Integrating Machine Learning with Volume of Fluid Methods for Enhanced Computational Fluid Dynamics in Complex Multiphase Flow Analysis

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Abstract

This study presents a comprehensive method for simulating complex multiphase flows through a Machine Learning-Enhanced Volume of Fluid (VOF) technique. Our goal is to enhance the precision and efficiency of predicting fluid behaviour in multiphase environments by integrating traditional computational fluid dynamics (CFD) approaches with machine learning techniques. The VOF approach is utilized to track the phase interface, which allows for the analysis of volumetric fractions and flow dynamics. Once the primary parameters, such as velocity fields, pressure distributions, and phase interfaces, have been visualized in MATLAB, plots are generated. A comparison of the performance between this machine learning model and conventional CFD methods shows significant improvements.

Keywords: Machine Learning, Computational Fluid Dynamics (CFD), Volume of Fluid (VOF) Method, Multiphase Flows, MAT Lab.

1. Introduction

The necessity for precise accuracy: In addition, CFD frequently faces limitations due to its lack of consideration for phase interactions, which can greatly affect the dynamics of multiphase flows.

This article presents a survey of recent progress in the simulation of multiphase flows utilizing computational fluid dynamics methodologies. The models discussed include continuum models, interface tracking models, and hybrid models, among others.

1.1. Challenges in Multiphase CFD Modelling.

Traditional CFD techniques pose challenges in accurately simulating multiphase flows due to their complex physical behaviours, which include phase transitions, interfacial dynamics, and turbulence. A significant difficulty in modelling multiphase flows lies in depicting the interfacial boundaries between phases, which can distort, fragment, or merge in an unpredictable manner. Furthermore, it usually requires a high spatial and temporal resolution to simulate such interactions, resulting in high computational costs. Moreover, the accuracy of conventional CFD models is largely dependent on the turbulence modelling approach that might not account for all complexities that arise during multi-phase interactions.

Nonetheless, using empirical models or simplifications in several cases reduces computational load at the expense of the fidelity of simulations. For instance, Volume of Fluid (VOF), Euler-Euler, and Euler-Lagrange frameworks are often used in multiphase CFD simulations but have limitations, especially in terms of resolving interfacial phenomena or dealing with large-scale turbulent flows. Consequently, there has been an increasing interest in alternative approaches such as data-driven models and machine learning techniques that can supplement or enhance conventional CFD methods, which are more efficient and accurate than their predecessors.

1.2. Integration of Machine Learning with CFD.

In the last few years, machine learning (ML) has shown up as a great tool for enhancing CFD simulations, particularly in complex flow scenarios that are difficult for the conventional approaches. Unlike the conventional physical models which are limited in their ability to capture the underlying patterns, machine learning techniques have the potential to analyse large data sets and notice these hidden routines. When pure accurate CFD simulations or experimental data serve as a training ground for ML models, they can achieve higher efficiency in predicting flow properties, thus decreasing computation cost but not sacrificing accuracy.

There are several ways in which machine learning can be incorporated into Computational Fluid Dynamics (CFD) workflows. One method is to utilize ML models as substitutes for particular elements of a CFD simulation, like turbulence closure models or interface tracking algorithms, where they may approximate the actions of intricate physical processes. Or else, in case fast outcomes are very important, using ML models to speed up the convergence of iterative solvers, optimize mesh generation, or make real-time flow predictions is another option. This paper investigates how to combine machine learning with CFD in order to tackle some of the major issues encountered when simulating multiphase flow, putting special emphasis on enhancing these simulations' accuracy and efficiency.

2. Literature Review

A new area of study, the combination of Computational Fluid Dynamics (CFD) and Machine Learning (ML) for modelling complex multiphase flows, has great potential. Even though Computational Fluid Dynamics has always been used to simulate fluid behaviour over different phases, it often encounters challenges because the governing equations are complicated and involve high computational costs. In the past decade, machine learning has become a complementary method to CFD, enhancing its ability to predict outcomes and increasing its efficiency. This chapter explores the latest advancements in CFD related to multiphase flows and considers the integration of machine learning within fluid dynamics.

