ABSTRACT: A bubble column reactor is simulated by a combination of Euler–Euler and adaptive network-based fuzzy inference system (ANFIS) method to develop an understanding of the machine learning (ML) technique in describing complex behavior of multiphase flow in bubble column reactors and for deep learning of input and output connections. In the validation stage of simulations, an intelligent bubble column is created that uses artificial intelligence nodes or neural network nodes, and the results of prediction indicated excellent agreement with computational fluid dynamics (CFD) simulation results. The hydrodynamic characteristics of the air bubbles and the amount of stress inside the bubble column reactor are used as the output of the ANFIS method. This study showed that when a three-dimensional bubble column is trained by a ML method, a similar CFD simulation can be created, which is independent of CFD source data. This type of smart simulation also enables us to avoid repeating the simulations with CFD methods that are time-consuming and computationally expensive for process modeling and optimization.

1. INTRODUCTION

Bubble column reactors are chemical/biochemical unit operations that can create multiphase flow, including liquid–gas and liquid–gas–solid interactions.1 This type of reactor is used in a variety of industries such as biotechnology, chemical, wastewater treatment, energy production, and bio/pharmaceutical manufacturing.2,3 In these industries, various processes are carried out in the bubble column reactors such as separation of one phase, bubbling flow, mixing, and chemical reactions between species. For instance, in the wastewater treatment industry, bubbles collide very fine solid particles and result in the movement of particles into the top of the bubble column. In addition, the amount of gas and liquid can be changed to keep microorganisms alive for biochemical applications such as production of biopharmaceuticals. In these types of reactors, spargers or orifices, that produce bubbly flow, are usually located at the bottom of the reactor for efficient processing.2–4 The orifice/sparger specifications, the diameter of the orifices, and their placement have a major effect on the hydrodynamics of reactors and need to be precisely designed.5

In addition to the orifices and the flow generated by orifices, other parameters affect the bubble column reactor hydrodynamics such as temperature, pressure, flow rate, and the size of the reactor. Changing these parameters can change the amount of gas production and fluid flow in reactors. Change in fluid circulation and gas hold up directly affects the efficiency of bubble column reactors. The study of the reactor hydrodynamics in the laboratory is expensive and time-consuming, and researchers are trying to model the fluid flow by novel computational tools such as computational fluid dynamics (CFD).6–8 A number of models, such as the finite volume (FV) method and lattice Boltzmann (LB) method for modeling of bubble column reactors, have been introduced over the last years using commercial software or numerical codes.9–11

Because of the existence of a turbulent flow regime inside bubble column reactors, a variety of methods have been used, and researchers have tried to fully model a bubble column reactor. Given that the capture of all dimensions of velocity in turbulence flows is complex, a number of mechanistic models such as the model of large eddy simulation and k–ε in mathematical models have been developed. For instance, in the large eddy simulation approach, large eddies are fully computed while small eddies are approximately resolved. In
the $k−\epsilon$ model, all the velocity flow fields are calculated based on approximation with lower computational costs. However, other models such as direct numerical simulation have not been fully used to solve bubble column reactors and understand all aspects of bubble column hydrodynamics. There are several studies about using turbulence models in the prediction of flow characteristics and bubble column hydrodynamics. They thoroughly explained all forcing schemes and turbulence models to predict the flow in the reactor. However, experimental observations for bubble dynamics, gas and liquid pattern, flow characteristics, and flow regime were investigated in many studies.

On the other hand, studying all parameters affecting the hydrodynamics of bubble column reactors using numerical techniques can be time-consuming and computationally expensive. We still need more speedy models to optimize the flow pattern in reactors. During filling reactors, harvesting products, and cleaning tanks and pipelines, hazardous materials can interact with operators, which is very dangerous. In this case, shortly, we need to empower robots to take control of the bubble column reactors. Regarding the existing issues, intelligent algorithms have been presented by a large number of artificial intelligence (AI) research, and these algorithms have recently been used in a variety of papers to create intelligent bubble columns.

