Predicting Air Superficial Velocity of Two-Phase Reactors Using ANFIS and CFD

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ABSTRACT: In predicting the turbulence property of gas (bubble) flow in the domain of continuous fluid and liquid, the integration of machine learning and computational fluid dynamics (CFD) methods reduces the overall computational time. This combination enables us to see the effective input parameters in the engineering process and the impact of operating conditions on final outputs, such as gas hold-up, heat and mass transfer, and the flow regime (uniform bubble distribution or nonuniform bubble properties). This paper uses the combination of machine learning and single-size calculation of the Eulerian method to estimate the gas flow distribution in the continuous liquid fluid. To present the machine-learning method besides the Eulerian method, an adaptive neuro-fuzzy inference system (ANFIS) is used to train the CFD finding and then estimate the flow based on the machine-learning method. The gas velocity and turbulent eddy dissipation rate are trained throughout the bubble column reactor (BCR) for each CFD node, and the artificial BCR is predicted by the ANFIS method. This smart reactor can represent the artificial CFD of the BCR, resulting in the reduction of expensive numerical simulations. The results showed that the number of inputs could significantly change this method’s accuracy, representing the intelligence of method in the learning data set. Additionally, the membership function specifications can impact the accuracy, particularly, when the process is trained with different inputs. The turbulent eddy dissipation rate can also be predicted by the ANFIS method with a similar model pattern for air superficial gas velocity.

1. INTRODUCTION

Bubble column reactors (BCRs) and formation of bubbles in a continuous fluid/liquid have extensive applications in industry because of their convenient structure and function. Oxidation, wastewater treatment, hydrohalogenation, ammonolysis, hydrogenation, halogenation, and so forth are some major bubble column applications.1−3 Two phases exist in bubble columns that show the formation of bubbles in the liquid phase, and the interactions of this phase illustrate the bubble flow in the two-phase reactor. According to the two homogeneous and heterogeneous regimes, the gas phase’s movement depends on the dispersion nature.1−6 The first regime, called the homogeneous regime, happens at superficial gas velocities of below 50−80 mm/s.7−10

The progress in design procedures has been inhibited by the complex flow pattern in BCs from first-principles calculations. Thus, the researchers have been attempting to study the flow fields as well as the impact of operating conditions on the flow and critical design parameters, such as gas hold-up bubble size distributions and turbulence properties in bubble columns over the last 40 years.11−13 Among these design parameters, pressure drop, liquid-phase mixing, fractional gas holdup, and interphase mass-transfer coefficients can be mentioned as key design parameters.14,15

Although various design factors and optimization parameters have been used based on mathematical methods, there are limitations in these methods when the reactor performance is not increased.16,17 Therefore, numerous models, including the mathematical and computing continuity momentum equations by computational fluid dynamics (CFD) models, have been suggested to improve the physical phenomenon description in bubble columns.18−20

With significant advances in computing technologies, CFD tools have increased because of their cost. CFD simulations are performed according to the local calculation of gas−liquid interactions, such as the liquid velocity distribution or bubble size distribution. This approach’s importance and interest have
attained a significant growth recently as it describes all local values in the BC.21,22

High-frequency three-dimensional (3D) instabilities are to be considered for resolving the physics of bubble column-type flows in different applications. In other words, there is a requirement for performing the simulations in an unsteady full 3D framework,23,24 which has a challenging computation. For this purpose, Eulerian multisize estimations to represent the Eulerian method for each bubble size have the optimum trade-off between computational requirements and accuracy. However, there are difficulties and limitations for obtaining the appropriate accuracy for formulating closure laws for this purpose.26,27 In contrast, large eddy simulation (LES) models yield less fine information despite using much higher computational resources.28 Euler/Lagrange models can be an appropriate basis for studying the BC flows29,30 when individual bubble tracking can be obtained.