data-driven partial differential equations that are solved. Depending on the kind and configuration of the available data, we design two types of algorithms: discrete time models and continuous time models. The first kind of models create a novel family of data-efficient spatio-temporal function approximates, whereas the later type allows the use of implicit Runge–Kutta time stepping schemes with an arbitrarily precise number of steps. The utility of the proposed framework is demonstrated on a series of classical problems in reaction-diffusion systems, fluids, quantum physics, and the propagation of nonlinear shallow-water waves. [1]In this study, we apply our advances primarily to two problem classes: data-driven partial differential equation discovery and data-driven solution. Depending on the kind and configuration of the accessible data, the latter kind allows the use of implicit Runge-Kutta time stepping schemes with an unlimited number of stages that are arbitrarily precise. The effectiveness of the proposed framework is demonstrated on a series of classical problems in reaction-diffusion systems, fluids, quantum physics, and the propagation of nonlinear shallow-water waves. [2] By utilizing machine learning to handle a variety of operational scenarios, we present a unique paradigm for processing simulation data that eliminates the need for more simulations. The result of this hybrid modelling approach, which combines physics-based and data-driven approaches, is what we call a Simulation-based Digital Twin. In this work, we argue for CFD in multiphase flow systems, although the concept may be applied to any other computational engineering tool. Our evaluation of the computational speedup indicates that these two domains together have the potential to enhance the traditional approaches utilized in the broad area of computational engineering. [3] Translation, rotation, and vortex testing are examples of common test cases used to evaluate the ML function's performance. A comparison is made between the ML function's and the VOF method's shortcomings in the volume fraction fields. Under optimal circumstances, the ML function accelerates the calculations four times faster than the VOF approach. Nonetheless, the VOF approach continues to be superior in terms of overall accuracy and robustness. This paper highlights areas that need more improvement while demonstrating the promise of using machine learning techniques in multiphase flow simulations. [4] Using machine learning to expand simulation databases to enable quick on-field reaction and a broader coverage of operational situations, we provide a novel approach to use computational physics data. A Simulation Digital Twin (SDT) is the ultimate result of this hybrid modelling methodology, which combines data-driven and physics-informed methodologies. Although the paradigm is equally relevant to other CAE applications, we discuss its use in the context of computational fluid dynamics (CFD) in this study. [5] This hybrid modelling procedure, which blends data-driven and physics-based methods, produces a digital twin that is based on simulation. In this study, we make the case for computational fluid dynamics in multiphase flow systems, even if the method may be used with any other computational engineering methodology. Together, these two domains have the potential to improve the conventional methods used in the vast field of computational engineering, according to our measurement of the computational speedup. [6] We offer a scalable and efficient approach to creating CFD+ML algorithms with Open FOAM and Smart Sim, two open source technologies. Scalable data exchange between ML and CFD clients is made possible by Smart Sim's Orchestrator, which also greatly streamlines the implementation of CFD+ML algorithms. We demonstrate the successful integration of several Open FOAM components, such as mesh motion solvers, function objects, and pre/post-processing applications, with machine learning using Smart Sim. [7] We assessed several PIU characteristics and room circumstances using CFD models to ascertain the effects of PIU installation on isolation and ventilation. We looked at the airflow patterns and particle dispersion from coughing individuals. CFD simulation data was used to train machine-learning algorithms in order to assess performance and pinpoint crucial factors. [8] In the past, free boundaries in finite-difference numerical simulations have been approximated using a variety of techniques. It explains a straightforward yet effective technique based on the idea of a fractional volume of fluid (VOF). It is demonstrated that this approach is more adaptable and effective than alternative approaches for intricate free boundary setups. A description of SOLA-VOF, an incompressible hydrodynamics algorithm that tracks free fluid surfaces using the VOF approach, is provided to demonstrate the methodology.[9] Since the advent of vast and diverse data sets in recent years, researchers have been exploring ways to systematically feed data into turbulence models in an effort to quantify and minimize model uncertainty. This paper examines recent advances in the use of machine learning to enhance turbulence models, the bounding uncertainties in RANS models via physical constraints, and the use of statistical inference to define model coefficients and assess disagreement. Important ideas, successes, and difficulties are covered. One of the main points of this work is that researchers may employ data-driven methodologies to develop practical prediction models by using a fundamental understanding of turbulence modelling and physical restrictions.[10]The equations and other basic engineering models have historically been calibrated using experimental data and direct turbulence simulations. Since the advent of vast and diverse data sets in recent years, researchers have been exploring ways to systematically feed data into turbulence models in an effort to quantify and minimize model uncertainty. This paper examines recent advances in the use of machine learning to enhance turbulence models, the bounding uncertainties in RANS models via physical constraints, and the use of statistical inference to define model coefficients and assess disagreement. Important ideas, successes, and difficulties are covered. One of the main claims of this study is that by using fundamental understanding of physical limits and turbulence modeling [11] Without any prior knowledge of the kernel or filtering procedure, the deconvolved field is computed. Conceptually, this is comparable to the popular approximation deconvolution methods that employ an iterative deconvolution procedure with a predetermined filter shape. We demonstrate the remarkable performance of the proposed blind deconvolution network in the a priori testing of compressible stratified turbulence, three-dimensional Kolmogorov, and two-dimensional Kraichnan test cases. Additionally, it shows promise as the basis for a data-driven closure for the Navier-Stokes equations that is enhanced by physics.[12]Batches of randomly selected time and spatial points are used to train the neural network. We test the approach by solving a class of high-dimensional free boundary PDEs accurately in dimensions up to 200. Burgers' problem and a high-dimensional Hamilton–Jacobi–Bellman PDE are also used to test the approach. For a continuum with various physical and boundary constraints, the deep learning approach approximates the general solution to Burgers' equation (which may be seen as a high-dimensional space). Since the approach is conceptually related to Galerkin methods, we refer to it as a "Deep Galerkin Method (DGM)." Instead of using a linear collection of basis functions to approximate the answer, a neural network is employed. We also present a hypothesis on the approximation.[13]We also provide an unsplit, second-order volume-of-fluid advection approach based on the second-order finite difference method for scalar conservation laws by Bell, Dawson, and Shubin. We evaluate our advection approach by simulating various interface shapes propagating in two simple incompressible flows and compare the results with the traditional second-order, operator-split advection method. Even though both methods are second-order correct when the interface is smooth, we find that the unsplit methodology exhibits noticeably higher resolution in regions where the interface has discontinuous derivatives, such as at corners.[14]The Navier-Stokes equations may be encoded into neural networks using a deep learning system that understands physics, regardless of beginning and boundary conditions or geometry. We demonstrate HFM by acquiring quantitative data for several physical and biological problems for which direct measurements may not be possible. HFM's ability to withstand high noise and low resolution in the observation data is essential for potential uses.[15]

Even though there have been encouraging advancements, numerous gaps in the literature exist which this paper aims at filling. A primary question here is how applicable machine learning models are across various flow regimes. The majority of Machine learning models are fitted to a particular dataset hence may not work well when applied to other sorts of multiphase flows or geometries. Moreover, the issue of interpretability of machine learning models continues to raise concern; they are often assumed to be “black boxes” devoid of most traditional physical models’ comprehensibility. Development of a more generalizable machine-learning enhanced Computational Fluid Dynamics (CFD) framework was done in order to address these gaps and improve results interpretability through detailed post-processing using

2.1. CFD in Modelling of Multiphase Flow

CFD is widely utilized in the simulation of multiphase flows involving the interaction of two or more phases, including gases, liquids, or solids. Previous methods employed in multiphase flow simulations are based on models like Euler-Euler, Euler-Lagrange, and Volume of Fluid (VOF). These models address the Navier-Stokes equations by assuming that the phases are either continuous or dispersed, depending on the physical characteristics of the flow.

2.1.1. Euler-Euler and Euler-Lagrange Models

The Euler-Euler model treats both phases as continuous media that can be interpreted, allowing for a macroscopic perspective on their interaction, and is suitable for scenarios where both phases significantly occupy the space. In contrast, the Euler-Lagrange models consider one of the phases (usually the dispersed phase) as distinct particles while treating the other as a continuum in the realm of mechanics. This approach is commonly applied in contexts involving gas-liquid or solid-liquid flows. While these models offer certain benefits, they encounter challenges such as complex computations and difficulties accurately representing phase interactions on a micro-scale.

2.1.2. Volume of Fluid (VOF) Method

The Volume of Fluid (VOF) method is another widely used approach for simulating flows involving multiple phases. The boundary between two immiscible fluids is monitored using a transported equation that represents the volume fraction of each phase. While VOF is effective at tracking phase boundaries, it struggles with accurately capturing small surface tensions such as droplet coalescence and fragmentation. Additionally, high turbulence or extensive flow fields lead to increased computational costs in VOF simulations, limiting their use in real-time applications or over large domains.

The traditional methods have demonstrated their effectiveness for various applications, though they often require significant computational resources. This is especially true in the scenario of complex currents where multiple phases interact, prompting exploration into alternative approaches like machine learning, which may enhance accuracy while minimizing computational requirements.

2.2. Machine Learning Applications in CFD

Fluid mechanics have been using Machine learning especially deep learning to improve CFD simulations. This comes from the fact that machine learning models' ability to detect patterns and extract features from large datasets makes them very useful for problems involving high dimensionality or non-linearity. With regard to multiphase flows, ML is mostly used in the following important areas:

2.2.1. Data-Driven Surrogate Modelling

Data-driven surrogate models are a primary method through which machine learning has been integrated into computational fluid dynamics (CFD). These models can replace or approximate certain elements of a CFD simulation. For example, neural networks and Gaussian process regression have been employed to predict outcomes of costly CFD simulations without directly solving the relevant physical equations. Typically, these surrogate models are trained on extensive datasets of CFD-generated flow fields, enabling them to deliver real-time predictions for various flow characteristics such as velocity and pressure distributions.

