The influence of the initial gas distribution on the dynamics of a three-phase fluidized bed reactor: Non-ideal gas condition

EDVCATIO PHYSICORVM
QVO NON ASCENDAM?

ISSN 1870-9095

L.P. Olivo-Arias[1], L.G. Araujo[2]
[1]Instituto Politécnico Nacional, Centro de Investigación en Ciencia Aplicada y Tecnología Avanzada.
Legaria No. 694 Colonia Irrigación, C.P. 11500 México D.F., México
[2]Instituto de Pesquisas Energéticas e Nucleares, IPEN-CNEN/SP
Av. Prof. Lineu Prestes, 2242-Butantã, São Paulo, SP CEP 05508-000, Brazil

E-mail: lolivoa1500@alumno.ipn.mx

(Recibido 9 December 2020, accepted 27 February 2021)

Resumen

La evolución hidrodinámica de un reactor de lecho fluidizado líquido-gas-sólido tridimensional (3D) se estudió mediante simulaciones de dinámica de fluidos computacional (CFD), y los resultados se compararon con datos experimentales anteriores. Las interacciones gas-sólido y líquido-sólido se calcularon utilizando el modelo de Euler-Euler, incorporando la teoría cinética para las fases sólidas. Los coeficientes de intercambio de momento para las interacciones fluido-sólido se calcularon utilizando el modelo de arrastre Gidaspow, y las interacciones fluido-fluido, utilizando el modelo de Schiller-Naumann. La fracción de volumen de gas prevista estaba de acuerdo con el modelo de Kumar y mostró un mejor comportamiento con el uso de una discretización de orden superior. Durante este estudio se empleó la correlación termodinámica de Peng Robinson para determinar las propiedades de los materiales a condiciones de alta severidad. Los resultados demostraron una consistente distribución de las fases, fue bastante uniforme y hubo una expansión razonable del lecho cuando se estableció una inyección de gas como condición inicial.

Palabras de claves: Dinámica computacional de fluidos, reactor de lecho fluidizado trifásico, condición de gas no ideal y modelo hidrodinámico.

Abstract

The hydrodynamic evolution of a three-dimensional (3D) liquid-gas-solid fluidized bed reactor was studied using computational fluid dynamics (CFD) simulations, and the results were compared with previous experimental data. The gas-solid and liquid-solid interactions were calculated using the Euler-Euler model, incorporating the kinetic theory for the solid phase. The momentum exchange coefficients for the fluid-solid interactions were calculated using the Gidaspow drag model, and the fluid-fluid interactions by using the Schiller-Naumann model. The predicted gas volume fraction agreed to the Kumar model and showed better performance with the use of higher-order discretization. Furthermore, the Peng Robinson thermodynamic correlation was used to determine the properties of the materials under high severity conditions. The results showed a consistent distribution of the phases, it was quite uniform and there was a reasonable expansion of the bed when gas injection was established as an initial condition.

Keywords: Computational Fluid Dynamics, Three-phase fluidized bed reactor, Non-ideal gas condition, and hydrodynamic model.

I. INTRODUCTION

The volume fraction of phases is an important transport property of three-phase fluidized beds and one of the main parameters to evaluate the hydrodynamic behavior of this type of system.

This behavior reflects the complex and individual interactions of the phases, such as fluid-fluid or fluid-solid momentum exchange during the bed expansion process. In this work, the volume fraction of the gas phase evolution is evaluated, under non-ideal gas consideration. Therefore, it must define what is the volume fraction of gas. This volume fraction is related to the gas flow rate vs. the total volume and the amount of gas present in the column at a given time. It is also one of the key variables to determine how intense the contact between phases is (e.g. gas-liquid or gas-solid) so that it may reach a stationary state or may vary periodically. Together with the size and form variables, the actual throughputs, feed distribution, and if there is packing or additional mixing, the values of the volume fraction determine the extent of the interfacial area, as well as the flow regimes. These, in turn, determine transport efficiency (heat & mass).