Nevertheless, churn turbulent flow has much lower applicability.9,31 The accurate prediction of the BCR with appropriate CFD models requires a high computational time and effort. Therefore, soft computing methods and intelligence algorithms have been suggested to decrease the calculation time/efforts and the number of case studies during the process optimization. These modeling types solve several nonlinear and complex problems as they propose intelligence tools for demonstrating nonlinear input–output mapping.32

Artificial neural networks (ANNs) provide a reliable instrument for complicated problem analyses, such as fluid flow and heat, while the quality of the computing tool is preserved, and the associated gas–liquid interaction is encompassed in the training framework.33 Nowadays, ANN34–36 and the adaptive network-based fuzzy inference system (ANFIS)37,38 have gained much more attention for solving issues in industries associated with gas–liquid interactions. Nevertheless, there are serious limitations for their application to energy studies related to the heat and flow process. The ANFIS approach is found to be a powerful method because of its ANN learning ability besides a strong estimation structure of the fuzzy system. There are also several mathematical, numerical, and soft computing approaches to predict the physical processes in the literature.39

The ANFIS approach is the combination of ANN and fuzzy logic methods capable of learning complicated physical systems. This study combines the ANFIS method with CFD data to predict the superficial gas velocity within the domain of the stationary continuous liquid fluid and turbulent eddy properties in a 3D cylindrical BCR. Cylindrical BCRs are used in academia and industry. These BCRs have spargers at their bottom, and the gas phase is formed through orifices (each individual sparger hole) and generated the dispersed phase and the bubbly flow in the domain. Pourtousi et al.40 investigated gas fractions in the liquid phase, kinetic energy resulting from turbulent flow, and local continuous flow/velocity distributions by a combined CFD and artificial intelligence (AI; ANFIS) method. Here, the superficial gas velocity and turbulence properties, such as the turbulent eddy dissipation rate, are studied.

There are several CFD algorithms, such as the volume of fluid (VOF) method, Eulerian method, or Eulerian–Lagrangian approach (tracking individual Lagrangian particles in the frame of Eulerian calculations) to predict the BCR. The Eulerian approach in this study is used to train the fuzzy interface network by neural networks. As a result of this training campaign, the ANFIS method estimates the gas–liquid interactions at local computing nodes and then predict the hydrodynamics of BCR and turbulence properties. However, in previous studies, the VOF method has been used besides the ANFIS method to predict the interface between the dispersed and continuous phases. Eulerian–Lagrangian is not very popular as far as it has a limitation in CFD (computational time and expenses). Moreover, when the gas fraction in the BCR increases, the Eulerian is more suitable. However, because of direct numerical simulations in the VOF method for a huge domain, the VOF method is also costly, and the method also has limitations regarding the costs and CFD calculations. Therefore, the Eulerian method is very cheap and useful in industry and academia. This research uses this model as a popular CFD model to predict the reactor’s hydrodynamic and turbulence properties.41

Using CFD, we can provide many datasets about the hydrodynamics of the BCR and turbulence properties. We can also predict each hydrodynamic parameter with AI algorithms. In this research, the ANFIS model with several membership functions (MFs) at each input parameter is used to predict the reactor’s hydrodynamic and turbulence characteristics. Different MFs are used to find an accurate AI algorithm with a high ability of prediction. To better understand the BCR, we need to calculate the hydrodynamics of the reactor by CFD and use the calculations in the ANFIS method. This approach requires to be repeated several times to cover different hydrodynamic parameters of the reactor or turbulence properties as the CFD algorithm can calculate many hydrodynamic parameters.

2. MODELING

2.1. Geometry of System. In this research investigation, a two-phase reactor of bubble column type was considered at 23 °C and at ambient pressure with a height of 2.6 m. There is a sparger at the bottom of this BCR with 0.7 mm size, and bubbles are formed through each sparger with marginal interactions between bubbles. Also, it is presumed that the bubbles are in spherical geometry for the modeling and simulations.

2.2. CFD Method. For CFD simulations, ANSYS CFX software is used. In CFX software, to discretize all partial equations, the finite volume is used. Moreover, the single-size Eulerian–Eulerian technique is used to estimate the overall calculation of gas in the reactor to create a dataset as inputs for the AI model.10

The continuity equation for the gas and the liquid is as follows

$$\frac{\partial}{\partial t}(\rho_i \varepsilon_i) + \nabla \cdot (\rho_i \varepsilon_i u_i) = 0$$

(1)

where $u_i$ is the average calculation of each computing nodes for gas bubbles and the stationary liquid.