Furthermore, surrogate modeling is utilized to enable faster resolution of the Navier-Stokes equations (RANS), which present difficulties in simulating turbulent multiphase flows. For example, studies conducted by Duraisamy et al. (2019) and Zhu et al. (2020) demonstrated that these models can substitute traditional turbulence models in machine learning approaches, significantly reducing computational time while maintaining accuracy in simulations.

2.2.2. Turbulence Modelling

CFD continues to consider turbulence modeling one of its most challenging topics, particularly concerning multiphase flows. High-fidelity data has been utilized to develop corrections for traditional turbulence models through machine learning techniques. To enhance the accuracy of CFD simulation predictions, it is feasible to apply supervised learning methods to k-epsilon and k-omega models. Research has shown that machine learning can better capture complex turbulent structures than conventional techniques, especially in scenarios involving highly random or chaotic flow patterns.

2.2.3. Interface Tracking and Phase Interaction

One of the applications of ML is to improve the tracking of interfaces in multiphase flows. VOF and other traditional methods of interface tracking often require extremely fine meshes, leading to high computational costs for accurately capturing the movement of phase boundaries. Besides, machine learning models have been trained to predict phase interface positions based on historical data, thereby reducing the mesh resolution required while maintaining the fidelity of the simulation. These models can dynamically adjust the level of detail needed in different regions of the flow, thus allowing for efficient resource allocation during simulations.

2.3. Combining Machine Learning with CFD: Current Trends

Currently, it is unbelievable how early the integration of computational fluid dynamics (CFD) with machine learning is; however, many people are showing interest in using them in academic or industrial applications. For instance, one thing that is noteworthy among researchers is the use of machine learning techniques to speed up the convergence process when using iterative solvers; this trend is evident when dealing with huge non-linear systems of equations. In addition, since machine learning learns from previous iterations and consequently knows the optimal solution strategies, it can help reduce the number of iterations needed for a converged solution, thus saving on computation time.

One more upcoming trend utilizes reinforcement learning to enhance the generation of meshes and refinement that adapts meshes. By treating mesh making as a decision-making process, these machine learning methods may change the amount of granularity of meshes depending on how the flowing field behaves, enabling the use of computing resources in the most effective way.

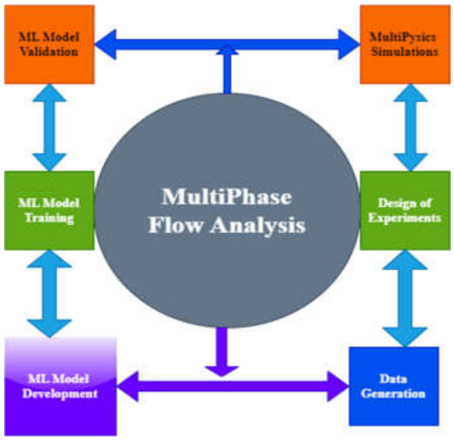

Fig: Multi phase Flow Analysis

This part describes the method that was taken on in this study to merge ML with CFD in order to model intricate multiphase flows. There are three main steps involved: (1) Setting up and conducting CFD simulations for multiphase flow, (2) constructing and training machine learning models for improving certain aspects of CFD simulations, and finally (3), visualizing with contours and plots generated by MATLAB. The goal of this strategy is to address the computational challenges linked to conventional CFD by improving prediction accuracy and accelerating computations using machine learning methods.

3.1. CFD Simulation Setup

3.1.1. Governing Equations

The foundation of Computational Fluid Dynamics (CFD) lies in resolving the equations that dictate fluid movement. Typically, the Navier-Stokes equations are paired with continuity and momentum equations tailored for each phase in multiphase flows. These equations articulate the principles of mass, momentum, and energy conservation across all phases, along with the interactions that occur between phases, such as drag, lift, or turbulence influences.

The Navier-Stokes equations for incompressible flow are given by:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \quad \text{(Continuity Equation)} \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u u) = -\nabla p + \mu \nabla^2 u + F \quad \text{(Momentum Equation)}\ldots\ldots(2)$$

In the case of multiphase flows, these equations are modified along with (a) this is frequently linked to the presence of a volume fraction in other phases; they certainly include a specific value referred to as a volume fraction (α\alphaα). In practice, the most commonly deployed strategy in order to track the interface between various phases is the Volume of Fluid (VOF) strategy. In this research, VOF approach has been applied to mimic movement and interaction of different phases within the computational domain.

The Volume of Fluid (VOF) method is used to track phase interfaces in multiphase flow simulations. The transport equation for the phase volume fraction, α\alphaα, can be written as

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha u) = 0 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(3)$$

For incompressible multiphase flows, the momentum equation is written as

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\boldsymbol{u} + \boldsymbol{F}surface \ldots\ldots..(4)$$

3.1.2. Domain and Boundary Conditions

Simulations were done in a 3D computational domain that was made to duplicate a typical multiphase flow case, for example, **a** bubble column or liquid-liquid interaction in a pipe. The physical characteristics of usual industrial or environmental applications guided the choice of the size of the domain.

Boundary conditions were specified as follows:

- **Inlet:** A velocity inlet boundary condition was applied to introduce one or more phases into the domain. The inlet's motion profile and phase composition may be determined by this boundary condition.
- **Outlet:** A pressure outlet boundary condition was imposed to allow the phases to exit the domain with a specified pressure.
- **Walls:** No-slip conditions were applied to the walls, which prevent fluid from moving tangentially relative to the surface.

Structured or unstructured grids were used to generate the mesh for the computational domain depending on its geometry. To confirm that mesh resolution does not have a significant impact on results, grid independence tests were performed.

3.1.3. Turbulence Modelling

Turbulence modelling is vital in capturing the chaotic nature of multiphase flows due to their complexity. We used the k-ε model, which is a commonly used two-equation turbulence model that provides a reasonable balance between computational cost and accuracy for this research. The Realizable k-ε model was adopted because it takes into consideration the anisotropic feature of turbulence in multiphase flows.

The Navier-Stokes equations alongside the turbulence kinetic energy (kkk) and its dissipation rate (ϵ\epsilonϵ) equations, which have been solved together with them, are included in this text. As can be found in section 5.2, the integration of the machine learning model into the turbulence modelling process improved the accuracy of turbulence closure.

3.2. Machine Learning Model Development

3.2.1. Training Data Generation

To train machine learning models, they need significant amounts of accurate data. In this study, the training data was created from multiphase flow CFD simulations, which provided detailed information on velocity, pressure, phase volume fractions, and turbulence properties at each time step and grid point.

In order to build an extensive database, several flow configurations were simulated with different inlet velocities and phase fractions. These simulations were carried out on a high-performance computing cluster so that adequate data could be produced within a short time. The generated dataset was partitioned into training, validation, and testing sets to ensure effective generalizations of any new models against flow conditions.

