gbell Learning function along with Fuzzy Mechanism in Prediction of Two-Phase Flow

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ABSTRACT: The integration of the computational fluid dynamics (CFD) and the adaptive network-based fuzzy inference system, known as ANFIS, is investigated for simulating the hydrodynamic in a bubble column reactor. The Eulerian–Eulerian two-phase model is employed as the CFD approach. For the ANFIS technique, a sensitivity analysis is done by varying the number of inputs and the number of membership functions (MFs). The x and z coordinates of the fluid location, the air velocity, and the pressure are considered as the inputs of the ANFIS, while the air vorticity is the output. The results revealed that the ANFIS with all four inputs and the MFs of five achieved the highest intelligence with the regression number close to 1. More specifically, gbell function in the learning framework is used to train all local computing nodes from solving Navier–Stokes equations. In the decision or prediction part, the fuzzy mechanism is used for the prediction of extra nodes that solve, which Navier–Stokes equations did not solve. The results show that the gbell function enables us to fully train all numerical points and also store data set in the frame of mathematical equations. Besides, this function responds well with the number of inputs and MFs for accurate prediction of reactor hydrodynamics. Additionally, a high number of MFs and input parameters influence the accuracy of the method during prediction. In the current study, gbell MF was studied to investigate its accuracy in the prediction of the two-phase flow. Also, different numbers of MFs were considered to investigate the level of accuracy and capability of prediction. ANFIS clustering methods, grid partition and fuzzy C-mean (FCM) clustering, are compared to see the ability of the method in prediction. To compare the accuracy of the ANFIS method with FCM clustering, the data were compared to the gaussmf function. The results showed that the method has high accuracy and that it could predict the flow pattern.

1. INTRODUCTION

Bubble columns have a wide range of applications as gas—liquid contactors or reactors in industries. Oxidation, chlorination, wastewater treatments, hydrogenation, and Fischer–Tropsch synthesis are the typical instances in this regard. Bubble columns possess numerous benefits, including easy manufacturing, geometrically simple, greater gas—liquid interfacial mass and heat transfer, lack of moving sections, cost-effective, and easy operation. Though a bubble column is still challenging, particularly, once scaling-up is required in terms of operating the present bubble columns since there is no complete comprehending of fluid mechanics within a bubble column. Two major CFD methods exist to predict the multiphase flows into the bubble column, including Eulerian–Lagrangian and Eulerian–Eulerian (EE) methods. EE is a practical than experimental approaches, improving our incomplete knowledge regarding the complex gas—liquid interaction happening into the reactors with the bubble column. Two major CFD methods exist to predict the multiphase flows into the bubble column, including Eulerian–Lagrangian and Eulerian–Eulerian (EE) methods. EE is a popular and proper option in industries for estimating bubble column hydrodynamics, such as efficiency and performance, owing to less computational work. The EE two-phase model was adopted as the CFD approach. The method is used in industries and academic

Received: July 4, 2020
Accepted: September 18, 2020
studies because of the low cost of its calculations. It can also provide an appropriate approximation of the gas flow in the liquid, or it can model huge bubble column reactors. The turbulence models could also be used in the EE method to study the turbulence characteristics of the flow. This method has very good capability in heterogeneous regime flows when the flow has turbulence behavior. It is also worth mentioning that the speed of predicting the flow increases when the EE is used beside Reynolds-averaged Navier–Stokes equations. Although the large eddy simulation methods have high accuracy, the time and cost of using them for predicting a flow are significantly higher.

Though the bubble dynamics and flow pattern are measured and estimated using numerous experimental, mathematical, and numerical techniques, some problems exist for complete prediction of the gas dynamics and liquid-flow pattern (break-up, bubble coalescence, shape, velocity, gas hold-up, and size) at every location of three-dimensional bubble columns on changing the operation circumstances, operation time, and flow regime. Computer capability and computation time are the main limitations of the computational methods to numerically simulate different operation circumstances and a large bubble column. Owing to these limitations, soft computing techniques were developed for estimating the bubble column hydrodynamics in different circumstances not experimented or simulated at each point of the bubble column.