Recently, several studies investigated coupling between machine learning (ML) and numerical calculation of Navier–Stokes equations for different physical problems, such as bubbly flow in bubble column reactors, velocity, and thermal distribution18 in the cavity and nanofluid problems. More specifically, researchers concentrated on the prediction of flow characteristics and turbulence behavior in the domain of multiphase flow (gas and liquid interactions). They found that the new coupling mechanism can potentially estimate the flow in the domain with a great degree of accuracy. For example, they found that tuning parameters in ML can change the accuracy and computational time of prediction.

The adaptive network-based fuzzy inference system (ANFIS) method is usually used as an intelligent algorithm in the prediction of phases inside bubble column reactors. Researchers have used the ANFIS model to simulate bubble column reactors for parameters such as gas hold-up, liquid velocity, turbulent kinetic energy (TKE), and microscopic parameters. This study follows Pourousi’s methodology24 that for the first time designed the method of an intelligent algorithm to predict the bubble column hydrodynamics including bubble formation, detachment, bubble interface, and overall bubble column hydrodynamics (such as liquid velocity, gas hold-up, and TKE). Azwadi et al. combined the ANFIS method with the LB method (mesoscale CFD modeling) in the simulation of fluid motion in a cavity. In this paper, an artificial bubble column reactor was designed and generated by the ANFIS method to enhance the understanding of a three-dimensional (3D) multivariable bubble column reactor. To the best of our knowledge, different parameters in the reactor have not adequately been trained with the ANFIS method, and there is a need to study the complicated relationship between parameters within the smart modeling framework. The shear rate, air mass flow rate, and the density of the medium are used as multivariable output parameters for the training process. We also analyzed different variables in the reactor through an AI framework to understand the influence of these parameters on the bubble column hydrodynamics.

2. RESULTS AND DISCUSSION

For validation of the ANFIS method, we verify the results in two different steps. First, we check training results, with 70% of all data. In this case, we consider 70% of data only for the training step and compare ANFIS results with CFD results. Second, we add up 30% remaining data to 70%, and we compare the full data set for test evaluation. This step is fully independent, and we can track all data set based on their location in the bubble column reactor. To understand the level of accuracy for the ANFIS model, we define different mathematical criteria. In this case, when the error is minimal, we can reuse the model for that specific data set and flow regime.

The flow pattern and the amount of gas hold up inside the bubble column reactor are illustrated in Figure 1. A sparger was used in this bubble column reactor for feeding the air bubbles. After sparging the air into the liquid, the gas is seen to be moving toward the reactor’s walls, and a rotary motion takes place in the bubble column reactor. Moreover, the flow pattern which is observed in the bubble column is an indication of fluid movement due to bubble collision. The bubble size is 3 mm for the single size Eulerian–Eulerian model and represents the average bubble size in the reactor. The input bubble size in the Eulerian model represents the average bubble size in the column.

The results in various directions are shown in Figure 2 and can be observed in the direction of 3D movement of the fluid in the reactor in the $x−y$ direction, in the $x−z$ direction, and in the $y−z$ direction. The amount of gas inside the column and the type of fluid movement can be observed in these directions.
The amount of air mass in the bubble column reactor is represented in Figure 2. As can be observed, there is a more considerable accumulation of air mass near the sparger. As the bubble column reactor advances further, the amount of air mass declines while its uniformity increases, bubbles are closer to the walls, and they create more diffusion and uniformity in the reactor. The bubbles appear spontaneously at the bottom of the bubble column reactor, and this is because of the kind of turbulence that takes place; a large amount of gas is produced at this point. However, there is usually no need for numerical models and CFD models that are utilized in the vicinity of the sparger. The latter is because of the turbulence in the current and the kind of sparger used at this point. A source point sparger was used in this research, and they could not be a precise representation of the sparger model as spargers are the source point. For an accurate model regarding the kind of sparger, volume of fluid and LB methods are required to indicate the interface and detachment.19,28

With regards to training, 70% of the aggregate air mass data was employed and included in the training process of the algorithm. As for the $R^2$ criterion, a considerable agreement was obtained. Subsequent to the training process, 30% of the remaining data is added to the training data, and the testing process is verified with the total data for the process of testing. By adding 30% of the data, which is not used in the training process, the ANFIS method adequately models it and assesses the ability of this method to predict the outcome. The power of this method is proven because $R^2$ does not change too much.

