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Hydrodynamic Analysis of Oxygen and Molten CuCl in the Cu-Cl Cycle Using a 3D CFD Model for Hydrogen Production

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Abstract - The increasing attractiveness of hydrogen as a substitute fuel has led to the necessity of investigating other technologies for hydrogen production. This work explores the hydrodynamics of the specific substances employed in the oxygen generation reactor, namely oxygen gas and molten CuCl, as part of the hydrogen production process using the copper-chlorine (Cu-Cl) cycle. The study utilizes a three-dimensional Eulerian-Eulerian Computational Fluid Dynamics (CFD) model. The objective of this study is to verify the precision of material simulations carried out in a prior investigation for the oxygen reactor. In the study, the researchers replaced the real materials with helium gas at a temperature of 90 degrees Celsius and liquid water at a temperature of 20 degrees Celsius in order to imitate the hydrodynamic properties of the real materials. The three-dimensional O2-CuCl CFD system accurately models the changes in gas holdup as the superficial gas velocity varies, with a maximum percent error of 29.9%. This inaccuracy is caused by the combined percentage errors resulting from the hydrodynamic dimensionless parameters utilized in the prior material substitutions, as well as the intricacy of the 3D multiphase system. Furthermore, the model suggests that the gas holdup values in the real materials are generally underestimated in comparison to those in the simulated materials.

***Keywords*:** Cu-Cl cycle; 3D CFD; gas holdup; superficial gas velocity; hydrogen production

1. Introduction

Hydrogen is expected to play a significant role in the future of sustainable energy due to its potential to reduce pollution and greenhouse gas emissions. The production of hydrogen gas from various fuel sources can generate greenhouse gases, but the emissions are much lower compared to those produced by gasoline and diesel vehicles. Thermochemical cycles, which can be integrated with nuclear reactors, offer a promising solution for thermally decomposing water into oxygen and hydrogen through multi-stage processes. The copper-chlorine (Cu-Cl) cycle, identified by Argonne National Laboratories (ANL) as a promising low-temperature cycle, requires a high-temperature heat source for the oxygen reaction [1-2]. This heat can be generated using non-polluting sources such as nuclear reactors or solar thermal energy. A practical and effective method for heating the oxygen reactor is to heat the molten salt within the reactor, which transfers heat from the molten CuCl to the solid Cu2OCl2 reactant particles. Various heat transfer mechanisms for the oxygen reactor have been investigated, with direct contact heat transfer from the oxygen gas to the molten CuCl identified as the optimal method [3-8]. In this approach, a portion of the oxygen gas produced during the reactor's decomposition process is heated to 530°C and reinjected into the reactor to transfer heat directly to the molten salt.

The Cu-Cl cycle's oxygen generation step is an endothermic process that requires a reaction heat of 129.2 kJ/mol and a temperature of 530°C [9]. Therefore, heat must be supplied to increase and maintain the reactor's temperature. Direct contact heat transfer using a Bubble Column Reactor (BCR) has been found to be the best method for the oxygen reactor. Bubble columns are beneficial for various industrial applications, but their scaling up, modelling, and designing is complex due to the need for detailed knowledge in areas such as kinetics, hydrodynamics, heat and mass transfer, and chemical reaction rates. One important characteristic to describe a bubble column's performance is the gas holdup, a dimensionless parameter representing the volume fraction of gas in the BCR [10]. This paper aims to investigate numerically, using 3D Computational Fluid Dynamics (CFD) simulations, the multiphase hydrodynamics of a direct contact heat transfer reactor between the oxygen gas bubbles and the molten CuCl salt in the oxygen reactor of the Cu-Cl cycle.

Studies on bubble column reactors have been conducted using both experimental methods and numerical simulations over the years. Li et al. [11] conducted hydrodynamic analyses on an air-water-glass bead slurry bubble column, both experimentally and using CFD. They employed a 2D axisymmetric two-fluid Euler k-ε model to simulate the reactor. Their findings revealed that the primary challenge in scaling up bubble columns is the variation in hydrodynamic characteristics with different column diameters. In larger-diameter columns, the axial liquid velocity significantly increases in the core of the column, while the gas holdup remains almost unchanged. Additionally, they observed an increase in turbulent kinetic energy with the scaling up of column sizes. Sarhan et al. [12] examined the impact of the physical and chemical properties of the liquid and gas phases on bubble formation and hydrodynamics in a bubble column reactor, using a combination of the population balance equation and a 3D CFD model. They used a Euler-Euler CFD model to approximate the experimental results of gas holdup in the reactor with different phase flows, achieving accuracy within ±7%. Their findings also indicated a slight increase in gas holdup as the gas phase density increased.

