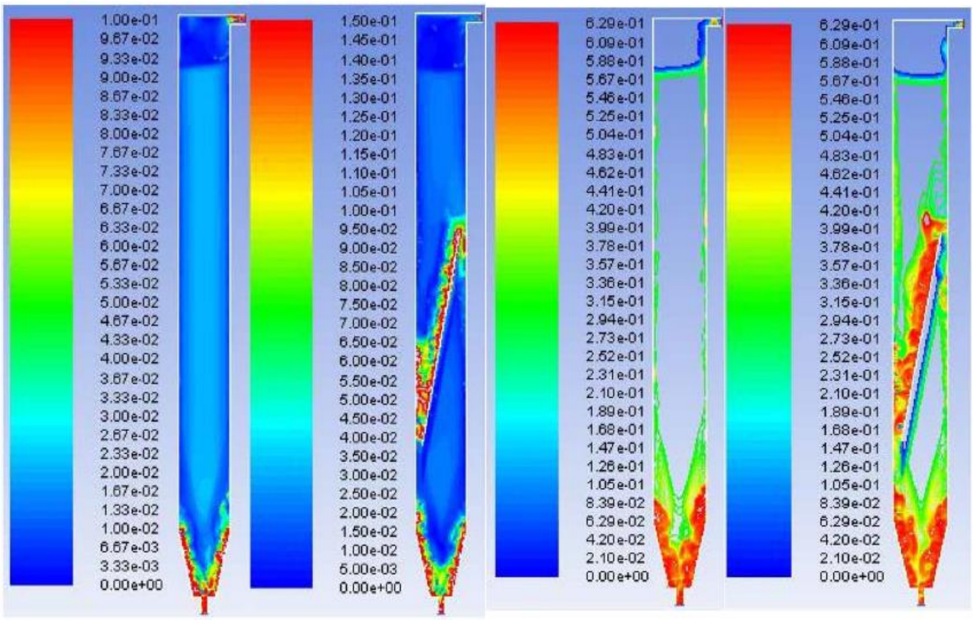


(a) (b) (c)

Figure 5. (**a**) Model Geometry, (**b**) Contours of the gas volumetric fraction as a function of time are displayed at z = 0, and (**c**) Detailed information on the gas outflow is provided [12].

4.2. Three-Phase Flow Dynamics in CFD Modeling of UASB Systems

Das modelled the reaction zones of UASB and MUASB (Modified UASB) reactors [15] to better understand their internal flow dynamics. These reactors, both featuring a reaction zone height of 70 cm and a square cross-section (7 cm × 7 cm), differ in that the MUASB reactor is equipped with baffles-slanted plates placed at heights ranging from 15 cm to 45 cm—to promote vertical mixing of the reactor contents. The reactor walls include two apertures (2 cm × 7 cm) along the vertical surface, further influencing the flow within the reactor. The momentum and continuity equations were solved using the ANSYS Fluent 6.3 software package after constructing the reactor geometry in the ANSYS Fluent GAMBIT pre-processor. Both UASB and MUASB reactors were modelled using two-dimensional computational domains to represent their reaction zones, with the UASB reactor consisting of 47,080 cells, 95,052 faces, and 47,973 nodes, and the MUASB reactor slightly more complex with 49,100 cells, 99,002 faces, and 49,903 nodes. The CFD model simulated the interaction between biogas (CH4), sludge granules, and wastewater, treating biogas as the primary phase and sludge and wastewater as secondary phases. The mixture model was employed to describe the relative velocities of the dispersed phases, solving the mixture momentum equation. The simulation procedure involved several steps: verifying a pressure-based, two-dimensional, implicit solver operating at a steady state, activating a realizable k-ε turbulence model, setting working parameters and material properties, enabling gravity, initializing the simulation, filling the reactor with the measured volumes of gas, sludge, and water, and finally running the simulation to achieve steady-state results. Initially, the sludge bed contained a 0.3-volume fraction of granular particles, which provided a pathway for gas entering the reactor. The solid surfaces, excluding biogas, were assigned wall boundary conditions, while a velocity-inlet boundary condition was applied to simulate liquid input. The reactor's outlet was defined using a pressure-outlet boundary condition, with a free slip for gas and no slip for sludge and wastewater. As illustrated in Figure 6, the simulation results show the maximum water velocity at the inlet, outlet, and baffle positions, along with the distribution of sludge volume fraction at the base of the tank and around the baffle. Notably, very little sludge was observed at the reactor's exit.



(a) (b) (c) (d)

Figure 6. The water velocity contour (in meters per second) is shown for both the (a) UASB and (b) MUASB systems. Additionally, the volume fraction of sludge granules (in percentage) is provided for both the (c) UASB and (d) MUASB systems [15].