According to Figures 3 and 4, no considerable alteration is observed in $R^2$ between training and testing, and the method leads to intelligence which represents the accuracy of the
model during prediction. In this case, the method is fully independent of training data during the prediction process. A possible solution is to filter the amount, either add to the number of rules or alter the type of membership function. In numerous research studies, this might be addressed through the inclusion of more rules. A massive effect on the prediction process could result from including more rules, and the negative parameter in the prediction process will be eliminated.

The contours are plotted in Figure 5a,b to show the amount of air mass adjacent to and in the middle of the wall. The proportion of air mass has a negative value at the side of the walls, the highest value is observed at the center, and generally, it can make the general prediction accurately. In Figure 5a,b, a process is demonstrated in general terms, and a view of the overall data and projection is inside the bubble column reactor.

In the case of other circumstances, the assessment is carried out in which the mesh position is an input parameter, and the output is shear, which is one of the significant parameters within the bubble column reactor. According to Figures 6 and 7, training and testing processes were relaunched. Using more data during training can provide an accurate model for the prediction process, while the overall computational time increases. In this case, the sensitivity study for the amount of training data can optimize the overall training time. So it is likely that we can lower the quantity of data to observe how much of our system can be intelligent and how data training can be in some cases with a truly small proportion of data, intelligent. Figure 8a,b is a representation of a projection in a situation where a systematic mesh refinement is implemented.

Figure 4. Testing the validation of the amount of air mass with the ANFIS model.

Figure 5. (a) X and Y labels represent the position of the computed gas in the bubble column reactor. (b) Prediction of the amount of air mass using the intelligent algorithm without using the CFD model.

Figure 6. Training the validation of the air shear strain rate with the ANFIS model.
to bridge the entire system with AI, and these meshes are not similar to CFD meshes.

Given that the system has achieved a rational intelligence, it is able to perform a projection process based on meshes on the nodes of the neural networks. A procedure for the level of stress or shear is seen to appear inside the system. This procedure is based on ANFIS intelligence, and ANFIS intelligence depicts this procedure. The level of stress in various segments of the reactor and how much it is along the wall and in the middle of the walls is shown in Figure 8.

In Figure 9, it is illustrated that when we use density as the output with just $2^3 = 8$ rule, the method with projection may not be performed with high accuracy, and projection is poor. The comparison of the data begins based on the AI nodes and CFD nodes. As observed in Figure 10, the nodes are usually aligned with each other, so the system error is too high.

### 3. CONCLUSIONS

Using smart modeling enhances understanding of multivariable analysis, including inputs and outputs and relation between parameters inside the bubble column reactor. This study uses intelligent algorithms, such as the ANFIS method, as a ML tool to learn the fluid flow inside a cylindrical bubble column reactor. Output parameters are selected based on information of meshes in the 3D bubble column reactor, and with the
procedure of the learning process and a proper validation criterion, the continuous domain of data is simulated by the ANFIS method. This nondiscrete domain of data enables us to provide the artificial bubble column domain, which is completely independent of the source data (CFD data). The artificial model of the multiphase bubble column reactor improves the optimization process, and it can decrease the computational time due to the physico independency of smart modeling/ML procedures. The mesh refinement algorithm, which is independent of the source data, can provide more data at different levels of the bubble column. This method improves the missing data in a different level of the column, and it is capable of generating a completely artificial bubble column reactor, which is not generated by the CFD database.