To predict the behavior of the phenomena in real-life applications, numerous soft computing methods were proposed, including support vector machines, neural networks, adaptive neuro-fuzzy inference systems, and evolutionary algorithms in several studies. In recent years, data-driven and intelligent approaches are progressively famous for predicting fluid characteristics. Among them, machine learning approaches were reported for delivering higher performance based on robustness, lower computation power, and accuracy to deal with large data and uncertainties. The machine learning approaches are mainly identified as powerful algorithms to deliver a comprehension for the nonlinear association between parameters. Numerous surveys report the hybrid and ensemble models as the future trends in machine learning as a result of their enhanced algorithms for greater efficiency.

ANFIS (adaptive network-based fuzzy inference system) is among these techniques attracting the researchers as a result of its capability for learning multifaceted associations with usages indicated in several studies. The accuracy of the ANFIS approach can be changed by altering the prediction model structure. Moreover, it can be adapted based on the association complexity. Either experimental or simulation results can be used by the ANFIS technique as training data for learning the phenomena performance. Successful training of the ANFIS model needs a proper training data set.

Every phenomenon in the CFD could be created in training, including the phenomena which have heat or mass transfer. However, before starting the training, the researchers need to start the analysis by using the experimental study or the CFD method, and after that, the data could be run in artificial intelligence (AI). The flow in heat and mass transfer can be predicted by using numerical and experimental studies, and it can be predicted and simulated by using AI. Also, flows with turbulence can be trained via AI; the turbulence characteristics, including kinetic energy, can be trained separately, and the behavior of the turbulence characteristics could be studied in the reactor. The neural network algorithm could train all CFD local nodes because of its high capability in learning. It could also provide the prediction stage of the data after the training process. Therefore, it could provide us with local prediction meaning that the method has a different capability compared to the typical regression methods. Also, the method could create nondiscrete predictions because of its high capability in training the large matrices and the high number of inputs.

The CFD method could address the two-phase flow, but for completing an optimization process, the AI method was used to reduce the repetition and examine the complexity of the flow inside the reactor. The two-phase flows have high capability in chemical engineering and wastewater treatment; when the two-phase flow or bubbly flow is created, the particle separation of waste particles takes place inside the tank. Optimization of such processes could provide suitable capability, particularly in industries. As the two-phase flows have widespread applications in chemical and petroleum engineering industries, the researchers consider the flow in numerical and AI simulations to provide suitable capability in industries. Therefore, researchers can optimize the processes, get the results faster, and reduce the cost of numerical studies.

Because numerical methods are time-consuming regarding the calculations, and sometimes researchers face limitations of the numerical methods, AI ability, besides the numerical methods, could train and predict the numerical data. When the optimization process is needed and researchers need to find out the answer very fast, the numerical method data that is trained via AI could provide the prediction. The local data set could be presented in the domain, which is similar to CFD. As different and particular number membership functions (MFs) could be used in the ANFIS algorithm, the researchers study the number of MFs in the study, and specifically, the $gbell$ MF was studied to create and measure its capability in prediction. The number of inputs and the number of MFs that were considered for the model could be the parameters that showed us the final accuracy of the $gbell$ MF. Also, by using different numbers of MFs and different numbers of inputs, the complexity of the flow could be studied with AI in the bubble column reactor. Therefore, these two significant parameters were considered to study the complexity and accuracy of the model.

In this study, the local calculation of reactor geometry was extensively used in the learning framework of neural networks. This local calculation was based on the numerical calculation of Navier Stokes equations throughout the domain of the bubble column reactor. More specifically, $gbell$ function was used in the training framework of neural networks, and after fully training the procedures, the fuzzy mechanism was involved in making decisions. Different parameters, such as the number of inputs and the number of MFs during the training method, were used for better accuracy of the method. For the training process, the $x$-direction and $z$-direction nodes were used, and the position of each of the CFD elements was trained with $x$-position and $z$-position. Also, air velocity and pressure were considered as the input parameters in training; therefore, four inputs were engaged in the training. Moreover, for investigating the accuracy and predictivity of the $gbell$ function, the training was completed with different number of input parameters. For the first time, we compared fuzzy C-means clustering (PCM) with ANFIS clustering grid partition method within the function of $gbell$, and the best condition
achieved for the ANFIS clustering grid partition system was compared to the FCM clustering to see how the ANFIS method could predict, especially, the bell function and create the pattern recognition.