The modeling, simulation, design, and control of three-phase fluidized bed reactors ─ where the estimation of hydrodynamic parameters play an important role ─ are often

limited by the lack of reliable measurement techniques. Such techniques are essential to obtain laboratory-scale data to validate with [1] and develop correlations to study the hydrodynamic behavior of industrial reactors. Therefore, researchers employ tools such as Computational Fluid Dynamics (CFD) to provide design information. This information is necessary to describe this type of variables concerning time and space, which can apply to multiphase systems.

Many simple studies evaluate the ideal gas conditions while using different correlations and comparing theoretical methods. This study aims to validate the experimental data from [1] at atmospheric and severe conditions using a non-ideal gas state. The combination of these models at different superficial gas velocities, while incorporating different conditions of 3D meshing and discretization schemes makes possible the definition of influences in an aspect such as the gas and solid volume fraction. As previously mentioned, the CFD is the most successful tool to determine these kinds of hydrodynamic parameters. To obtain an agreeable simulation, it is necessary to select reliable physics models to calculate the converged solution.

The flow field predicted by CFD simulations showed fair agreement with the experimental results. The gas volume fraction profile predicted by the researchers matches closely with the experimental data reported by [2], at the center region of the column, and slightly varies at the wall region of the column. This may be due to the effect of the wall on the gas volume fraction. The researchers conclude that the gas volume fraction profile decreases when the radial position increases.

A 3D transient model reported results developed to simulate the local hydrodynamics of a three-phase fluidized bed reactor (liquid-gas-solid) using the CFD method. The CFD simulation predictions are compared with the experimental data reported by other authors [3].

Some featured works for a non-bubbling system will be mentioned in this research, [4] and [5]. CFD simulations of gas-liquid-solid fluidized beds have been performed in a fully three-dimensional, unsteady multiple-Euler framework through the commercial software FLUENT. The simulation results were compared with experimental data obtained from laboratory scale three-phase fluidized beds. The significance of implementing accurate numerical schemes, as well as the choice of available k–e turbulence models (standard, RNG, realizable), solid wall boundary conditions, and granular temperature models were investigated. The results indicate that to minimize numerical diffusion artifacts and to enable valid discussions on the choice of physical models, third-order numerical schemes need to be implemented. The best prediction of flow characteristics was obtained with a laminar model formulation accounting for the solid phase viscosity and the molecular viscosities of the two fluids.

Additionally, a robust model, which uses the Reilly correlation, has been proposed; this correlation covers a wide range of liquid, gas, and particles properties and flow conditions to evaluate the gas volume fraction and incorporated it for a non-ideal gas model, employing different superficial gas velocities, which are operating conditions that are used in real fluidization process.

II. HYDRODYNAMIC MODEL

The governing equations of the two-fluid model can be derived by conditional ensemble averaging of the local instant conservation equations of multi-phase). This results in two sets of mass, momentum, and energy balances. In the present case, the flow is assumed to be isothermal, hence the energy balances are not needed. Furthermore, there is no interfacial mass transfer between the air and water phases.
It is available on Ansys 18.2 platform.

A. Schiller-Naumann drag model

This model is used for modeling of drag between fluid phases in multiphase flow. The drag function $f_{D,lg}$ is given as:

$$f_{lg} = \frac{C_D Re}{24}, \tag{1}$$

$f_{D,lg}$ stands for the drag force, $C_{D,lg}$ is the drag coefficient between the liquid and gas phases the drag coefficient, and Rel is the liquid Reynolds number. The value of the coefficient $C_{D,lg}$ can be calculated (for a given Re range), as follows:

$$C_{D,lg} = \frac{24(1 + 0.15\mathrm{Re}^{0.687})}{\mathrm{Re}}, \quad \mathrm{Re} \leq 1000, \qquad C_{D,lg} = 0.44 \quad \mathrm{Re} > 1000, \tag{2}$$

Morsi and Alexander described the drag coefficient for smooth spherical particles as in the Schiller and Naumann model, but with eight different correlations over eight successive ranges of Re. In this model, the Re domain is divided by eight successive Re ranges using adjusting eight corresponding corrections. This is done to minimize the deviation between the experimental data and the adjusted correlation.