Li and Zhong [13] carried out a three-dimensional, time-dependent computational fluid dynamics (CFD) analysis of three different bubble column reactors, using a Eulerian-Eulerian-Eulerian approach for a three-phase system (air-water-glass powder). They studied the hydrodynamics in relation to time step, momentum discretization schemes, and wall boundary conditions. The models they used were Gandhi et al. (height: 2500mm, static height: 1500mm, diameter: 150mm), Rapure et al. (height: 2000mm, static height: 1000mm, diameter: 200mm), and their own model (height: 800mm, width: 100mm, depth: 10mm). They employed the RNG k-ε turbulence model for their simulations. Their findings indicated that the best conditions for matching experimental results were using a no-slip condition, momentum discretization with the second-order upwind scheme, and a time step of 0.001s.

Pu et al. [14] conducted a two-dimensional CFD simulation of a molten salt bubble column to explore the hydrodynamics and direct heat transfer characteristics of a two-phase flow model (air-molten salt). They utilized a Euler-Euler multiphase model with a k-ε turbulence model. During the simulation, they varied the superficial gas velocity, static liquid heights, operational pressure, and inlet gas temperature. They observed that increasing either the superficial gas velocity or the operational pressure led to a rise in both the molten salt temperature and its rate of increase over time. Conversely, as the static liquid height increased, the rate of increase in the average molten salt temperature decreased. Additionally, enhancements in superficial gas velocity or operating pressure increased the volumetric heat transfer coefficient, while an increase in static liquid height decreased it. Zhang and Luo [15] developed a two-phase (air-water) CFD model to study the distribution of local gas-liquid slip velocities in a bubble column, focusing on how they relate to heat transfer in a heterogeneous regime. Their research also looked into how these slip velocities changed on average over time when factors like the superficial gas velocities, axial positions, and the size of the bubble column were altered. They used a CFD-PBM (population balance model) simulation with an RNG k-ε turbulence model for their study. They found that increasing the superficial gas velocities led to higher local gas-liquid slip velocities in the area where flow was fully developed. When the superficial gas velocities were higher, the slip velocities were more influenced by the position across the radius of the column. Near the centre of the column, the slip velocities were lower than in the fully developed flow areas. The slip velocities were not significantly affected by the height along the axis in the fully developed flow areas.

Li et al [16] explored the effects of a circular heat exchanger on the hydrodynamics of a pilot-scale slurry bubble column reactor using a 2D CFD PBM model. They used a Euler-Euler multiphase model with an RNG k-ε turbulence model for their simulations. The reactor they studied had a diameter of 30 cm, a height of 200 cm, and the circular heat exchanger was 108 cm tall. Paraffin oil and catalyst particles were used in the simulation. They observed that the gas phase was distributed noticeably, local circular vortices were formed, and the slurry was circulated strongly due to the presence of the circular heat exchanger tube. The bimodal profile of the gas holdup in the radial direction was caused by the specific layout of the circular gas distributor. Moreover, the circular heat exchanger tube increased this distribution, leading to a higher gas holdup, which in turn facilitated momentum transfer. Zhou et al. [17] explored how particles influence gas-liquid flows in a slurry bubble column by developing a conceptual model known as the particle-dependent dual bubble size (PDBS) model. This model was designed to examine the effects of changes in viscosity and density caused by the addition of particles and the impact on the bubble drag coefficient due to the presence of particles. The model incorporated a three-phase system of air, water, and glass beads. The study found that an increase in slurry viscosity and density led to greater stability, as evidenced by a delayed transition to a higher flow regime. The research concluded that a higher concentration of solids in the slurry results in a reduction in gas holdup.