2. CFD METHOD
The EE-based two-phase model was utilized to understand the liquid and gas interaction. In this trend, each phase was preserved as a continuum in the considered domain. Momentum transport and ensemble-averaged mass equations for each step are the basis for the framework of Eulerian modeling.\(^{32,37}\)

Continuity equation\(^{32,37}\)

\[
\frac{\partial}{\partial t} (\rho L \epsilon_X) + \nabla \cdot (\rho L \epsilon_X \mathbf{u}_L) = 0
\]

(1)

Momentum equation may be written as\(^{32,37}\)

\[
\frac{\partial}{\partial t} (\rho L \epsilon_X \mathbf{u}_L) + \nabla \cdot (\rho L \epsilon_X \mathbf{u}_L \mathbf{u}_L) = -\nabla (\epsilon_X \mathbf{p}_L) - \epsilon_X \mathbf{v}_L + \epsilon_X \rho_L g + M_{ik}
\]

(2)

The exact interfacial force within\(^{32,37}\)

\[
M_{iL} = -M_{iG} = M_{D,L} + M_{T,D,L}
\]

(3)

The exact explanation of interfacial force models employed in this work could be found in the study of Tabib et al.\(^{47}\)

Within the 20 previous years, \(k-\epsilon\) model was extensively utilized in explaining the flow outline in the bubble columns. Therefore, the results of using the model show that this model is low-cost and sufficiently reliable. This turbulence model was considered in our work for whole simulations. All turbulence model elements were the same as in the study of Pourtousi et al.\(^{26}\)

3. GEOMETRICAL ARRANGEMENT
In this work, a cylindrical shape bubble column reactor is utilized with the diameter and height of 0.288 and 2.6 m, respectively, similar to the study of Pfeifer and Becker.\(^{48}\) The superficial velocity of gas phase is \(5 \times 10^{-3}\) m/s at the ambient circumstance. For the complete data regarding the boundary circumstances such as outlet pressure and walls in this work, one can refer to the study of Pfeifer and Becker. To model a 3-D bubble column reactor, we model an industrial bubble column reactor, and for comparison and validation of the study, we used the obtained model from Pfeifer and Becker to have a CFD result that has its capacities in the industrial domain. This bubble column reactor has more than 2 m of length, and it could create different flows, including a homogeneous flow regime. A homogeneous regime was created in the study. This flow regime has spherical bubbles that are similar in size and shape. Therefore, the model used in this study is very similar to Pfeifer and Becker’s model, and the results were compared to their model. The inlet boundary situation is the same as Tabib et al.’s work.\(^{47,48}\)

A hexahedral grid-based structured grid is utilized all over the domain. The type of grid in this work is the same as the study of Laborde-Boutet et al.\(^{49}\)

The best mesh used in the system was nonstructured in the bubble column, which was created and repeated by a similar pattern in all of the levels of the bubble column. As this mesh has been used in different studies, the researchers of the study used this mesh to create a two-phase flow between the liquid and the gas in the column. One of the capabilities of this mesh is that creating the nonstructured mesh is easier than creating a structured mesh with a fixed pattern and design. Therefore, creating a nonstructured mesh needs less time, which is according to the size of the mesh, and could appear along with the bubble column reactor.