$$C_{D,lg} = a_1 + \frac{a_2}{\mathrm{Re}} + \frac{a_3}{\mathrm{Re}^2}. \tag{3}$$

For $\mathrm{Re} \geq 10000$ the corresponding values for a_1, a_2 and a_3 coefficients are 0.5191, 16662.5, and 5416700, respectively [6].
As aforesaid, the transport equations were solved numerically in the turbulent flow regime. Therefore, it is necessary to model the turbulent energy exchange and dissipation. To do this, the k-epsilon model and the wall function standard took into consideration [1, 7].

Cubic equations of state [8] are a convenient means for predicting real fluid behavior. In this research, the Peng Robinson correlation will be used and the behavior of real gas and the influence on gas volume fraction will be analyzed.

B. Selected Gas volume fraction Correlations

For the gas phase [9], this correlation was considered for the estimation of α(g), since is appropriate for a wide range of gas velocities of the physical properties of both the gas and the liquid phases used.

$$\alpha_g = 296{u_g}^{0.44}{\rho_l}^{-0.98}{\sigma_l}^{-0.16}{\rho_g}^{0.19} + 0.009, \quad (4)$$

$$\alpha_g = 0.5056{u_g}^{0.47}\left(\frac{0.072}{\sigma_l}\right)^{2/3}\left(\frac{0.001}{\mu_l}\right)^{0.05}. \quad (5)$$

Where ρ_j is the mass density of the phase j = (l), (g), superficial gas velocity u_g is the gas and liquid surface tension σ_l and μ_l is the dynamic liquid viscosity.

Hikita proposed the model given in [9], employed for a gas volume fraction correlation, covering a wide range of fluid properties. These fluids were all aqueous mixtures or were highly polar organic liquids.

III. NUMERICAL METHODOLOGY

The three-dimensional (3D) computational domain was discretized by hexahedral cells as follows: 41,800 cells for the coarse mesh, and 100,000 cells for the fine mesh, with cell boundary layers close to the walls where the velocity gradients increased, and a finer resolution was necessary. In a similar study performed by the Gidaspow drag model and k-epsilon Standard turbulence model, the maximum cells of these dimensions were found to be adequate to achieve mesh-independent results. The solution was initialized from all zones as depicted in Fig. 1.

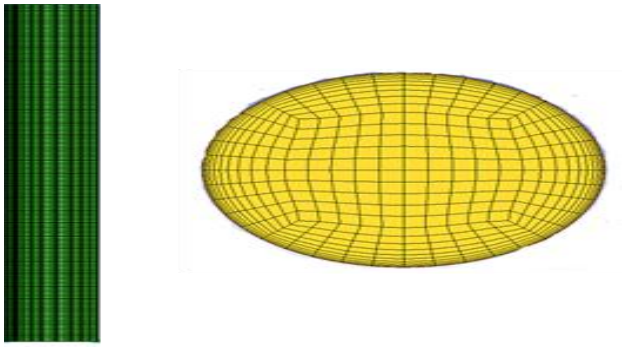

FIGURE 1. Computational domain meshing.

IV. RESULTS AND DISCUSSION

Non-Ideal Gas Consideration

The simulation of the gas volume fraction in a three-phase fluidized bed reactor at high severity conditions of pressure, where the superficial gas and liquid velocities are kept constant, has a strong effect on the hydrodynamic parameters. The results (Figures 2 and 3) show how they were affected during the bed expansion. This condition was necessary to establish how a fluidized bed reactor operates in the industrial field.

The equation of state of the non-ideal gases for CFD simulations of hydrogen at 1MPa includes appropriate real gas relations based on the Peng-Robinson correlation. Table 1 shows the physical-chemical properties employed in this investigation.

TABLE I. Physical properties of Hydrogen, by Peng Robinson correlation.