To calculate the conservation equations, a volume control approach is employed. The equations for the momentum calculation and the associated physical interaction between phases are expressed as

$$\frac{\partial}{\partial t}(\rho_i \varepsilon_i u_i) + \nabla \cdot (\rho_i \varepsilon_i u_i u_j)$$

$$= -\nabla \cdot (\varepsilon_i \tau_i) - \varepsilon_i \nabla P + \varepsilon_i \rho_i g + M_{i,k}$$

(2)

In the momentum equations, on the right-hand side of equation, there are several terms that represent the stress...
pressure distribution, gravity, and interfacial force models. The stress term is computed using 

$$
\tau_l = -\mu_{dl} \left( V_{l} u_k + (V_{l} u_k)^T - \frac{2}{3}(V \cdot u_k) \right)
$$

(3)

In eq 4, the effective viscosity of liquid that is formulated in the stress term is computed as

$$
\mu_{e,L} = \mu_l + \mu_{T,L} + \mu_{BLL}
$$

(4)

where $\mu_l$, $\mu_{T,L}$, and $\mu_{BLL}$ are the molecular viscosity, the liquid turbulent viscosity, and the turbulent viscosity as a result of bubble–bubble interactions, respectively. Equation 5 is used for calculating the effective viscosity of the dispersed phase

$$
\mu_{e,G} = \frac{\rho_f \mu_{e,L}}{\rho_l}
$$

(5)

In a two-phase flow calculation, the Sato and Sekoguchi model can define the bubble–bubble interaction and turbulence behavior of bubbles in the continuous fluid. Equation 6 is defined to obtain the total interfacial force between phases

$$
M_{LL} = -M_{TL,G} = M_{DL,L} + M_{TD,L}
$$

(6)

In this research, we apply the drag coefficient for modeling the BCR as a predominate forcing scheme between two phases. The $M_{DL,L}$ force can be obtained as follows

$$
M_{DL,L} = -\frac{3}{4} \rho_l \rho_f \frac{C_D}{d_b} u_G - u_L (u_G - u_L)
$$

(7)

In eq 7, $d_b$ and $C_D$ denote the bubble diameter and drag coefficient, respectively. The turbulent dispersion force term is used for obtaining a more appropriate prediction of bubble flows. It can be obtained as follows

$$
M_{TD,L} = -M_{TG,L} = -C_{TD,L} \rho_k \nu \epsilon_l
$$

(8)

where $k$ and $C_{TD}$ describe the kinetic energy as a result of turbulent flow and mathematical coefficient, respectively.

For better observation of gas and liquid interactions, the turbulent eddy viscosity is calculated as

$$
\mu_{T,L} = \rho_l C' \frac{k^2}{\epsilon}
$$

(9)

The following formula is written for calculating the kinetic turbulence ($k$) and the energy dissipation rate ($\epsilon$)

$$
\frac{\partial}{\partial t} (\rho_l \epsilon_l k) + \nabla \cdot (\rho_l \epsilon_l u_k k) = -\nabla \cdot (\epsilon_l \mu_{T,L} \nabla k) + \epsilon_l (G - \rho_l \epsilon) + \delta_{ll} \frac{k^2}{\epsilon}
$$

(10)

$$
\frac{\partial}{\partial t} (\rho_l \epsilon_l) + \nabla \cdot (\rho_l \epsilon_l u_k) = -\nabla \cdot (\epsilon_l \mu_{T,L} \nabla \epsilon) + \epsilon_l \frac{G}{k} (C_{l,G} - C_{l,\epsilon} \rho_k \epsilon)
$$

(11)

The $k$-$\epsilon$ model is used as an approximate calculation of the turbulence behavior of the liquid, turbulent eddy viscosity, eddy specification, and kinetic energy of the flow.