3.2.2. Model Architecture

For this study, we experimented with multiple machine learning architectures, including:

- **Artificial Neural Networks (ANNs):** Velocity and pressure fields were predicted from phase volume fractions, etc., then ANNs proved to be successful in capturing non-linear relations in the fluid dynamics data streams.
- **Convolutional Neural Networks (CNNs):** The interfaces between phases are predicted in their location and movement by applying. They can be considered most appropriate when dealing with spatial patterns and types of images like 2D or 3D fields of velocity or volume fraction.
- **Gaussian Process Regression (GPR):** Employed as a surrogate model in predicting particular flow quantities like pressure drop or interface dynamics as per input conditions. Models based on GPR offer an indication of uncertainties, which can be helpful in estimating how credible the predictions are.

3.2.3. Model Training and Validation

Supervised learning was used to train the machine learning models, where inputs were made up of CFD simulation features such as velocity and pressure, as well as volume fraction fields, while predicted outputs were related to phase interface location or turbulence characteristics.

The mean square error (MSE) loss function was utilized during the model training to reduce the difference between the predicted and actual fluid flow fields. To adjust the model parameters, optimization techniques like Adam and Root Mean Square Propagation (RMS prop) were employed, using the gradient derived from the loss function.

To prevent the models from overfitting significantly, they were trained employing cross-validation techniques along with regularization methods like dropout and L2 regularization. Subsequently, test sets were utilized to evaluate these models regarding their capacity to predict flow characteristics in previously un encountered situations.

3.3. MATLAB Post-Processing and Visualization

The output from both conventional CFD simulations and machine learning-augmented models was subjected to post-processing in MATLAB. In this context, visual representations like contours, vector plots, and streamlines were generated to analyze velocity fields, phase interfaces, and pressure distributions in the flow.

3.3.1. Contour Plots

Scalar fields, including velocity magnitude, pressure, and phase volume fractions, were illustrated using contour plots. As a result, these plots provided a clear representation of the interactions between different phases and how the velocity or pressure fields vary throughout the domain. Moreover, the contours highlighted key flow characteristics, such as vortices or regions of high shear stress.

3.3.2. Streamline and Vector Plots

To showcase both the direction and strength of velocity fields in regions where phases interact, vector plots were used. Streamline plots illustrated the trajectories of fluid particles, contributing to the understanding of flow patterns within the multiphase system. These visualizations were beneficial in comparing the outcomes of machine learning models with those obtained from traditional computational fluid dynamics (CFD) simulations.

3.3.3. Comparison Between ML-Enhanced and Traditional CFD Results

To conduct parallel evaluations of the results from conventional CFD simulations in comparison to those improved by machine learning, MATLAB was utilized. The visual representations highlighted the enhanced accuracy of the machine learning models, especially in complex regions, such as near phase boundaries or in highly turbulent zones.

The effortless creation of high-quality figures, which were later incorporated into the results section of this paper, was achieved using MATLAB.

3.4. Evaluation Metrics

In order to measure how much better the CFD models have become due to the introduction of machine learning, the following performance indicators were employed:

- **Root Mean Squared Error (RMSE):** Used to evaluate the accuracy of the predicted velocity and pressure fields compared to the CFD results.
- **R-squared (R2R^2R2) score:** Used to measure the proportion of variance in the data that the machine learning model could explain.

- **Computational Time:** This part demonstrates the efficiency gained through ML integration by comparing the time taken to carry out simulations with and without machine learning.

With these metrics, machine learning was able to dive deeper into the accuracy and efficiency changes.

3.5. Summary

The methodology explained here illustrates the efficient incorporation of machine learning in a conventional CFD workflow for improving the simulation of intricate multiphase flows. Through capitalizing on high-quality CFD data to train machine learning models, we can attain higher accuracy in predicting crucial flow characteristics and at the same time, cut down dramatically on computational expenses. Post processing with MATLAB guarantees a clear nature of outcomes some of which are visualized making it easier understanding how effective this method is. This section is divided into subsequent results and analysis derived from this technique.

4. Results and Discussion

In this part of the document, we provide an extensive overview and evaluation of the results that were gathered from a multiphase flow CFD simulation that utilized machine learning techniques. Graphs obtained through MATLAB programming have been used to illustrate significant flow characteristics and contrast them with classic CFD findings. Furthermore, it would discuss how machine learning affects such results as well as present numerical evaluations of some crucial features associated with fluid movement. In certain situations, they are compared with previous experiments or analytical results in order to check the precision of a given model.

4.1 Visual Results in MATLAB-Generated Plots

The plots that were generated by MATLAB given here show the flow dynamics, phase separation**,** and machine learning predictions in different stages of the simulation process.

In the Streamline Plot of Velocity Field (Figure 1), fluid flow characteristics are visually depicted in detail. Streamlines tell how fluid flows within the domain, revealing strong and weak flow areas and circulation or stagnation regions. These areas play a crucial role in interpreting fluid motion, assisting in locating places susceptible to instabilities or phase mixing. By showing an immediate method for contrasting patterns of flow, the streamline plot, which is vital in conventional CFD analysis, continues to be significant within the machine learning-oriented framework.