UASB reactors with different deflector designs have been modelled by **Brito** in [16] using Ansys CFX® to assess their impact on reactor hydrodynamics. One design featured an inverted V-shaped deflector with pipes connected below, which could cause flow obstruction and uncontrolled gas release, potentially leading to leaks. An alternative design placed the pipes atop the deflector to prevent gas-liquid interface formation and associated issues. **Figure 7** shows the geometry segmentation. Two 3D meshes were created for simulations, as shown in **Figure 8**: one with an upward deflector angle (67,875 elements) and one with a downward angle (81,630 elements). The study applied the Eulerian-Eulerian approach to examine the reactor's hydrodynamics in a dispersed multiphase model, focusing on the interaction between liquid (water), gaseous (biogas), and solid (sludge) phases. The biogas, composed of 70% methane and 30% carbon dioxide, and the sludge were modelled as spheres with a diameter of 0.003 m. The drag coefficient was calculated based on established correlations, with the system's mass flow rate set at 0.004 kg/s and the liquid, gas, and solid phases occupying 91%, 6%, and 3% of the volume, respectively. The simulations accurately represented the reactor's flow dynamics compared to the mathematical model, demonstrating effective modelling of upward and downward deflector inclinations.

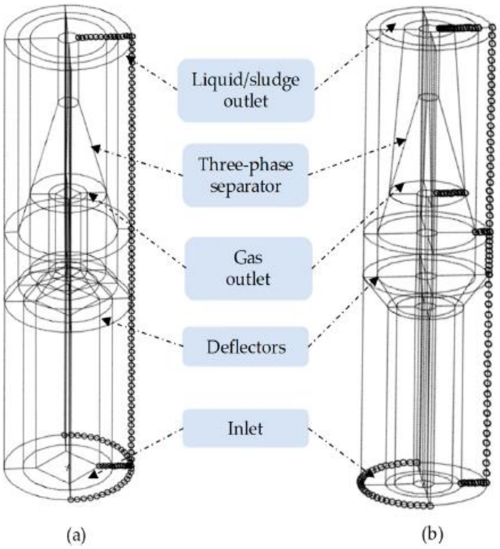
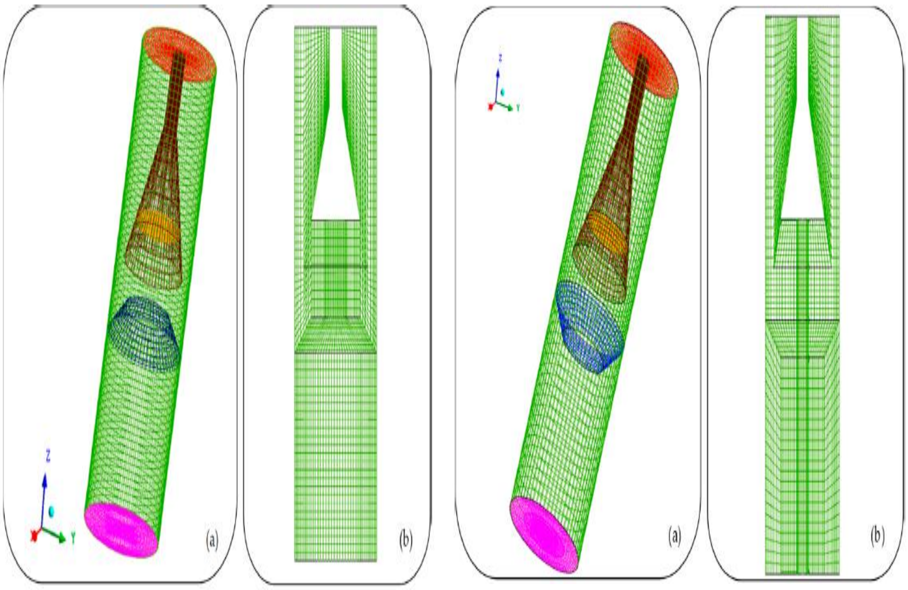


Figure 7. The geometric arrangement of two scenarios: (a) the deflector inclined in an upward direction and (b) the deflector inclined in a downward direction [16].



(i) (ii)

Figure 8. The mesh depiction includes deflector inclination in two directions: (i) upwards and (ii) downwards. (a) an overview, (b) a plan in the yz plane [16]

Chen investigated the gas-liquid-solid Eulerian model in [17], wherein granular sludge was treated adiscrete and virtual objects were modelled as continuous phases. The study simplified the system by neglecting bubble rupture and aggregation based on an assumption of uniform bubble size derived from a single-bubble model. To analyze the reactor's flow dynamics, velocity cloud processing was employed to assess the flow field and velocity distribution. The CFD model successfully predicted sludge particle velocity and volume fraction during the startup phase of the High H/D Anaerobic Inoculated Packed Bed Reactor (HHAIPBR). The model was run for fifty seconds at an average flow rate of 0.1 litres per minute, with the results illustrated in **Figure 9.** The simulation indicated that sludge particle velocities at the base of the HHAIPBR ranged from 12 to 20 m/s, with the inner cylinder showing velocities between 4 and 10 m/s and the outer cylinder ranging from 0 to 4 m/s. As corroborated by experimental data and CFD simulation results, the High H/D HHAIPBR demonstrated effective regulation of dissolved oxygen (DO) dispersion, which was essential for maintaining active bacterial populations.