Wodolazski [18] conducted a 3D CFD simulation of a slurry bubble column reactor to investigate the flow dynamics of syngas in a three-phase system (syngas, paraffin oil, solid particles). The study utilized a Eulerian-Eulerian approach with a k-ε turbulence model, focusing on parameters such as superficial gas velocity, initial solid particle concentration (ranging from 10% to 50%), gas holdup, and bubble size distribution. The findings indicated that an increase in slurry concentration led to a decrease in axial gas holdup. Furthermore, a higher slurry concentration resulted in a reduced rate of bubble breakup. The study also noted an approximate parabolic relationship between the effects of gas velocity and the axial solids holdup profile. Matiazzo [19] conducted a comprehensive 3D computational fluid dynamics (CFD) study focusing on the complex gas-liquid flow within a churn turbulent regime. The research aimed to evaluate the accuracy of various models in predicting essential factors such as drag closures, breakup, and coalescence of bubbles.

Ertekin et al. [20] adjusted variables like the column diameter, ranging from 0.19 meters to 3 meters, and the superficial gas velocities, which varied from 0.03 meters per second to 0.25 meters per second. Yan et al. [21] employed three different optimized drag models to simulate the hydrodynamics in a high-pressure, air-water bubble column. They explored the impact of varying superficial gas velocities (0.121, 0.174, 0.233, and 0.296 meters per second) and reactor pressures (0.5, 1.0, 1.5, and 2.0 MPa) on the radial gas holdup. The findings from 2D and 3D CFD simulations were compared with experimental data obtained using the electrical resistance tomography method.

Adam and Tuwaechi [22] developed a two-phase, gas-liquid, Eulerian-Eulerian, k-ε mixture turbulence CFD model to investigate the effects of gas holdup and superficial gas velocity on the hydrodynamics. They observed that increasing the time step resulted in a higher volume fraction. A finer mesh with a grid resolution of 0.005 provided more detailed insights. Pourtousi et al. [23] examined the bubble column regime, focusing on the effects of varying superficial gas velocities (0.0025 – 0.015 meters per second) and bubble diameters (3, 4, 5, and 5.5 millimetres) on the flow pattern predictions from Euler-Euler simulations. They created a 3D air-water CFD simulation for a slurry bubble column with a height of 2.6 meters and a diameter of 0.288 meters.

Due to the challenges associated with using the actual materials of the oxygen production reactor (O2 gas and molten CuCl) for laboratory experiments, Abdulrahman conducted dimensional analysis studies based on the Buckingham pi theorem. This analysis was aimed at stimulating the actual materials of the oxygen production reactor with more suitable materials that are safe for laboratory use. He identified helium gas at 90˚C and liquid water at 22˚C as the simulated materials. These materials can replicate the behaviour of the actual materials in terms of hydrodynamics and heat transfer within a specific margin of error [24-25]. Abdulrahman has conducted experiments and 2D CFD simulations to investigate the hydrodynamics of the slurry bubble column reactor with direct contact heat transfer between the helium gas at 90ºC and the slurry of water and alumina particles at 20ºC. The parameters that he studied were gas holdup, transition velocity and the volumetric heat transfer coefficient in addition to the temperature distribution of the helium gas inside the slurry bubble column [8, 26-35]. Abdulrahman and Nassar provided a review of the Eulerian approach for CFD analyses of bubble column reactors [36]. Also, they have developed a 3D CFD simulations for the oxygen production reactor a slurry bubble column reactor with helium gas, water liquid, and alumina solid particles. They have investigated the effects of superficial gas velocity, static liquid height and solid concentration on gas holdup using the simulated materials of helium gas and liquid water [37-40].

Based on a thorough review of existing literature, it's clear that 3D computational fluid dynamics (CFD) simulations focusing on the thermal hydraulics of oxygen bubble column reactors with the actual materials in the copper-chlorine (Cu-Cl) cycle have not been conducted previously. Moreover, previous CFD studies on the oxygen bubble column rector performed by Abdulrahman and Nassar [37-40] have been focused on simulated materials of helium gas and liquid water instead of the actual materials of oxygen gas and molten CuCl. This paper aims to investigate the 3D CFD simulations for the actual materials of the oxygen production reactor in Cu-Cl cycle of hydrogen production and compare the results with that of simulated materials to validate the material simulations created by Abdulrahman [24-25].

2. CFD Analysis

In this study, the computational fluid dynamics (CFD) simulations are carried out for a three-dimensional system using a Eulerian-Eulerian model and a Eulerian sub-model, along with a pressure-based solver. The specific equations employed in the CFD analysis are presented in Table 1. These equations are formulated for the gas phase only. Since the equations for the liquid phase are similar to those for the gas phase, they are not repeated for brevity.

Table 1: Details of equations used in the 3D CFD simulations.