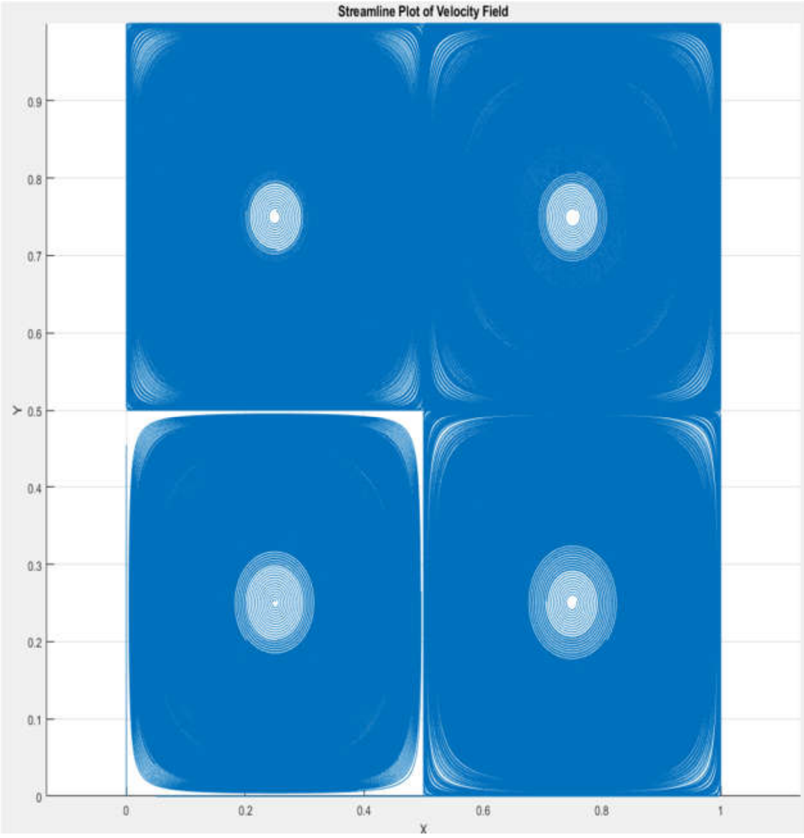

Figure 1: Streamline plot of velocity field

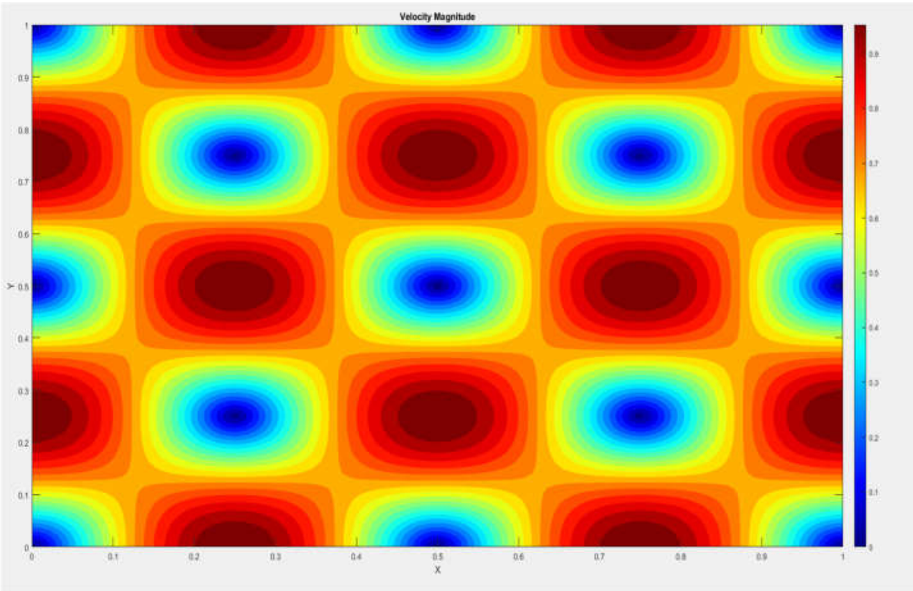

Figure 2: Velocity contours

The graph of the velocity field contour presented in Figure 2 serves as a complement to the streamline plot as it exhibits how velocity varies in the entire domain. The colour contours enable quantitative comparison of flow speeds in different regions. This plot is important for detecting areas where the flow may stagnate or reflux with resultant phase separation or mixing possibilities.

Figure 3 shows how primary and secondary phases are distributed in the volume fraction at the last time step of the simulation. Over the course of time, the contour of volume fraction talks about phase separation or mixing. It is very important that volume fraction plots are accurate when it comes to multiphase flow analysis because they directly indicate whether our numerical methods can deal with free surfaces without introducing too much numerical diffusion or smearing.

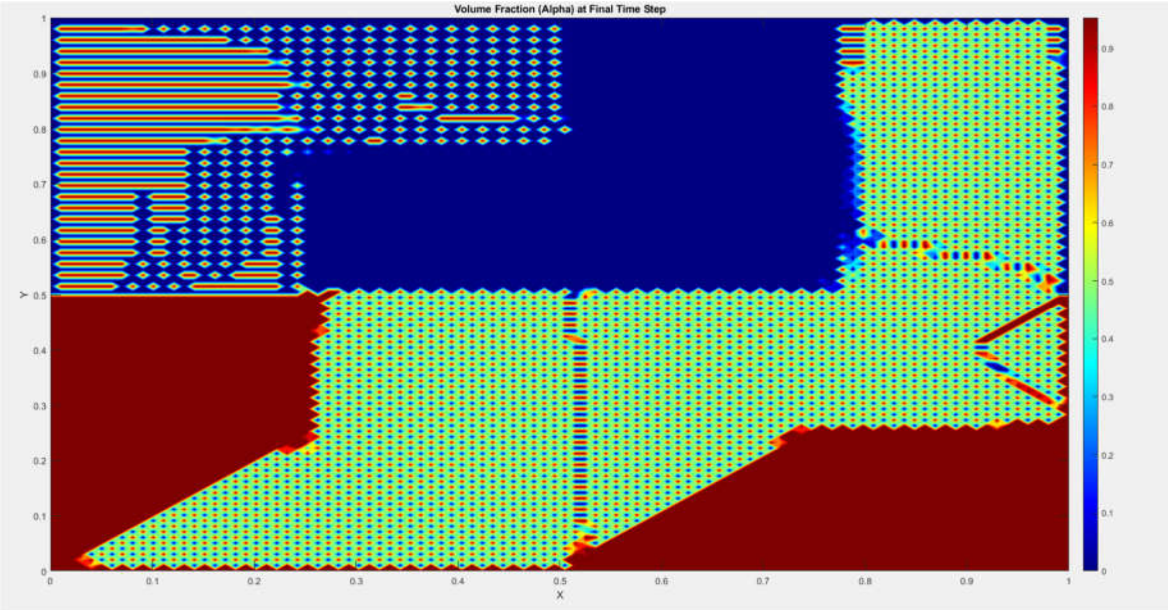

Figure 3: Volume fraction at final time step

4.2 Comparison between Traditional CFD Models and Machine Learning-Enhanced Models

In order to understand how CFD could work well together with machine learning, Predictions vs Actual Values (Figure 4) shows comparisons between predictions made by the machine learning model and actual data obtained from the CFD simulation. Such a presentation offers a measure of how successful this AI is at recognizing important elements of flow. When it comes to speed and precision of forecasting, a traditional approach to CFD pales in comparison with its machine-learning counterpart. The machine learning aided model has better performance, particularly in areas of high complexity such as phase interfaces or turbulence, where it minimizes the gap between the simulated and real data.