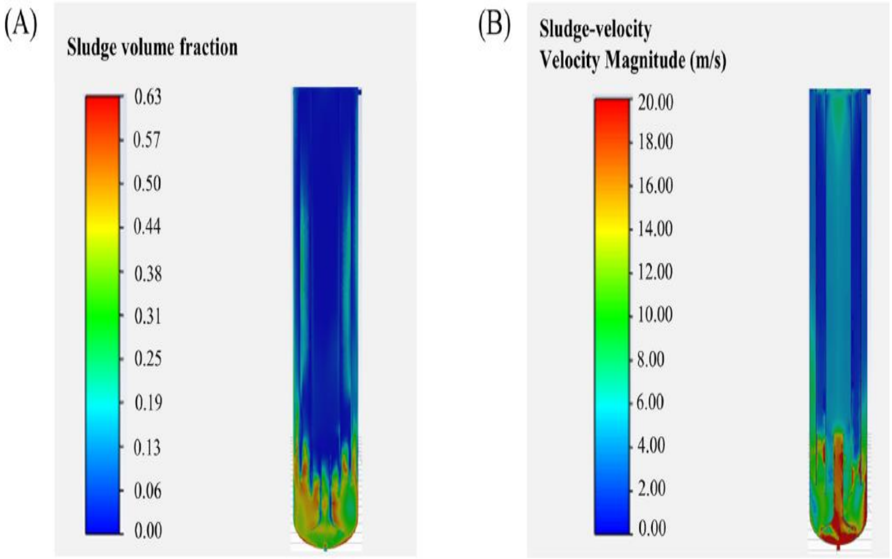


Figure 9. CFD simulation: (A) Distribution of sludge volume fraction, (B) The distribution of velocity of sludge particles [17].

5. Conclusion

This study systematically evaluates single-phase, two-phase, and three-phase CFD modelling approaches for simulating UASB reactors in wastewater treatment. The comparative analysis reveals that:

1. **Single-Phase Models**: While useful for preliminary assessments, single-phase models offer limited insights into the complex interactions between solid, liquid, and gas phases. These models typically provide basic hydrodynamic behaviour but may lack accuracy in predicting detailed phase interactions.
2. **Two-phase models** enhance the simulation by incorporating interactions between liquid and gas phases. These models offer a more accurate view of flow dynamics and turbulence. However, they may still fall short of accurately capturing the behaviour of solid phases and their interactions with the liquid and gas.
3. **Three-Phase Models**: The three-phase models provide the most comprehensive representation of UASB reactor dynamics, including solid, liquid, and gas phases. These models, particularly those

utilizing the Eulerian-Eulerian approach, demonstrate superior accuracy in predicting velocity distribution, volume fraction, and turbulence. They effectively capture the complex interplay of phases, making them the most reliable for detailed reactor simulations.

The study identifies several gaps in current research, particularly regarding integrating and validating these models against experimental data. The findings suggest that while three-phase models offer significant advantages in accuracy, there is still room for improvement in model calibration and the incorporation of additional physical phenomena, such as bubble dynamics and sludge granulation. Overall, this research underscores the importance of selecting the appropriate modelling approach for accurate simulations of UASB reactors. Enhanced CFD modelling practices will contribute to a better understanding and optimization of reactor performance, leading to improved wastewater treatment outcomes and more efficient bioenergy production.

6. Challenges and Future Perspectives

Simulating the movement of multiple phases in anaerobic granular sludge reactors presents ongoing challenges, particularly in managing momentum transfer at phase interfaces. Integrating multiphase CFD models with biokinetics models is crucial for accurate biogas production simulations. The Anaerobic Digestion Model No. 1 (ADM1), which predicts biomass degradation and biogas production, requires a three-phase approach to account for biomass and biogas interactions. Variations in granule density due to biogas production affect granule movement and wash-out, highlighting the need for more precise modelling. While current studies mainly use the Eulerian-Eulerian approach, a Lagrangian method may better capture biogas generation by incorporating gas injection sites in the sludge bed. Future research should explore this method's feasibility. Developing a comprehensive model that combines hydrodynamics with biochemical kinetics and mass transfer models could improve reactor design and optimization. The successful alignment of mathematical models with real reactor behaviours underscores the potential for enhanced CFD modelling practices in advancing wastewater treatment and bioenergy production.

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