Properties	*Hydrogen @ 1MPa*
Density ($kg \cdot m^{-3}$)	0.3722
Heat Capacity ($J \cdot kg^{-1} \cdot K^{-1}$)	14570
Viscosity ($kg \cdot m^{-1} \cdot s^{-1}$)	1.533E-5
Enthalpy ($kJ \cdot kg^{-1} \cdot mol^{-1}$)	5044
Thermal Conductivity ($W \cdot m^{-1} \cdot K^{-1}$)	0.3104

The axial gas velocity showed the highest concentration of the phase from the bottom to the middle of the catalyst bed. Under severe conditions, a better distribution of hydrogen was reached. However, the flow was observed to be too close to the wall in an atmospheric state. The high pressure inside the system provoked this condition (Fig. 2).

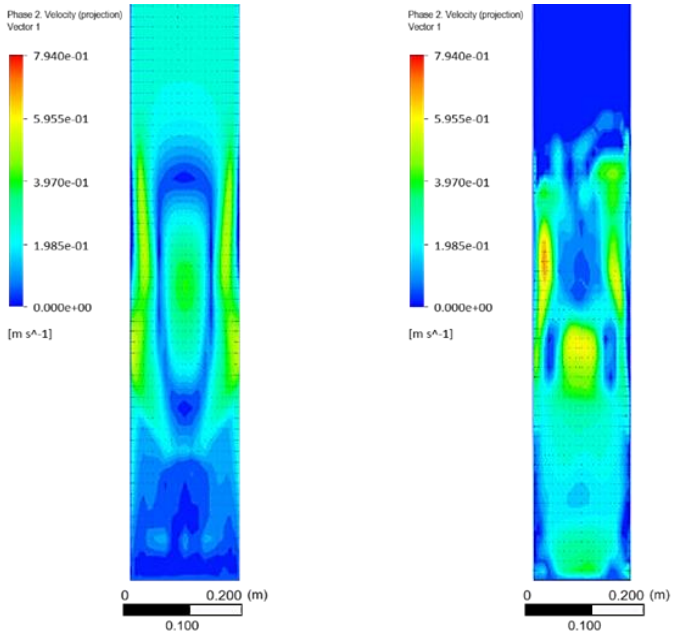

FIGURE 2. Contour of gas axial velocity 0.05 $m \cdot s^{-1}$ at atmospheric (left) and severe (right) pressure until 25 s of simulation. Simulations with a three-phase system were performed up to 25 s on the same solid concentrations at 1 MPa and 298 K. These particles were kept in suspension by hydrogen injections from the bottom of the column and mixing with liquid and solid phases.

The contours of the fluid-solid phase during the bed expansion process, at severe conditions, are shown. The

Gidaspow model was affected during the simulation at high pressure providing a non-uniform distribution. The highest concentration of solid had settled in the center of the domain, with part of the gas expanding to the outside zone of the catalyst bed (Fig 3).