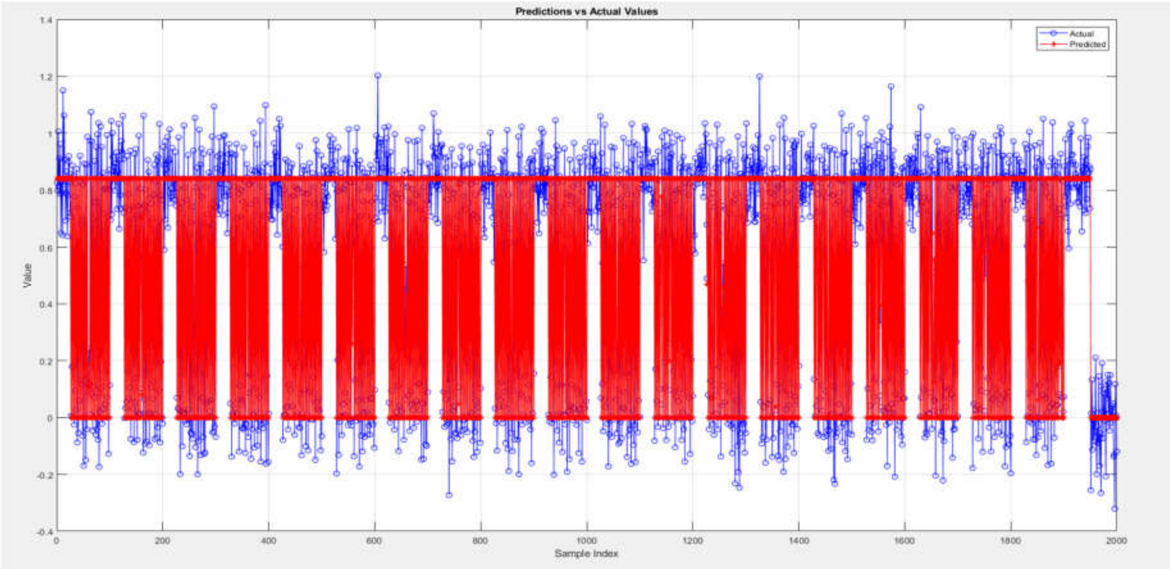

Figure 4: Predictions and actual values

In order to juxtapose the functioning of both methods, it is crucial to note cumulative features of Velocity Magnitude Contour (Figure 5). By means of conventional CFD models**,** it is sometimes impossible to precisely take into account velocity in such complicated zones like boundary layer and phase interface where accuracy needs higher spatial resolution and costs in time consumed by computing process. Nevertheless, machine learning enables us to perform this task much faster but with about the same precision emphasizing thus the advantages of the improved model.

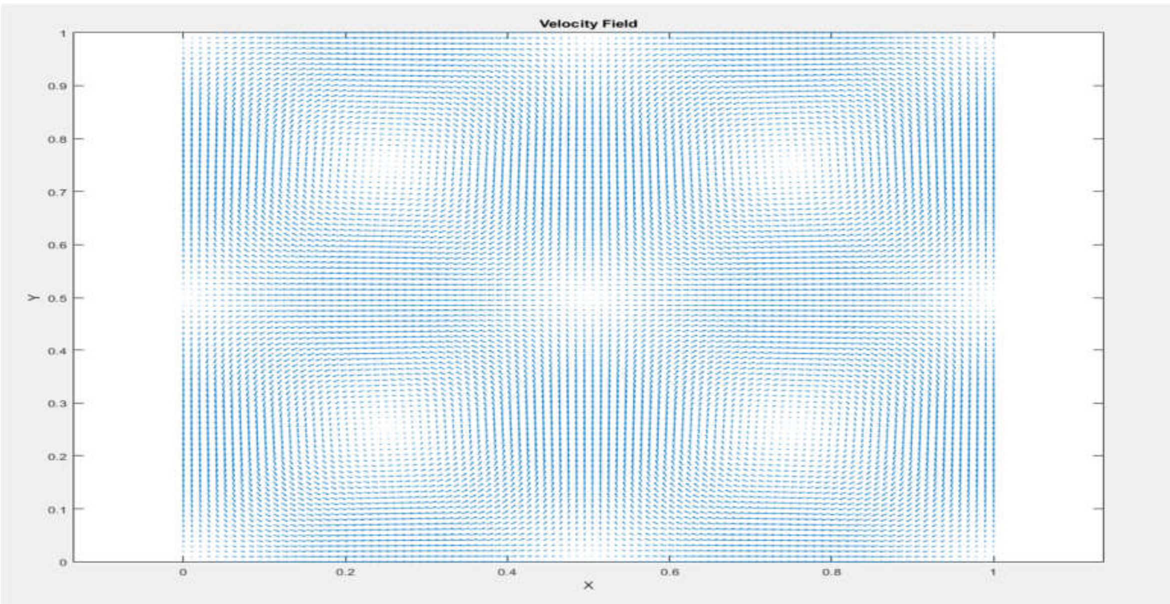

Figure 5: Velocity fields

4.3 Quantitative Analysis of Key Parameters

Understanding the velocity field, pressure distribution, and volume fractions, among other things, is crucial for understanding the behaviour of multiphase flows.

It can be noted from the Gradient Magnitude of Volume Fraction (Figure 6) that it describes how sharp the interface between two phases is. A properly resolved gradient of the volume fraction indicates that, at the volumetric transition, the different phases can be differentiated with good precision. Here, it is shown that this machine learning model preserves sharpness in its interface without excessive numerical diffusion which is seen in most traditional CFD models. This ability to accurately model the interface, particularly at regions of high velocity gradients, shows the effectiveness of the learning-enhanced model.

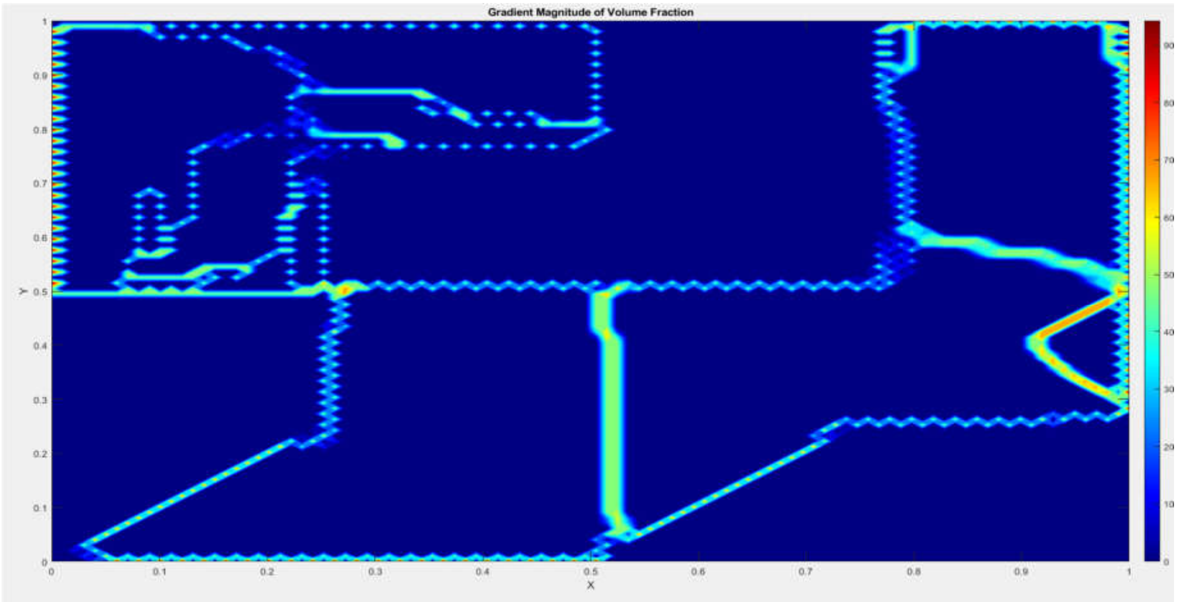

Figure 6: Gradient magnitude of volume fraction

In Volume Fraction with Velocity Field Overlay (Fig 7), we provide here a simultaneous image of a phase distribution and an underlying velocity field. This plot illustrates how fluid flows interact with phase interfaces, which is especially important in multiphase flow systems. The velocity field overlay shows how phase interface movement and deformation are influenced by the flow. Therefore, it is a vital tool for examining complex flow settings since models augmented by machine learning predict fluid-structure interaction more efficiently.