The method of ANFIS or other ML methods can be used only as assistance tools besides numerical models (solver of Navier–Stokes equations). As the calculation of flow with CFD can be very time consuming and complicated, and analysis of CFD results is very complex; ML methods can play a central role in facilitating all complex calculations.

4. COMPUTATIONAL METHODS

4.1. Geometrical Structure. In this work, an industrial bubble column was studied, which has a height of 2.6 m. At the bottom of the bubble column reactor, a sparger is designed and embedded for generating bubbles. The diameter of the orifice hole is 0.7 mm, and these orifices are arranged in a regular shape.20 The operating pressure and temperature of the bubble column are designed based on ambient conditions. The top surface of the reactor is opened and connected to the air. The superficial gas velocity is set at 0.015 m/s, which shows the homogeneous flow regime with approximately spherical bubbles (uniform shape) and almost similar size. For further information about a homogeneous flow regime based on superficial gas velocity and the bubble column dimension, Kantarcı et al.30 fully explain the regime based on different operating conditions. The schematic picture of the reactor with numerical boundary conditions is shown in Figure 11.

Our basic assumption is based on the separation of bubbles from the orifice domain to a completely spherical shape. Bubbles are separated from the orifice without collision and coalescence due to low superficial gas velocity and homogeneous flow regime; therefore, they possess a completely spherical shape. This assumption is very useful to use a single-size Eulerian model which can calculate the flow field faster than the multisize Eulerian method. On the other hand, these bubbles will not be subject to the channeling process during separation from the orifice. In this case, the size of bubbles after detachment is dictated from sparger specifications, particularly the sparger size.

The channeling process is a process that commences when a bubble is separated from the orifice at the time of separation of the next bubble, so it creates a channel in the first bubble, and we have several bubbles that are detached from the orifice together. Spherical separation of bubbles gives us the ability to use the single Eulerian–Eulerian method and simple interfacial force models such as single drag coefficient without lift, wall lubrication, and virtual mass terms in our numerical calculations and compute the Navier–Stokes equations with fewer source points and interfacial force models in the momentum equations.31

4.2. CFD Modeling. In CFD modeling, the Eulerian–Eulerian method was used to simulate the bubble column reactor hydrodynamics and flow pattern. This is a single-dimensional Eulerian–Eulerian method. Because all bubbles that are separate from the orifice are completely spherical, one can use such a model. In eq 1, the continuity equation is described. This equation can be used to calculate the volume of available gas or the volume of available liquid. In the second equation, the equation shows the momentum-transfer calculation, and this equation can calculate the amount of gas and liquid phase. To the right of the equation, there are different forces within this equation. The first force to be observed is the force of tension, and afterward, the force is the gravity of the earth, and the pressure can be calculated. Finally, the amount of force applied between the bubble and the liquid can be calculated.

The continuity and momentum-transfer formulations are presented below, which gives $\epsilon_k$ the fraction and $u_k$ presents the average velocity of the discrete phase and the continuous phase

$$\frac{\partial}{\partial t}(\rho_k \epsilon_k) + \nabla \cdot (\rho_k \epsilon_k u_k) = 0 \tag{1}$$

The derived equation for the momentum transfer in the gas phase and the liquid phase is as follows

$$\frac{\partial}{\partial t}(\rho_k \epsilon_k u_k) + \nabla \cdot (\rho_k \epsilon_k u_k u_k) = -\nabla p + \epsilon_k \rho_k g + M_{jk} \tag{2}$$

This equation can calculate the amount of gas and liquid phase. To the right of the equation, there are different forces. The first force to be observed is the force of tension, next force is the gravity of the earth, the pressure can be calculated, and finally, the amount of force that occurs between the bubble and the liquid can be calculated.32 We have tension, and in this equation, the term of stress is observed for the bubble phase and the dispersed phase and matrix, and it is expressed as follows.

$$\tau_k = -\mu_{eff} \left( \nabla u_k + (\nabla u_k)^T - \frac{2}{3} I (\nabla u_k) \right) \tag{3}$$

The effective viscosity of the matrix phase is indicated by $\mu_{eff}$ and calculated by the following equation.