Description [reference]	Equation
Volume equation [41]	$V_g = \int_V \alpha_g dV$
Continuity equation in 3D Polar coordinates (r, θ, y) [8]	$\nabla . V_g = \frac{\partial v_{r,g}}{\partial r} + \frac{v_{r,g}}{r} + \frac{1}{r}\frac{\partial v_{\theta,g}}{\partial \theta} + \frac{\partial v_{y,g}}{\partial y} = 0$
Momentum equation in 3D Polar coordinates [8]	$\rho_g \alpha_g \left(\frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r}\frac{\partial v_r}{\partial \theta} + vy \frac{\partial v_r}{\partial y} - \frac{v_\theta^2}{r}\right) = -\alpha_g \frac{\partial P}{\partial r} + \alpha_g \frac{\mu_{g,eff}\partial(\nabla. \cdots}{3\partial r}$
	$\rho_g \alpha_g \left(\frac{\partial v_\theta}{\partial t} + v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r}\frac{\partial v_\theta}{\partial \theta} + v_y \frac{\partial v_\theta}{\partial y} + \frac{v_r v_\theta}{r}\right) = -\alpha_g \frac{1}{r}\frac{\partial P}{\partial \theta} + \alpha_g \frac{\mu_{g,eff}}{3r} \cdots$
	$\rho_g \alpha_g \left(\frac{\partial v_y}{\partial t} + v_r \frac{\partial v_y}{\partial r} + \frac{v_\theta}{r}\frac{\partial v_y}{\partial \theta} + v_y \frac{\partial v_y}{\partial y}\right) = -\alpha_g \frac{\partial P}{\partial y} + \alpha_g \mu_{g,eff} \left[\frac{1}{r}\frac{\partial}{\partial r}\left(r \cdots\right.\right.$
Energy equation in 3D Polar coordinates [8]	$\alpha_g \rho_g C \left(\frac{\partial T_g}{\partial t} + v_{r,g} \frac{\partial T_g}{\partial r} + \frac{v_{\theta,g}}{r}\frac{\partial T_g}{\partial \theta} + v_{y,g} \frac{\partial T_g}{\partial y}\right) = \bar{\bar{\tau}}_g : \nabla V_g + k_g \left(\frac{1}{r}\frac{\partial}{\partial r} \cdots\right.$
Effective density	$\hat{\rho}_g = \alpha_g \rho_g$
Drag force [41]	$M_D = \frac{\rho_g f}{6\tau_b} d_b A_i (V_g - V_l)$
Interfacial area [41]	$A_i = \frac{6\alpha_g (1-\alpha_g)}{d_b}$
Schiller-Naumann drag equation [42]	$C_D = \begin{cases} \frac{24(1+0.15\Re_b^{0.687})}{\Re_b} & \Re_b \le 1000 \\ 0.44 & \Re_b > 1000 \end{cases}$

The setup dimensions of the reactor in this paper are based on the Helium-Water bubble column reactor studied by Abdulrahman [26-28], but the material properties have been adjusted to match those of oxygen and Cupreous Chloride. According to Abdulrahman's property comparison [24-25], the O2-CuCl system and the Helium-Water (He-H_2O) systems are similar. To ensure comparability, the superficial gas velocity of the O2-CuCl system is fine-tuned to maintain the same Reynolds number as that of the He-H_2O system. The reactor used in this study has a cylindrical shape, with a diameter of 21.6 cm and a height of 91.5 cm. The gas is introduced into the bubble column reactor through a six-arm sparger-type gas distributor, with each arm featuring 12 orifices of 0.3 cm diameter, totalling 72 holes.

In this study, the turbulence model employed is the Reynolds-Averaged Navier-Stokes (RANS) models, such as k-ε and k-ω, which are known for being the least computationally expensive approaches for estimating complex turbulent flows. These models are capable of simulating a broad variety of turbulent flows and heat transfer processes with an acceptable level of accuracy. Specifically, the RNG k-ε model is chosen for its enhanced accuracy and reliability over a larger range of flows compared to the standard k-ε model. This model is particularly suitable for simulating churn turbulent flow, which is the focus of this study. The k-ε sub-model utilized is the dispersed turbulence model, selected due to the significant difference in phase densities between liquid and gas and the low gas phase concentrations. Additionally, this turbulence model is less computationally expensive than the per-phase turbulence model. The standard wall function is applied for wall boundary conditions, as it is commonly used in industries and provides reasonable results for a variety of wall-bounded flows.