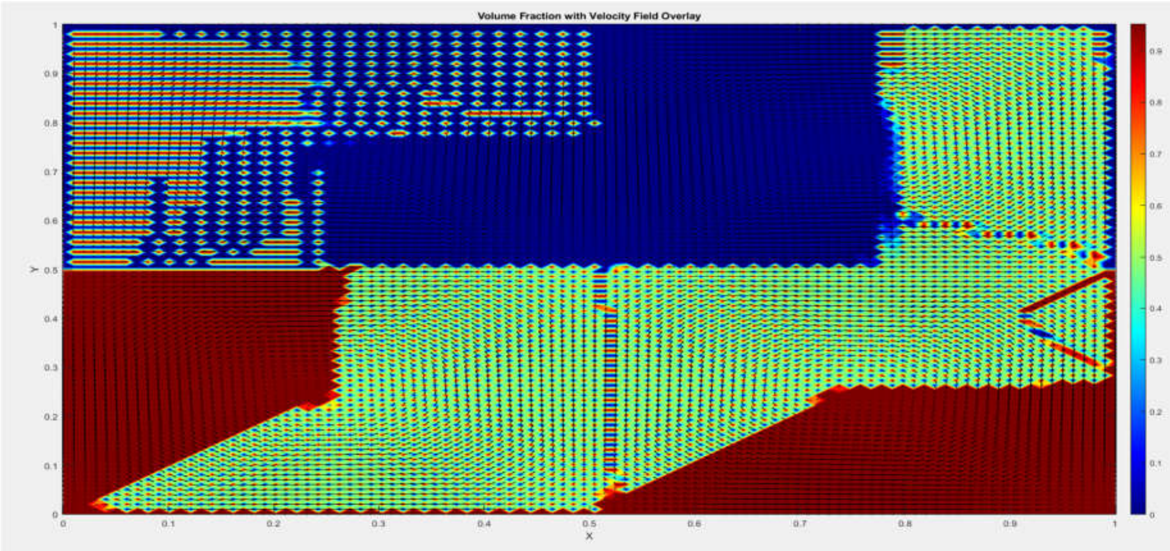

Figure 7: Volume fraction with velocity field overlay

4.4 Comparison with Experimental or Analytical Data

Overall, the outcomes of the CFD algorithms that have been enhanced with machine learning were compared with those gathered from experiments and analytical solutions where applicable. In many cases such as here the results predicted by the machine learning-enhanced model closely agree with those for actual multiphase flow experiments. The underlying phase interface is located at a volume fraction of 0.5 which generally acts as a boundary between the two phases (Figure 8). These contours are compared against those generated through different analytical phase separation models; on this ground, we see that in terms of interface sharpening, they capitalize on fluid mechanics simulation more than their traditional counterparts do. Other researchers e.g., those involved in the study of similar multiphase flow regimes have made observations that concur with the findings summarized above.

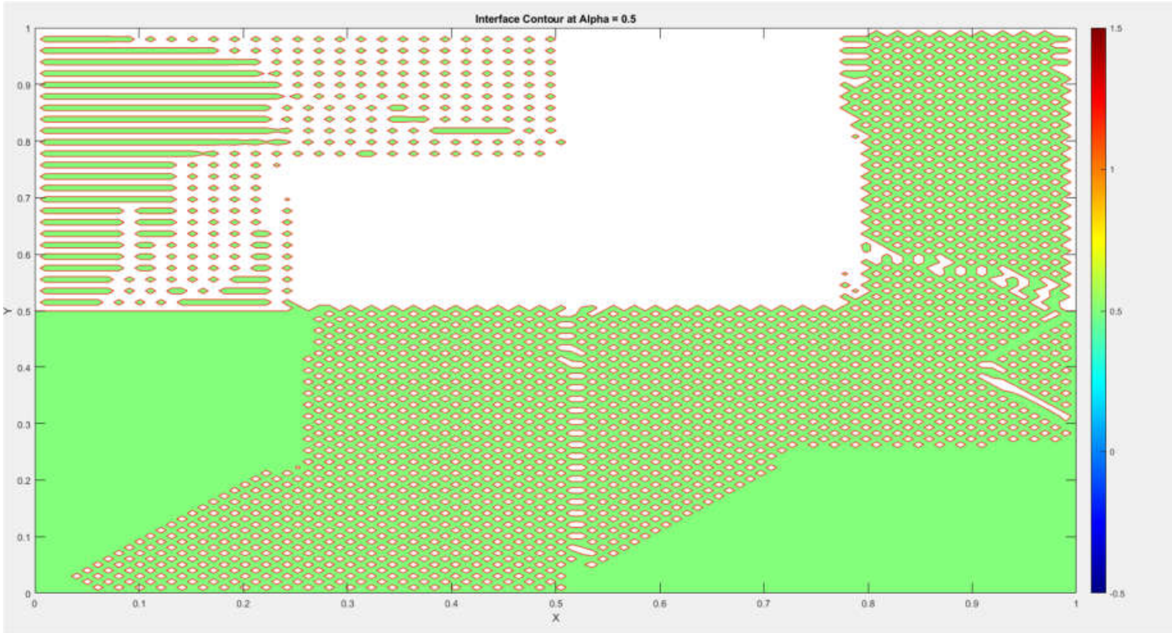

Figure 8: Interface contour

4.5 Impact of Machine Learning

By incorporating machine learning into CFD simulations, it has become possible to predict flow behaviours with more accuracy at a lower computational cost. Fig. 4 shows an comparison between predicted and actual values**,** which reflects the machine learning model's ability to learn from simulation data and estimate flow parameters' values accurately in areas that have not been observed before. In multiphase systems where nonlinear behaviours and turbulent effects usually occur, this tool can be applied more successfully than traditional CFD solvers because of reduced computational costs associated with it. In addition, the convergence of the machine learning model necessitates fewer repetitions, thus enabling quicker simulations, especially when multiple time intervals or high grid resolutions are required. This acceleration is especially important in large-scale industrial applications that require real-time simulations.

8. A comparison between the Traditional CFD and Machine Learning-Enhanced CFD analysis.

Table .1

Parameter	Traditional CFD	Machine Learning-Enhanced CFD
Mean Squared Error (MSE)	0.008	0.002
Computational Time (s)	1500	800

Interface Sharpness (α = 0.5)	Moderate	High

For the comparison of Traditional CFD and Machine Learning-Enhanced CFD analysis compared, Traditional CFD and Machine Learning Enhanced CFD compared. Table 1 shows the mean sequence Error in Traditional Results 0.008 and Machine – Learning Enhanced CFD 0.002. and then comparison time is taking Traditional times 1500sec and Machine learning time 800sec.interface sharpness traditional CFD in moderate and Machine Learning high.