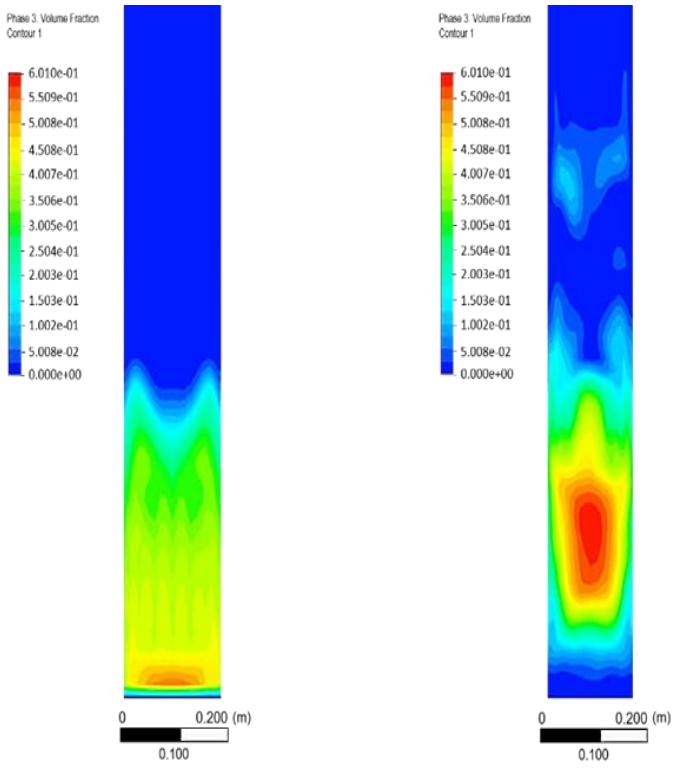

FIGURE 3. Contour of solid volume fraction at atmospheric (left) and severe (right) pressure Gidaspow drag model, for a simulation time of 25 s.

Figures 4 and 5 show the calculation of the gas distribution along the reactor using the Morsi-Alexander and Shiller-Newmann fluid-fluid interaction drag models (using the value of 0.05 m·s^{-1} for the superficial gas velocity).

There was a significant bed expansion during the hydrogen-water interaction from the initiation to the end of the simulation (25 s), reaching a quasi-steady state for Shiller Newmann almost 30% and for Morsi-Alexander 25%. This indicates that despite using severe pressure conditions for the hydrogen and altering the fluidized bed system, significant results can be obtained in the same way, as in the case of an atmospheric system. This is a strong suggestion that the selection of the real gas by Peng Robinson correlation was appropriate to obtain vital information of gas distribution within a height from zero to 0.7 m, which would generate stability on the interaction of the phases.

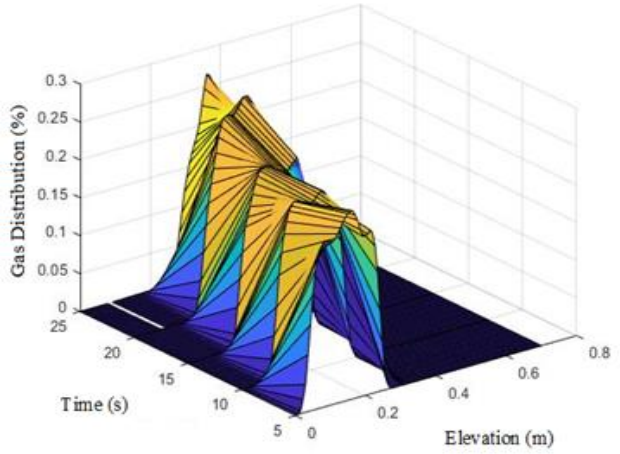

FIGURE 4. Gas Distribution employing Shiller-Naumann drag model at a severe condition of pressure

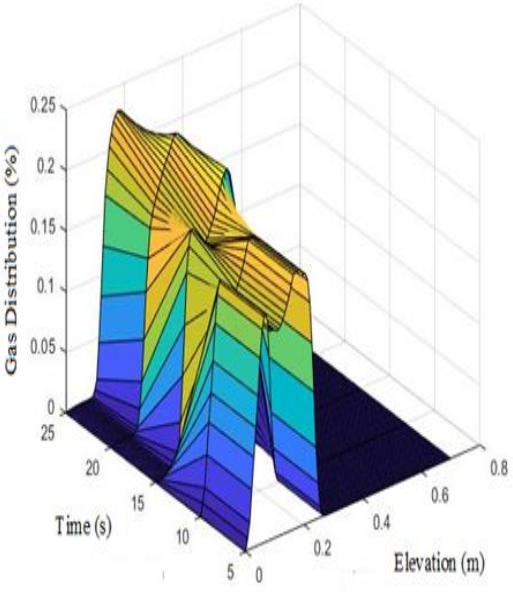

FIGURE 5. Gas Distribution employing Morsi-Alexander drag model at a severe condition of pressure

The aim in this section is to improve results for the gas volume fraction employing two correlations from the changes of the superficial gas velocities. In Figure 6, the proposed model by Hikita and Reilly is compared, from the estimation of superficial gas velocity at u_g = 0.032 m·s^{-1} and u_l = 0.02 m·s^{-1}. The Hikita results, obtained in this study for air and water, are acceptable, but they fail to give very adequate prediction (within 20%) of the measured gas volume fraction in Reilly. It may be reasonable to expect, therefore, that correlations that apply well in aqueous systems might show a more accurate prediction of gas volume fraction (more than 50%).