Figure 11. Schematic picture of the bubble column reactor with ring spargers.
The molecule viscosity, $\mu_{T,L}$ is the turbidity viscosity, and $\mu_{BLL}$ is the viscosity based on the bubble-induced turbulence. The effective dispersive phase viscosity $\mu_{eff}$ is expressed as follows:

$$\mu_{eff} = \mu_{L} + \mu_{T,L} + \mu_{BLL}$$  \hspace{1cm} (4)$$

where $\mu_{L}$ is the molecular viscosity, $\mu_{T,L}$ is the turbidity viscosity, and $\mu_{BLL}$ is the viscosity based on the bubble-induced turbulence. The effective dispersive phase viscosity $\mu_{eff}$ is expressed as follows:

$$\mu_{eff} = \frac{\rho_T}{\rho_L} \mu_{eff}$$  \hspace{1cm} (5)$$

For interactions between the dispersed phase and the continuous phase, the total interfacial force $M_{f,L}$ is expressed as:

$$M_{f,L} = -M_{L,G} = M_{D,L} + M_{T,D,L}$$  \hspace{1cm} (6)$$

More details about the CFD model can be found elsewhere.\textsuperscript{14}

4.2.1. Grid. We used nonuniform meshes in the bubble column reactor to mesh the bubble column reactor in CFD study. The nonuniform mesh structure used is similar to the study of Laborde-Boutet et al.\textsuperscript{33} This mesh structure is nonuniformly created for the height and then duplicated for other levels of the reactor, almost same procedure as Laborde-Boutet et al., but the aspect ratio of mesh structure for the current study is not similar with Laborde-Boutet et al. We used the ANFIS structure to learn all data from nonstructure CFD meshes, and then, we created the new mesh structure of AI.

4.2.2. Mesh Sensitivity and Discretization Method. In this study, the FV method is used to discretize all complex and nonlinear equations within the framework of ANSYS-CFX software. After meshing the domain, this method of discretization is used to discretize equations for each computing node. For the mesh sensitivity study, different size of meshes is considered. For example, number of elements in the reactor $\approx$ 16,000, 43,000, and 80,000. The best results are achieved in 43,000 number of elements based on validation with the gas hold up in the domain with the existing literature. The results show that as superficial gas velocity increases in the reactor, the amount of gas hold up in the tank is increased. This finding is consistent with the existing experimental and numerical results in previous studies.\textsuperscript{26,27,34}

The velocity—pressure framework is used for all simulations by a SIMPLEC procedure. The high-order differencing schemes of total variation diminishing are also utilized to decrease numerical diffusion in the domain of the two-phase reactor. The gas-dispersed phase is sparged for 1400 s, and the results are time-averaged after 100 s of CFD simulation. To investigate the impact of different CFD time steps on the numerical results and liquid and gas flow pattern finding, we study different time steps, and we found that time step equal to 0.1 is appropriate for this study. For convergence of the current numerical method, we select $10^{-6}$ error number for solving continuity and momentum equations.

4.3. Adaptive Network-Based Fuzzy Inference System. The ANFIS method is one of the tools that are employed to simulate physical/biological phenomena. In many works with the ANFIS approach, Takagi and Sugeno model has been used to describe the ANFIS method.\textsuperscript{35} To begin the learning stage, the data allocated for learning is first categorized at various levels of membership formations (MFs). As shown in Figure 12, the output of each membership function as a signal from the first layer of the model is multiplied together and represents the AND rule. According to this rule, after multiplying signals together, the second layer is appeared in the ANFIS model. The function $ith$ rule can be expressed as:\textsuperscript{9,32}

$$w_i = \mu_{A_0}(X) \mu_{B_0}(Y) \mu_{C_0}(Z)$$  \hspace{1cm} (7)$$

where $w_i$ represents the output of learning feedback, and $\mu_{A0}$, $\mu_{B0}$, and $\mu_{C0}$ also denotes the input of learning feedback.