For the setup and boundary conditions in ANSYS Fluent, the study uses ANSYS 2021 R1 to simulate the 3D Bubble Column Reactor (BCR). A hexahedron mesh is employed for the Bubble Column Reactor (BCR), and mesh independence is conducted to ensure that the largest mesh size is selected to minimize computational expenses while achieving acceptable results. The final mesh comprises 26,825 nodes and 24,396 elements, leading to a 3% difference in the gas holdup when using finer meshes. The simulated SBCR has three boundaries: the inlet, outlet, and wall conditions. The single inlet boundary condition is set with a specified superficial gas velocity and is assumed to have a gas holdup of 1. The outlet pressure is set to atmospheric pressure, and a no-slip condition is applied to the walls of the reactor for both phases. The turbulent kinetic energy and dissipation rate at the inlet and outlet are specified using 5,000 iterations, as they are challenging to estimate for turbulent models.

3. Results

3.1. Gas holdup versus superficial gas velocity

Figure 1 shows the three-dimensional curves of the gas holdup α_g versus the U_{gs} and the H. Figure 2 depicts the effect of varying the U_{gs} (0.0283, 0.0567, 0.085 m/s) on the average gas holdup while varying the H *(45, 55, 65cm)* for an O_2- CuCl system. Figure 3 shows the contours of the cut sections of the BCR taken in the centre of the XY, and ZY planes. Additional cut sections are taken at various heights on the ZX plane within the reactor at heights 10, 20 and 30 cm from the base of the reactor to allow for a more detailed contour of α_g. It is clear from the contours that the gas holdup is not symmetrical on the XY, ZY and the ZX planes demonstrating that the behaviour of the gas holdup is strongly three dimensional. From the figures, it can be observed that the physical behaviour of α_g with U_{gs} is the same for that of Helium-Water system, in which α_g increases by increasing U_{gs}.

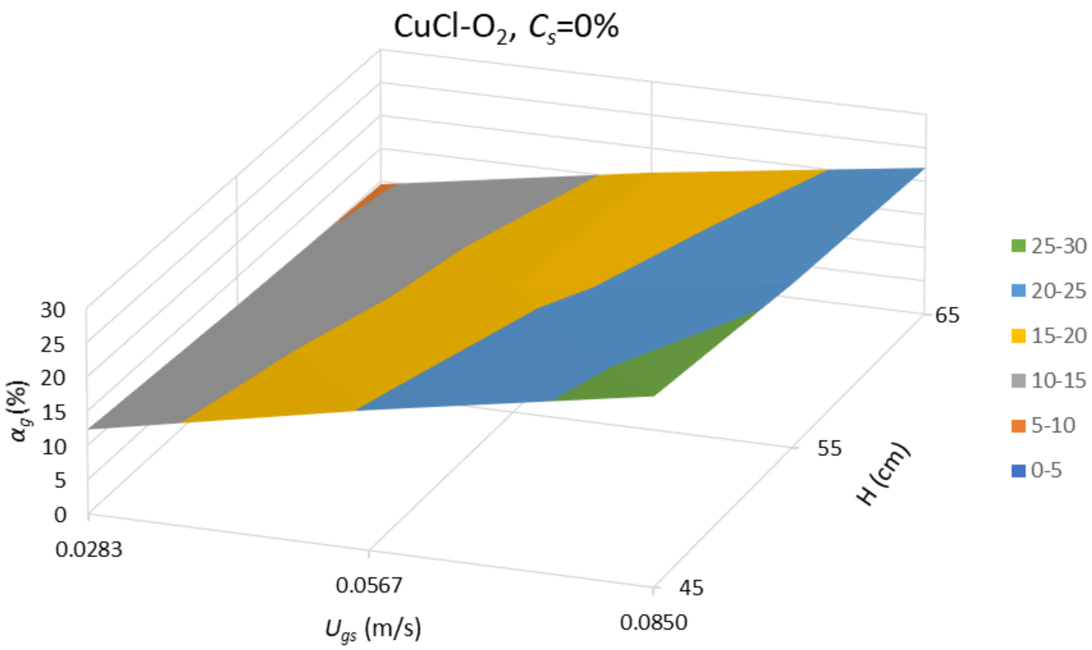

Fig. 1 Average Gas Holdup Versus Superficial Gas Velocity and Static Liquid Height of CuCl-O_2 system.