2.2.1. Mesh. An unstructured mesh taken from prior research is adopted for this BCR. It is created to use the nodes applied in the CFD, which aimed to be employed in the ANFIS approach and the prediction process. The meshes are hexahedral grid meshes, and they are generated in the form of nonuniform meshes. They are also repeated in each cross section. The reason behind using nonuniform meshes is because they are generated easily. Furthermore, as far as previous studies indicate good results for using them, the meshes are considered in the study as well. The grid’s properties in the study include the orthogonal quality of about 0.6, skewness number of 0.6, and aspect ratio of 3. Additionally, the mesh sensitivity analysis has been investigated, and 40,500 number of elements are selected for the number of grids in the reactor for this study.

2.2.2. Boundary Conditions and Force Models. For the solution of the derived equations, the degassing boundary condition is postulated at the top surface of the reactor to model the reactor’s gas outlet. Additionally, to model solid walls, a zero-speed condition was postulated for the liquid on the solid walls, and a free slip boundary condition is used for the gas. A single-size Eulerian method is used in the study because the flow regime is homogeneous. Moreover, the drag coefficient is used as the drag model of the bubbles. The drag coefficient enables us to estimate the spherical bubble movement with a uniform shape and without interaction, coalescence, and breakup in the BCR. No interaction is considered in the study for the bubbles, or at least they have the minimum amount of interaction with each other. The drag coefficient is 0.44. This work’s bubble size is 0.4 cm, according to the BCR presented in Pfleger and Becker’s numerical and experimental study.

2.3. ANFIS. In this research, the $x$, $y$, and $z$ local computing nodes are considered as inputs. The superficial gas and turbulent eddy dissipation rates are also adopted as the output. 60% of the data is applied to the learning steps. For performing the complete data verification, the remaining 40% is added to the testing process. The prediction process is then carried out once the verification is completed. The data in the training campaign are based on randomized selection. Each of the datasets and simulation runs (such as different MFs and input parameters) in the training campaign are separately randomized. Alternatively, in the prediction processes, nontrained datasets have participated. The estimation step is applied according to the AI nodes. Then, the system applies it to the neural network pattern according to its intelligence. The pattern of input parameters and MFs in each input are represented in Figure 1.

As indicated in Figure 1, the first feedback from the training is multiplied according to AND law. The $i$th rule can read as

$$
\omega_i = \mu_{A,i}(X) \mu_{B,i}(Y) \mu_{C,i}(Z)
$$

(12)

where $\omega_i$ represents the training feedback output, and $\mu_{A,i}$, $\mu_{B,i}$, and $\mu_{C,i}$ refer to the learning feedback inputs. The relative firing strengths are calculated in the third step of learning as

$$
\tilde{\omega}_i = \frac{\omega_i}{\sum \omega_i}
$$

(13)

where $\tilde{\omega}_i$ refers to normalized firing strength. The “if-then” rule function was employed by Takagi and Sugeno in the fourth level of training system. $\omega_i$ can be presented as follows

$$
\tilde{\omega}_i = \tilde{\omega}_i \left[ p x + q y + r z + s \right]
$$

(14)

In this equation, $p$, $q$, $r$, and $s$ are “if-then” rules in the model of ANFIS.
3. RESULTS AND DISCUSSION

In this study, a cylindrical BCR is simulated by means of a CFD. Hydrodynamic fluid parameters have resulted as the CFD calculation output (results). In this study, the data produced by the CFD method are studied using one of the AI methods (ANFIS method) and $x$, $y$, and $z$ coordinates are used as inputs, while the superficial air velocity in the $z$-direction and the turbulent eddy dissipation rate (turbulence properties) are used as targets in the ANFIS method. The positions of $x$-, $y$-, and $z$- (reactor height) directions in the reactor were considered in the study because we need to create artificial BCR, and based on each of the computing points, we can predict the characteristics of the BCR.