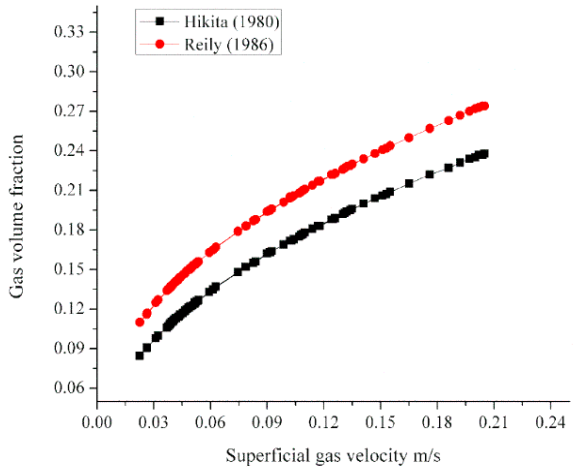

FIGURE 6. Comparison between of Hikita and Reilly's correlations of Gas volume fraction vs superficial gas velocity u_g = 0.032 m·s^{-1} and u_l = 0.02 m·s^{-1}.

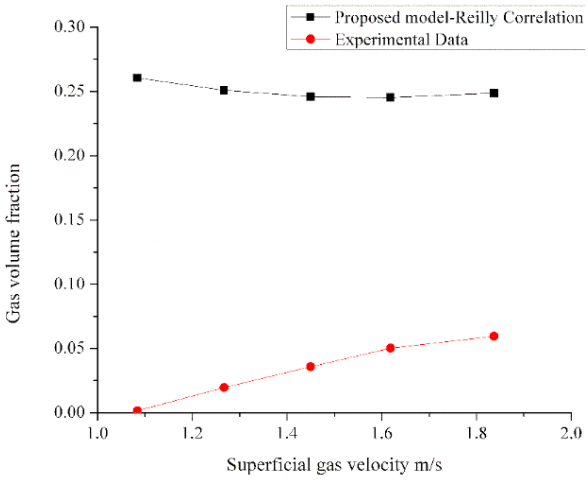

FIGURE 7. Comparison between experimental data and Reilly's correlation of Gas volume fraction vs Superficial gas velocity at u_l 0.06 m·s^{-1}

The comparison between experimental data and the proposed model for gas volume fraction vs superficial gas velocity at u_l = 0.06 m·s^{-1} is represented in Figure 7, by employing the same boundary conditions. It shows an increased value of the gas volume fraction when the Reilly correlation is incorporated, which causes a great impact on the bed expansion when the system operates at 1 MPa. For such systems, it has been found that the bed expansion increases with the superficial liquid velocity. Additionally, by introducing the gas into a liquid-solid system, the bed can expand or contract, depending on the properties of the solid and liquid velocity. Similar behaviors have been reported for a fluidized bed reactor operated at high pressures.

It showed a tendency towards expansion with the introduction of the gas phase for all pressure conditions, reporting similar results for 2.1 and 3.0 mm glass beads particles at low superficial liquid velocities.

A phenomenological model was selected to determine hydrodynamic parameters in the fluidized bed system. For that, we employed Reilly's correlation for an organic-hydrogen-catalyst system and water-catalyst-hydrogen, with a wide range of gas velocities and particle diameter. The objective was to obtain the gas phase volume fraction during the fluidization process. Some results, obtained from the simulations, are represented and plotted between the gas volume fraction versus the superficial gas velocities in different stages.

In Figures 8, 9 and 10, the gas volume fraction was evaluated. This can bring to the conclusion that a relationship between two hydrodynamic parameters exists for each different boundary conditions selected and the value of the volume fraction is almost the same as predicted by the correlation.

As much as the superficial gas velocity increases, the volume fraction will obtain a significant increase which will lead to an increase in fluidized bed expansion.