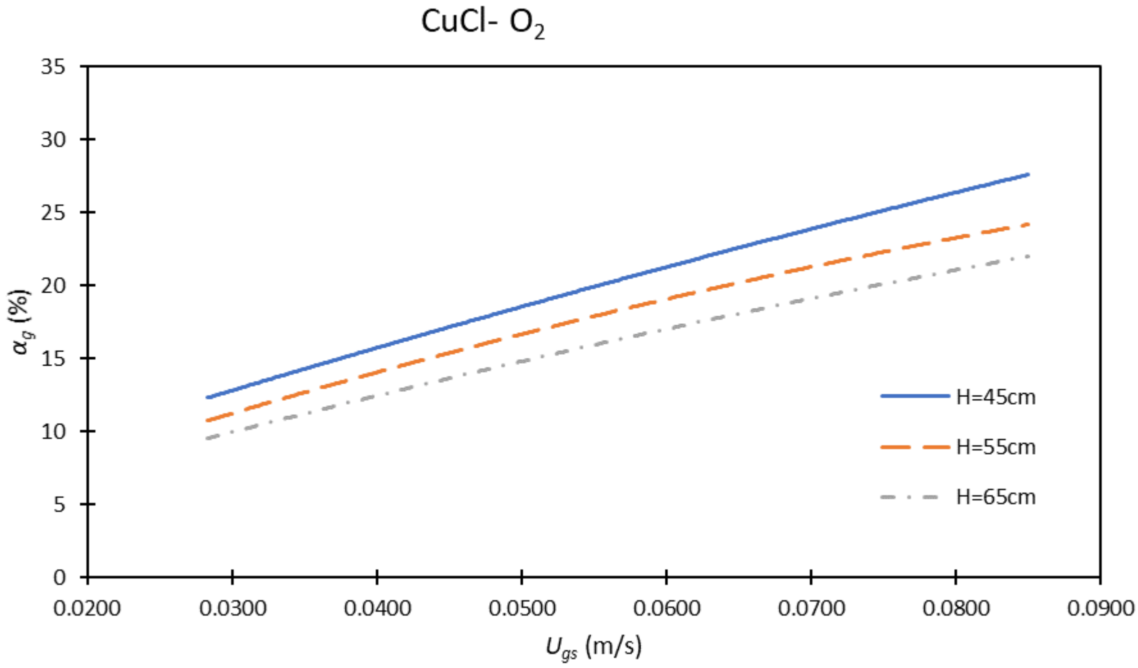

Fig. 2 Average Gas Holdup Versus Superficial Gas Velocity of CuCl- O_2 system.