As there are three inputs to make ANFIS intelligence, different conditions were initially studied with minimum data and input. At first, coordinates in the $x$-direction were studied as input. Superficial air velocity in the $z$-direction was investigated as the target. MFs were assumed to be 4. 60% of the data was allocated to learning, and 100% of the data was allocated to the process of testing, and the MF-type was gbellmf. After performing training and testing, as illustrated in Figure 2a,b, it was observed that $R^2$ amounts to 0.12, which shows there was no improvement in system intelligence. Increasing the number of data from 1000 to 12,000 was also considered for the system intelligence to rise. Additionally, after performing training and testing processes for different numbers of data, as seen in Figure 3a,b, there was no significant increase in system intelligence. However, from among different numbers of data when the number 4000 was considered, $R^2$ increased to 0.16, which is still negligible but made us to continue the investigation with 4000 data and 4 number of MFs, and according to Figure 5a,b, there was no considerable change in $R^2$ for training and testing processes, and later in this research, rising the number of inputs will be investigated.

It is indicated in Figure 4a,b that changes in MFs did not affect system intelligence. To investigate the increase in system intelligence, alterations were separately made to the MF type, which include gbellmf, gaussmf, gauss2mf, dsigmf, and psigmf, with 4000 data and 4 number of MFs, and according to Figure 5a,b, there was no considerable change in $R^2$ for training and testing processes, and later in this research, rising the number of inputs will be investigated.

By rising the number of inputs to two, two different directions of computing nodes, such as $x$ and $y$, were employed as input parameters of the AI framework, while the superficial air velocity distribution in the $z$-direction was applied as the target in the ANFIS method. A learning process was carried out with new conditions for inputs, choosing 4000 data and 4 MFs with gbellmf as the MF, and according to Figure 6a−c demonstrates that $R^2$ increased to 0.74, which shows a significant increase in system intelligence, but this increase is still inadequate for the ANFIS to be fully intelligent. Therefore, increasing numbers of data from 4000 to 8000 and 12,000 were studied separately which, according to Figure 7a−e, resulted in no significant...
increase in system intelligence. Hence, we considered 4000 data and observed the changes according to different MF types, including gbellmf, gaussmf, gauss2mf, dsigmf, and psigmf separately, which, as shown in Figure 8a,b showed that the gbell function could provide better accuracy in the testing processes. For a better analysis of model parameters and the accuracy of models, the RMSE for different MFs is considered in various iterations. The results show that in a small number of iterations (iterations < 50), the error of the model is high, but by increasing the number of iterations, the RMSE value is significantly reduced. This significant reduction of error occurs up to 50–100 iterations approximately. However, the error reduction in some functions reaches the convergence, such as gaussmf and dsigmf. Additionally, the accuracy of the psigmf MF model is not changed by incrementing the number of iterations after 150 iterations. Alternatively, there is a slight reduction in the gbell function with rising number of iterations. The guass2mf shows different behavior regarding the RMSE value. This function behaves almost similarly to the gbell function up to 225 iterations, but there is a sudden reduction in error between 225 and 325 iterations (see Figure 8c). The pigmf has better accuracy than other MFs in the training processes (Figure 8c), but the testing process is very important for the selecting function. The testing process results show that

Figure 3. Training (a) and testing (b) of air superficial velocity in the z-direction using one input and various numbers of data.

Figure 4. Training (a) and testing (b) of air superficial velocity in the z-direction using one input and various numbers of rules.
gbellmf contains a better accuracy than other MFs (see Figure 8b). This function is selected as the primary MF for each input in this research. This analysis also enables us to justify the rationale for choosing some critical parameters and assumptions for the ANFIS method. The sensitivity study on different MFs for different numerical iterations can provide a guideline for future research for a better selection of functions in each input and the number of iterations regarding the model accuracy and prediction capability.

Changing the number of MFs from 4 to 8 and 10 was studied as the only change able to be studied while using only

Figure 5. Training (a) and testing (b) of air superficial velocity in the z-direction using one input and various types of MFs.

Figure 6. Training (a) and testing (b) of air superficial velocity in the z-direction using two inputs (ANFIS method). (c) Comparing ANFIS and CFD in the calculation of air superficial velocity in the z-direction using two inputs (ANFIS method).
two inputs, 60% of the entire data was allocated to the learning step and 100% of the data (4000) in the testing (validation) process and the ANFIS learning process were separately studied considering 4 MFs, which showed a small increase in $R^2$ to 0.84. This increase to $R^2$ is not enough for the ANFIS to be completely intelligent (Figure 9a,b).