An increase in pressure in the system immediately increases the number of collisions between the phases, which influences a lot the hydrodynamics parameters. Pressure has also been found to have a major influence during gas-solid interactions. The gas volume fraction had a uniform distribution along the reactor presenting an increase of high superficial gas velocity and a good distribution of gas along the reactor.

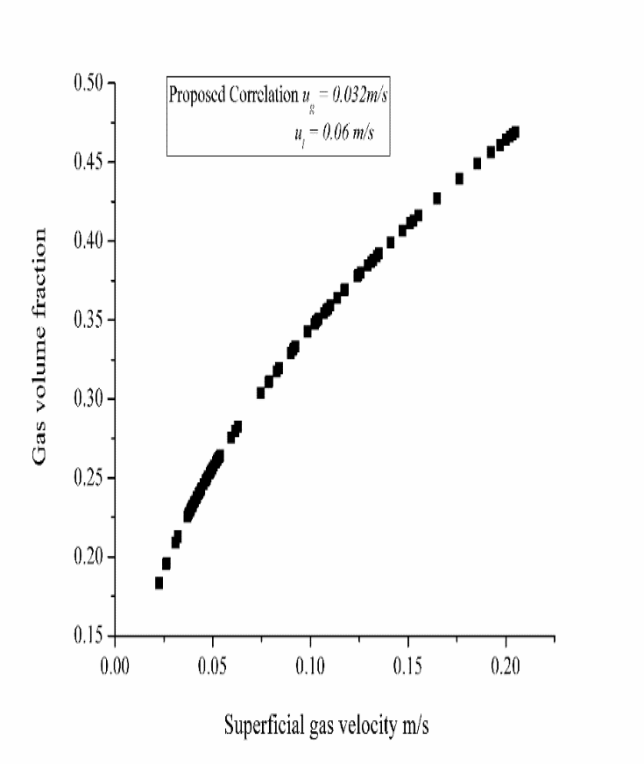

FIGURE 8. Gas volume fraction vs superficial gas velocity u_g = 0.032 m·s^{-1} and u_l = 0.06 m·s^{-1}.

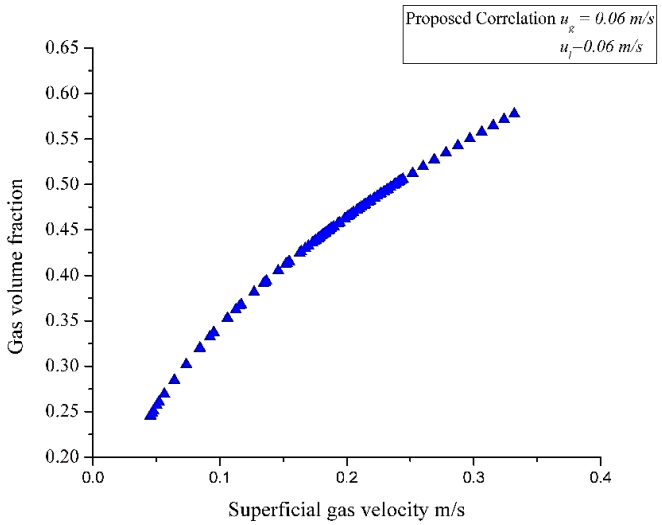

FIGURE 9. Gas volume fraction vs superficial gas velocity at u_g = 0.06 m·s^{-1} and u_l = 0.06 m·s^{-1}

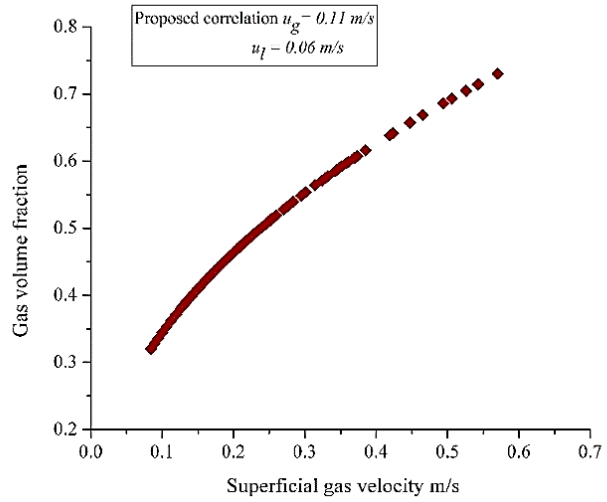

FIGURE 10. Gas volume fraction vs superficial gas velocity at u_g = 0.11 m·s^{-1} and u_l = 0.06 m·s^{-1}