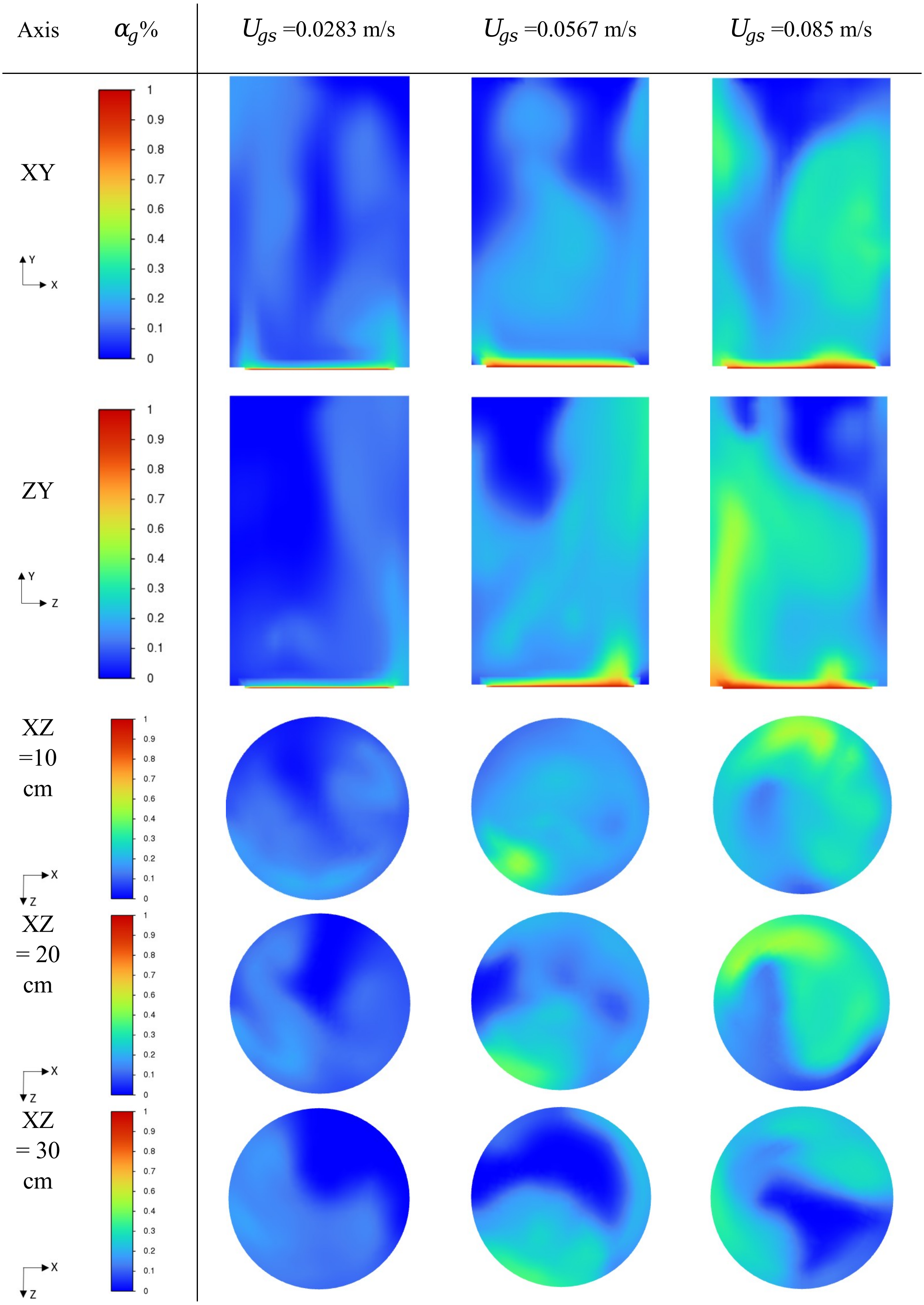

Fig. 3 Oxygen-Cupreous Chloride Gas Holdup Contours for H=45cm.

3.2. Comparison of the 3D Water -Helium CFD system and the 3D Couperus Chloride-Oxygen CFD system

Table 2 shows the comparisons in the results of the hydrodynamics dimensionless groups between the actual materials (CuCl and O_2) and the simulated materials (He and H_2O) according to the study of Abdulrahman [24-25]. The highest error in the dimensionless groups is coming from the density ratio of gas to liquid which is equal to 11.311%. Table 3 shows the values of the gas holdup calculated for both the actual and simulated materials with the percentage of errors created from the difference between them. It can be seen that the highest percentage error is 29.9%. Also, it can be seen that the values of the gas holdup in the actual materials are usually underpredicted those in the simulated materials. The superficial gas velocities of the actual materials were adjusted to have the similar effects of those in the simulated materials. The high percent error can be explained by the accumulation of the percent errors produced from each of the hydrodynamic dimensionless parameters as shown in Table 2, and also due to the complexity of the multiphase system in 3D. The 3D CuCl-O_2 simulation was able to successfully simulate the trends and behaviour within the SBCR.

Table 2 Dimensionless groups of actual and experimental material percent error [24-25].

Dimensionless Group	Actual Material	Experimental Materials	Error%
$\frac{\rho_g}{\rho_l}$	0.000121	0.000135	11.311
$\frac{\mu_g}{\mu_l}$	0.021756	0.023	6.908
$\frac{\Re_l^2}{We_l}$	76473868 (D_R=1m)	76085070 (D_R=1m)	0.508

Table 3 Comparison between the Water-Helium system and Cupreous Chloride- Oxygen superficial gas velocity and gas holdup with the calculated percent error for static liquid height of 45 cm.