4. AI METHOD
ANFIS is a fuzzy inference structure for precise prediction of the nonlinear and complex behavior of the systems.\(^{50-52}\)

Different fuzzy reasoning can be selected among which the if-then rules proposed in ref 53 is used for ANFIS. In this study, the \(x\) and \(z\) coordinates of the fluid location, the air velocity, and the pressure were considered to attain the air vorticity as the output. The inputs were classified into different MF numbers in layer 1. The signals incoming from layer 1 were multiplied based on the AND rule as the second layer of the node function.\(^{14}\) For example, the function of the ith rule can be expressed as\(^{30}\)

\[
w_i = \mu_{Ai}(x)\mu_{Bi}(z)\mu_{Ci}(v)\mu_{Di}(p)
\]

(4)

in which \(w_i\) represents the out-coming signal of the second layer’s node and \(\mu_{Ai}\), \(\mu_{Bi}\), \(\mu_{Ci}\), and \(\mu_{Di}\) refer to the signals coming from implemented MFs on inputs, \(x\) coordinate, \(z\) coordinate, \(v\) velocity of air, \(p\) pressure, to the second layer’s node.

Relative amount of each rule’s firing strength is determined in the third layer, which is equal to each layer’s weight over the overall quantity of all rules’ firing strengths\(^{37}\)

\[
\bar{w}_i = \frac{w_i}{\sum w_i}
\]

(5)

in which \(\bar{w}_i\) is the normalized firing strengths. Layer four used the function of a consequence if-then rule presented by Sugeno and Takagi.\(^{53}\) In the prediction of the ANFIS stage, the fuzzy logic method was used. The high capability of fuzzy logic in the decision can lead to suitable capability in the prediction. The fuzzy logic method also could provide a better understanding of the kind of phenomenon and its complexity in a flow. It could also provide the relationship between the inputs and outputs, which enables the researchers to have a better understanding of the system.

Therefore, the node function is given as\(^{53}\)

\[
\bar{w}_f = \bar{w}(\delta x + p z + q y + r s + s)
\]

(6)

in which \(\delta\), \(p\), \(q\), \(r\), and \(s\) represent the parameters of the if-then rules and termed as the consequent parameters. The parameters are updated using a hybrid learning algorithm where the gradient descent technique was used to update MF parameters, and least-squares estimate technique was used to update the consequent parameters.\(^{26}\)

5. RESULTS AND DISCUSSION
The CFD method has been used to simulate a 3D bubble column reactor. The simulation results have been considered as inputs and output of the ANFIS AI. The parameters including \(x\) and \(z\) coordinates of the fluid location, the air velocity, and the pressure were the first, second, third, and fourth inputs of the ANFIS, respectively. In addition, the air vorticity was the output.

Seventy percent of the obtained data from the CFD was used in the training stage. The remained 30 percent plus 70
percent of the data were used in testing, evaluation, or validation of the study. Figure 1a shows the training of the system for the different number of MFs. Also, Figure 1b indicates the testing process for various number of MFs. The two figures do not reveal significant differences, and they show that when the number of MFs increases, the system sends intelligent signals. The training process was continued for three and four inputs. For the best prediction of ANFIS intelligence, the sensitivity analysis was done by varying the number of inputs and MFs. Figure 1a,b shows the ANFIS training and testing regression with two inputs (i.e., x and z) and the number of MFs of 2, 3, 4, and 5. Enhancing the number of MFs from 2 to 5, the regression number \( R \) increases from 0.68552 to 0.98955 for the training process. Similarly, by a little difference, \( R \) increases from 0.67288 to 0.98078 for the testing process.

Increasing the number of the inputs to three (i.e., x, z, and air velocity), more accurate prediction of the output is found. For example, according to Figure 2, for MFs equal to 2, the regression number increases significantly \( (R = 0.966) \). Increasing the number of MFs to 5, the regression number increases again \( (R = 0.998) \).

With the increment of the inputs to four (i.e., x, z, air velocity, and pressure), the most accurate prediction of the ANFIS is achieved (Figure 3). In this case, the \( R \)-value approaches 1. Besides raising MFs, no significant changes are seen in \( R \) values. Figure 4 shows a continuous prediction of the air vorticity by fitting surface to the predicted results. So, the air vorticity is evaluated by the ANFIS as a function of the inputs without using the CFD method. This, in turn, facilitates the calculation of the air vorticity and saves the computational efforts.