V. CONCLUSIONES

The momentum interchange was analyzed by evolution and distribution along the catalytic bed, employing the Shiller-Newmann correlation. This is the most suitable model to evaluate the fluidization process.

Simulation results indicated a uniform distribution of the solid phase in the cross-section in 25 s of real flow time to allow a fluidization process. The contour of the solid volume fraction showed an ascend at the center of the bed and a descend near the walls. This represents an effect on operation variables at atmospheric conditions.

The superficial gas velocity and material properties play an important role in the hydrodynamic parameters of liquid-gas-solid fluidized bed reactors. The predicted values from the present CFD model match the experimental results found in the literature. The key for a successful simulation is the choice of a correct model i.e. the Gidaspow drag force in liquid-gas-solid fluidized beds. The Gidaspow model provides the closest results to the experimental data among all models.

Among the considerations taken into account during the hydrodynamic study in a three-phase fluidized bed reactor, a non-ideal gas consideration, it can be concluded that the parameters changed when applying severe conditions for higher pressure, the gas volume fraction showed an irregular behavior during the interaction between phases, unlike a system operated at atmospheric conditions, where variables had better control and fewer deviations from the final results during the simulation process were observed.

By incorporating a more robust model at different superficial gas velocities, a good agreement was obtained with what was initially predicted, during the analysis under real gas conditions. It showed significant results, with a theoretical proposal based on a correlation for the volume fraction of the gas phase.

REFERENCES

[1] Kumar, A., *CFD modeling of gas–liquid–solid fluidized bed,* (B. Tech, NIT, National Institute of Technology, Rourkela, India, 2009), pp. 1 – 57.

[2] Krishna, R., Ellenberger, J., *Gas holdup in bubble column reactors operating in the churn-turbulent flow regime,* AIChE Journal **42**, 2627-2634 (1996).

[3] Akita, K., Yoshida, F., *Gas Holdup and Volumetric Mass Transfer Coefficient in Bubble Columns*, Effects of Liquid Properties. Industrial & Engineering Chemistry Process Design and Development **12**, 76-80 (1973).

[4] Zhang, K., Brandani, S., Bi, J., & Jiang, J., *CFD simulation of fluidization quality in the three-dimensional fluidized bed,* Progress in Natural Science **18**, 729-733 (2008).

[5] Hamidpour, M., Chen, J., Larachi, F., *CFD study on hydrodynamics in three-phase fluidized beds-Application of turbulence models and experimental validation*, Chemical Engineering Science **78**, 167 – 180 (2012).

[6] Du, W., Bao, X., Xu, J., & Wei, W., *Computational fluid dynamics (CFD) modeling of spouted bed: Assessment of drag coefficient correlations,* Chemical Engineering Science **61**, 1401-1420 (2006).

[7] Panneerselvam, R., Savithri, S., & Surender, G. D., *CFD simulation of hydrodynamics of gas–liquid–solid fluidised bed reactor,* Chemical Engineering Science **64**, 1119-1135 (2009).

[8] Smith, J. M., Van Ness, H. C., Abbott, M. M., & García, C. R., *Introducción a la termodinámica en ingeniería químic*a, Quinta Edición, (McGraw-Hill, México, 1989).

[9] Reilly, I. G., Scott, D. S, De Bruijn, T. J. W., Jain, A., Piskorz, J., *A Correlation for Gas Holdup in Turbulent Coalescing Bubble Columns*, Can. J. Chem. Eng. **64**, 705-718 (2018).