Water-Helium		**Cupreous Chloride-Oxygen**		**Percent Error**
U_{gs} **(m/s)**	α_g**(%)**	U_{gs} **(m/s)**	α_g**(%)**	**(%)**
0.05	16.0	**0.0283**	12.3	29.9
0.1	24.4	**0.0576**	20.4	19.6
0.15	31.3	**0.085**	27.6	13.3

In Fig. 4, it can be noticed that the behaviour of the gas holdup with the superficial gas velocity and static liquid height is similar in both systems of H_2-H_2O and O_2-CuCl, where the gas holdup increases with increasing the superficial gas velocity and decreases with increasing the static liquid height. At lower velocities the gas holdup values were more closely clustered at different static liquid heights. However, as the superficial gas velocity increased the gas holdup values were more separated at different heights.

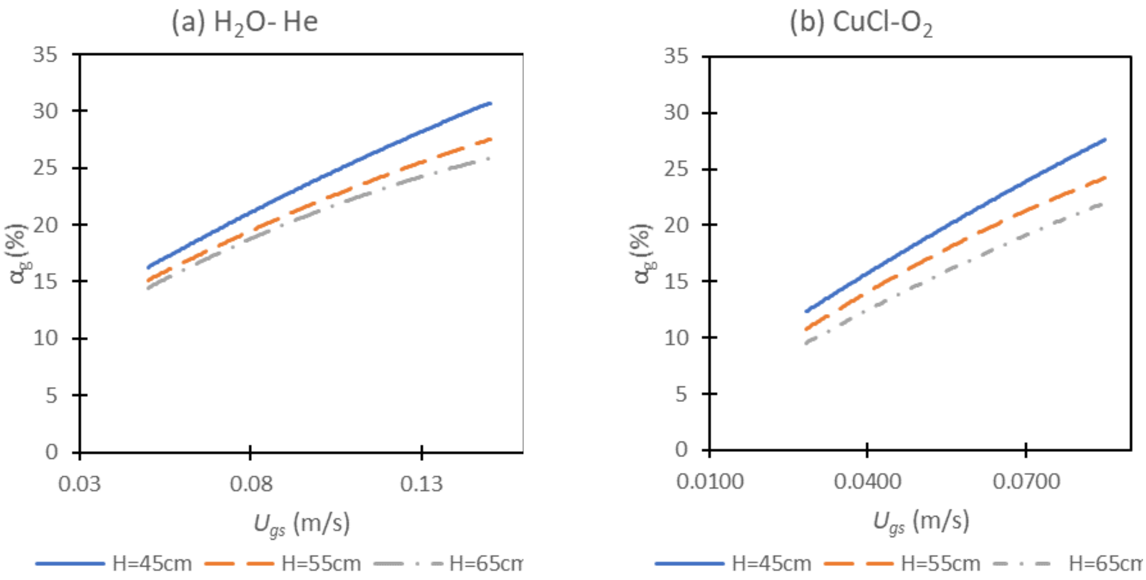

Fig.4 Comparison between the effects of superficial gas velocity on gas holdup for different static liquid heights (a) Water-Helium data, (b) Cupreous chloride-oxygen data.

4. Conclusions

The aim of this study is to validate the use of substitute materials, specifically helium gas and liquid water, in place of the actual materials, namely oxygen gas and molten CuCl, within the oxygen bubble column reactor for the thermochemical copper-chlorine (Cu-Cl) cycle of hydrogen production. The validation is carried out through 3D computational fluid dynamics (CFD) simulations using ANSYS Fluent software, focusing on the CuCl-O_2 system at varying superficial gas velocities. It is concluded that the patterns of gas holdup as a function of superficial gas velocity are consistent across both 3D CFD simulations. Also, for the 3D CFD results of the O_2-CuCl system, the gas holdup tends to be underpredicted compared to the 3D CFD results of the He-H_2O system.

List of Symbols

A_i	Interfacial area concentration
C	Specific heat
C_D	Drag coefficient
d_b	Bubble diameter
g	Gravitational acceleration
H	Height
Mi	Total interfacial forces between the phases
P	Phase pressure
$Q_{g,l}$	Intensity of heat exchange between the gas and liquid phases
Re	Reynolds number
T	Temperature
v	Velocity field
V_g	Volumes of gas
V_l	Volumes of liquid
U_{gs}	Superficial gas velocity
α_g	Gas holdup
μ_{eff}	Effective viscosity
μ_g	Dynamic viscosity gas
μ_l	Dynamic viscosity liquid
ρ_g	Density, gas
ρ_l	Density, liquid
$\bar{\bar{\tau}}:\nabla v$	Viscous stress tensor contracted with the velocity gradient

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