The ANFIS framework contains five layers of communication. Figure 12 shows that the first layer implements the fuzzification structure, while the second layer presents fuzzy patterns in the system. In the third layer, the membership structures are normalized for simplifications. The fourth layer summarizes all fuzzy rules, and finally, the last layer finalized the results of fourth layers. The ANFIS method is used for input and output data in this study. Inputs are considered as mesh positions in the bubble column reactor, and outputs are based on the amount of air mass and shear inside the bubble column reactor. The analysis process was used for the ANFIS method, and we first examined this process based on training; we used 70% of the data, and we evaluated the system with 70%. This was examined with various error criteria such as $R^2$, root mean square error (RMSE), and MSE. After examining the data, we added 30% of the remaining data to 70%, and we analyzed the whole data, and again, we considered all the criteria for the error. When the error rate reaches acceptable levels or the system arrives at an acceptable predictor for the prediction process, we have defined a process called the prediction process, and the whole bubble column reactor or domain is artificially computed. According to the intelligence obtained through the learning process, we made the final prediction based on new AI nodes. This suggests that in a chemical or mechanical process, we can reduce the repetition to optimize that process and reduce repetition or how we can simulate some modes. We will examine several situations in the CFD state and then use the data for AI and give AI the remaining states and will recommend optimization. In the third stage for learning, the relative firing strengths of each rule are defined using eq $8$:\textsuperscript{35}

$$\bar{w}_i = \frac{w_i}{\sum (w_i)}$$  \hspace{1cm} (8)$$

where $\bar{w}_i$ is normalized firing strengths. Takagi and Sugeno\textsuperscript{35} suggested the If-Then rule function for the fourth step of learning. The mesh formula in the ANFIS can be modified as follows:\textsuperscript{35}

$$w_i = w_i(pX + q_i Y + r_i Z + s_i)$$  \hspace{1cm} (9)$$

where $p$, $q$, $r$, and $s$ are parameters related to “If-Then rules”.

![Figure 12. ANFIS method for the simulation of the amount of air mass at different neural nodes.](image)
The RMSE equation, where \( N \) shows the number of test levels, can be calculated as follows:\(^{19,29}\)

\[
RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (\text{actual output} - \text{estimated output})^2}
\]

\[(10)\]

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The authors declare no competing financial interest.

**NOMENCLATURE**

- \( C_D \): coefficient of drag force for dispersed phase
- \( C_{TD} \): turbulent dispersion coefficient for dispersed phase
- \( C_{1} \): turbulent dissipation energy equation
- \( C_{2} \): constant in turbulence modeling of dispersed phase
- \( C_{u} \): constant in bubble-induced turbulence modeling of dispersed phase
- \( d_b \): dispersed phase size
- \( D \): size of reactor
- \( D_S \): ring sparger size
- \( g \): gravitational force in modeling
- \( H \): height of reactor in modeling
- \( k \): turbulent kinetic energy for modeling of dispersed phase
- \( M_I \): interfacial force
- \( M_D \): drag force for modeling of dispersed phase
- \( P \): pressure in the reactor
- \( MF \): membership function for ANFIS modeling
- \( RMSE \): root mean square error for ANFIS modeling

**GREEK SYMBOLS**

- \( \epsilon \): turbulent energy dissipation rate per unit mass; \( \epsilon_1 \): phase hold-up; \( \overline{\epsilon} \): average phase hold-up; \( \mu \): molecular viscosity; \( \mu_{bp} \): bubble-induced viscosity; \( \mu_{eff} \): effective viscosity; \( \rho \): density of phases; \( \rho_{T} \): turbulent viscosity; \( \tau_{0} \): shear stress of phase; \( \kappa \): volume of dispersed phase

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