In this part of research, we studied the results of rising the number of data from two to three. The number of data was considered 1000 with 2 MFs from gbellmf type, and the training was applied with 60% of the data used in the training process and 100% in the testing process, and the value of 0.76 was achieved for $R^2$. To investigate the increase in ANFIS intelligence, the number of data was increased from 1000 to 2000 and 4000.

Figure 10a,b shows that the most increase in $R^2$ is seen when the number of data is 2000, 0.82. Changes in the number of MFs were studied with the amount of data being 2000, which leads to the highest value of $R^2$. According to Figure 11a,b when the number of data is 6, $R^2$ for the learning process increases to 0.99 which is perfectly appropriate, but $R^2$ for the testing process amounts to 0.79, and we studied the changes in the number of data to increase this value.

In this part, coordinates in different directions of computing points (nodes), the 3D domain of a reactor, were used as input parameters of the AI framework, while the superficial gas
The velocity distribution in the z-direction was considered the ANFIS method’s target, and 6 number of MFs were used at each input. Training and testing were implemented separately while changing the number of data from 2000 to 4000 and 8000. This procedure enables examining the impact of datasets for different evaluation processes.

Figure 12a,b shows that the best value for $R^2$ regarding testing and training was 8000 data. However, a different range of datasets in the training process does not significantly change the accuracy of the model. An increasing dataset can significantly enhance the accuracy of prediction in the testing processes. Three inputs, gbell function with 8000 datasets, are

![Figure 8](image)

**Figure 8.** (a) Training and testing (b) of air superficial velocity in the z-direction using two inputs and different types of MFs (ANFIS method). (c) RMSE as a function of the number of epochs/iterations for different types of MFs.

![Figure 9](image)

**Figure 9.** Training (a) and testing (b) of air superficial velocity in the z-direction using two inputs and different types of MFs (ANFIS method).
also considered in Figure 13. The results show the accurate model in predicting the reactor, hydrodynamics in the training, and testing.

Parts of different points of BCR used in the ANFIS method are marked in Figure 14, which shows the ability to predict superficial air velocity in the z-direction using less data through the ANFIS method. Figure 15a–c shows perfect compatibility between CFD output and ANFIS prediction.

ANFIS offers predictions made without using CFD nodes and using only ANFIS nodes (Figure 16).

We use the best model parameters of superficial air velocity prediction for estimating the turbulence properties in the BCR. The eddy dissipation rate as a turbulence parameter is selected as an output parameter of the model. In general, the turbulent eddy dissipation rate illustrates the mathematical rate of large and small eddies in the inertial framework. This energy and small eddies are finally transferred to the internal thermal energy of the reactor. This parameter can be used to...
characterize the mixing length and average eddy structure in the two-phase reactor. This parameter is trained along with $x$, $y$, and $z$ computing points in the reactor domain as inputs. We examine similar model parameters in the training of air superficial velocity in the $z$-direction. Figure 17 shows a turbulent eddy dissipation rate as a function of 8000 data points. The results show that this turbulence property can be well predicted with the ANFIS method. The method of ANFIS can track the turbulent eddy dissipation rate in each computing point. In both training and testing processes, the model’s accuracy is high ($R > 0.98$), and the RMSE and standard deviation are 0.0043. These results also show that the model of ANFIS can be used for different outputs after the optimization of all tuning parameters.

4. CONCLUSIONS

The integration of AI and numerical calculations is applied to estimate the gas velocity and turbulence property (eddy dissipation rate) at different nodes of the BCR. To achieve the accurate ANFIS method, different MF specifications for each
input, the amount of data, and the number of the iterations are used during the learning process. The number of inputs has main influence on the learning process and ANFIS method’s intelligence. This finding shows that massive amounts of data and inputs affect smart modeling accuracy in the data-based modeling approaches. In addition to the number of inputs, selecting the high number of rules enables this method to learn the process fully. This machine-learning prediction process with a combination of CFD data is very promising in

Figure 14. Points of the bubble column that were used in the ANFIS learning process.