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**Figure 1.** (a) Training of ANFIS using two inputs and diversity of number of MFs. (b) Testing of ANFIS using two inputs and diversity of number of MFs.

**Figure 2.** (a) Training of ANFIS using three inputs and diversity of number of MFs. (b) Testing of ANFIS using three inputs and diversity of number of MFs.
Figure 5 makes a comparison between the air vorticity contour of the CFD prediction and that of the ANFIS one. The results reveal that the air vorticity contours predicted by both methods are similar in almost all locations. In order to study the \textit{gbell} function in the ANFIS method with grid partition clustering framework with \textit{gbell} function, we compared it with the FCM clustering gauss function, and we compared the two methods to study the capability of \textit{gbell} in...
prediction and its accuracy. As shown in Figure 6, in testing and training of the grid partition, clustering with \textit{gbell} function showed higher accuracy compared to FCM clustering. Figure 7 shows that the two methods were compared with each other in the pattern recognition method, and the CFD data were compared in different methods, which were FCM with grid partition clustering, \textit{gbell} MF, and FCM clustering \textit{gaussmf} function, to see how the methods could predict the flow pattern in a reactor. As shown in the figure, the air vorticity was considered as a function of total data, and the grid partition clustering with \textit{gbell} function showed high capability in prediction and flow pattern and could significantly match with the CFD data.

The FCM clustering method also has suitable capability, and generally, the results showed that the ANFIS technique possesses great capability in learning and prediction, and
when the gbell function was used, the method showed suitable behavior.

6. CONCLUSIONS

This study aimed to investigate the link of CFD and the ANFIS for the understanding and simulation of hydrodynamics in a bubble column reactor. The EE CFD model was used, and the bubble column was 3D. In the model, gbell MF was used. The model was changed with each of the inputs and the number of MFs to study the accuracy of gbell function. After achieving the accuracy of the model, it was compared with FCM clustering in order to compare the methods and their accuracy. The pattern recognition in the ANFIS method was also studied, and it was compared to FCM clustering. Although there are lots of other methods for simulating bubble columns, and a variety of machine learning algorithms exist that can be used. The statistical methods, including regression, could be used for simulation, but we employed ANFIS algorithm to train the data collected using CFD simulations and run the prediction stage of the data. The method has a high capacity because of two features, which are suitable learning of the neural networks and prediction of the fuzzy logic system. As shown in previous research studies, the method has a high capability in the prediction of AI results, and it could provide mathematical correlation; therefore, we could have the mathematical formulas relating to the predicted flow. The flow in the bubble column reactor was homogeneous; therefore, the bubbles were created in spherical and uniform shapes. For decreasing the time of CFD, a single size Eulerian method was used. The method could provide us with a suitable prediction for the CFD. Also, for the bubble column reactor, only one size was considered for the calculations; but when the regime changes to heterogeneous flow, the multisize Eulerian method is needed. A sensitivity analysis was done on the ANFIS method by changing the number of inputs and the number of MFs during the training and testing process. The x and z coordinates of the fluid location, the air velocity, and the pressure were taken as the inputs for ANFIS, while the air vorticity was the output.

The results obtained from prediction from grid partition clustering and gbell function showed that the method has high capability in the prediction of the flow. It also has high accuracy. Similar to FCM clustering, this method predicted the flow in the reactor. This method beside gaussmf function could perform better than the FCM clustering. The gbell function in grid partition clustering could be better than this method in the prediction of the flow and air vorticity in the reactor. The limitation of the study is that each of the regimes inside a reactor needs separate training to provide the condition that is suitable for the flow and turbulence characteristics in AI. Also, in the prediction process, a similar condition could be predicted, and the complexity of the flow and the relationship between inputs and outputs can be found. For a better understanding of the flow inside the reactor, we need to use deep learning algorithms or autoencoder algorithms; so the meaning and the complexity of the inputs and outputs could be found.

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Notes

The authors declare no competing financial interest.

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