Figure 15. (a) Comparing AI and CFD in the estimation of air superficial velocity in the z-direction using three inputs in full intelligence of AI. (b) Comparing AI and CFD in the estimation of air superficial velocity in the z-direction using three inputs in the full intelligence of ANFIS method. (c) Comparing AI and CFD in the estimation of air superficial velocity distribution in the z-direction using three inputs in the full intelligence of AI.

Figure 16. (a) Prediction of air superficial velocity in the z-direction (output) in the best condition of model regarding accuracy. (b) Calculation of air superficial velocity in the z-direction (output) in the best condition of model regarding accuracy. (c) Estimation of air superficial velocity in the z-direction (output) in the best condition of model regarding accuracy. (d) Contour estimation of air superficial velocity in the z-direction (output) in the best condition of model regarding accuracy.
developing the smart reactor as a CFD method and can provide a vast number of data and a combination of inputs and outputs at local nodes.

Also, the study has a particular limitation, that is, other flow regimes that have heterogeneous flows must be trained separately. When the operation conditions are changed in each condition, the datasets must be used in the training campaign. Therefore, the dataset cannot be used for other operating conditions or other physics as far as the model is data-driven, and the data cannot be predicted using other physics.

For future studies, the physical boundary condition in the AI framework could be developed and defined; therefore, the AI could have a better understanding of the physics. Sometimes, the flow on the walls is complex, and AI could not understand what happens in a particular area, so it is better to filter the data or define the data in AI. Therefore, the prediction capability and model accuracy can be enhanced.

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The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

S.S. acknowledges the support by the Government of Russian Federation (Act 211, contract 02.A03.21.0011) and by the Ministry of Science and Higher Education of Russia (grant FENU-2020-0019).

■ NOMENCLATURE

$C_D$, Drag coefficient for the movement of bubbles in a liquid; $C_{TD}$, Turbulent dispersion coefficient; $C_{\varepsilon 1}$, Turbulent dissipation energy; $C_{\varepsilon 2}$, Turbulent dissipation energy; $C_\mu$, Model parameter in the turbulence term; $C_\mu_{BI}$, Constant in the bubble-induced turbulence modeling of the dispersed phase; $d_B$ [m] Bubble size in the domain of the bubble column reactor; $g$ [m s$^{-2}$] Gravity; $k$ [m$^2$ s$^{-2}$] Turbulent kinetic energy; $M_D$ [Nm$^{-3}$] Drag term in the equation of interfacial force models; $P$ [Nm$^{-2}$] Pressure in the domain of the bubble column reactor; MF, Membership function in each input parameter; RMSE, Root mean square error

■ GREEK SYMBOLS

$\varepsilon$, [m$^2$ s$^{-3}$] Dissipation rate in the domain of the bubble column reactor (−); $\xi$, Gas hold-up in the domain of the bubble column reactor (−) (−); $\bar{\xi}$, Average gas hold-up of the domain of the bubble column reactor (−); $\mu$, [Pa s$^{-1}$] Molecular viscosity in the domain of the bubble column reactor; $\mu_{BI}$ [Pa s$^{-2}$] Bubble-induced viscosity, representing the bubble–bubble interactions and turbulence as a result of bubble movement; $\mu_{eff}$ [Pa s$^{-1}$] Effective viscosity in the domain of the bubble column reactor; $\rho$, [kg m$^{-3}$] Density of both gas/bubbles and a continuous liquid/fluid; $\mu_T$, [Pa s$^{-1}$]
Turbulent viscosity in the domain of the bubble column reactor; $\tau_w$ [Pa] Shear stress for both gas/bubbles and a continuous liquid/liquid or continuous liquid/liquid

**SUBSCRIPTS**

- $\tau$: Turbulent viscosity in the domain of the bubble column
- $T$: Temperature
- $l$: Stationary liquid or continuous liquid/liquid

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