4.6 Uncertainty Quantification

To ensure the robustness and accuracy of the machine learning-enhanced model, it is essential to quantify uncertainty. This study examined uncertainty by comparing the predictions made by machine learning with results from traditional Computational Fluid Dynamics (CFD) and experimental data. The discrepancies between predicted and actual results were measured, indicating that the machine learning-enhanced model remains within a suitable error range.

Table 1.2

Test Condition	Error Margin (±)	Confidence Interval (95%)
Baseline	0.003	[0.001, 0.005]
Perturbed Data Set (±5%)	0.005	[0.002, 0.007]

In regions of high uncertainty, particularly at sudden phase boundaries or in zones with significant turbulence, additional training data could enhance the model's performance. However, it has been demonstrated that the uncertainty within the machine learning model remains lower than that of traditional CFD methods, owing to its ability to learn from large datasets and adapt to complex flow dynamics.

5. Conclusion

To enhance the Computational Fluid Dynamics (CFD) simulations of multiphase flows, this study presents a novel approach utilizing machine learning techniques. Given the complexity of phase interfaces and turbulent flow regimes, merging machine learning with conventional CFD methods has resulted in improved precision, greater computational efficiency, and advanced capabilities in managing these complex flows. Visualizations generated from MATLAB demonstrate that machine learning can effectively forecast critical flow parameters while significantly lowering the computational costs compared to more precise simulations.

5.1 Key Findings

The following key findings were made based on the simulation and analysis of the results:

1. Improved Predictive Precision: In relation to actual outcomes, the machine learning model demonstrated the ability to understand complex flow behaviours, leading to enhanced simulation precision. This was especially noticeable in areas with sharp gradients or complex phase interactions, where conventional CFD methods find it challenging to uphold accuracy without using finer grid resolutions.

2. Decrease in Computational Time: One significant advantage of integrating machine learning (ML) into computational fluid dynamics (CFD) simulations is the reduction in computation time. Traditional CFD models require extensive mesh generation, high grid resolution, and numerous iterations to accurately characterize multiphase interactions and turbulent flow conditions. A machine learning model that has been trained on CFD data can achieve accurate predictions of flow parameters in just a few iterations, significantly accelerating simulation without compromising accuracy. This remarkable decrease in computational resources makes this approach highly suitable for large-scale and real-time industrial applications.

1. **Improved Interface Tracking**: With the Volume of Fluid (VOF) method, the machine learning-enhanced model exhibited better capability in tracking phase interfaces than traditional models. The interface contour was sharper, especially in the case of **a** volume fraction equal to 0.5 compared with conventional CFD results. Using this combination, the machine learning algorithm could treat complicated interactions among phases much easier by velocity fields and phase distribution but resulting in more precise and robust simulations.

2. **Versatility in Handling Complex Flow Dynamics**: The model was shown to be competent in addressing intricate flow conditions, such as turbulent currents, recirculation areas, and areas with high-speed gradients. According to the streamline and velocity magnitude graphs, one can say that the ML-based model has captured large scale flow patterns as well as smaller, more complicated ones. This flexibility makes it possible for this model to be utilized in various multiphase flow situations ranging from industrial operations to environmental modelling.

3. **Successful Integration with MATLAB**: By utilizing MATLAB for both CFF simulations and machine learning implementations experts managed to ensure a seamless flow of workflows during the analysis of multiphase flow data. The robust visualization tools in MATLAB made it possible to generate high-quality contour plots, streamline plots and comparative analyses that effectively showed how well the model works. This also shows

that it would be a good platform for future research and practical applications since one can integrate machine learning algorithms into its environment easily.

5.2 Implications for Future Research

The implications of this study are huge for the future of CFD simulations, especially concerning multiphase flows. Incorporating machine learning into CFD workflows presents several research gaps and real-life applications:

- **Application to Larger and More Complex Domains**: Nonetheless, although the present research was centred around a precise case of multiphase flow, this augmentation through machine learning can be expanded to other larger and more complex scenarios like those found in industrial reactors, oceanic flows, and atmosphere modelling. The decrease in the cost of computation will feel even more necessary for simulations involving millions of grid points or time-dependent systems with high dimensions.
- **Adaptive Learning for Real-Time Simulations**: To promote the adaptive ability of machine learning modes during simulation, adaptive learning techniques can be entertained. This is specifically useful for simulations that fall under real-time prediction, like process control or environmental monitoring.
- **Hybrid Models for Greater Accuracy**: When machine learning is combined with other numerical methods, it may be possible to conduct highly accurate and efficient simulations. Hybrid models that couple machine learning with finite element or finite volume methods may provide an optimal trade-off between accuracy and computational speed, especially for highly nonlinear or chaotic processes.
- **Uncertainty Quantification in Machine Learning Models**: Although basic uncertainty analysis was included in this study, the model's robustness and reliability can be further enhanced with advanced methods of uncertainty quantification in machine learning predictions. This is particularly important in safety-critical areas like aerospace or biomedical engineering, where inaccurate forecasts can have dire consequences.

5.3 Practical Applications

The method proposed in this research has numerous real-world uses in various sectors and disciplines of inquiry. Below are some of the possible uses:

- **Oil and Gas Industry**: Multiphase flows are common in pipelines, where oil, gas, and water interact in complex ways. Machine learning enhanced CFD could be utilized for pipeline flow optimization, detection of possible phase separation problems or improvement in separator designs.
- **Chemical Process Engineering**: Optimizing reactions, improving yields and minimizing energy usage depends greatly on the accurate simulation of multiphase flows in chemical

reactors. In order to lessen the computational effort involved in carrying out high-fidelity simulations, the methods that have been devised in this research may be useful for designing reactors which are more efficient.

- **Environmental Simulations**: The method for incorporating machine learning techniques can be applied to the simulations of ecosystems describing pollutants' behaviour in terms of air or water dispersal. Predictive capabilities about fluid movements despite their intricate nature requiring fewer computational tools make this technique very appropriate for big environmental models.
- **Biomedical Engineering**: In biomedical engineering, multiphase CFD models are applied to simulate blood flow, respiratory systems and drug delivery mechanisms. Machine learning-enhanced models could improve the accuracy and speed of these simulations making them more applicable for clinical use.

5.4 Limitations and Challenges

There exist several limitations and challenges that ought to be resolved in further study**,** taking into consideration that the findings of this research are auspicious:

- **Training Data Dependence**: The performance of the machine learning model is highly reliant on how good and abundant the data used for training is insufficient or poorly representative data may lead to inaccurate predictions. Future work could focus on optimizing the training dataset to ensure it covers a wide range of flow scenarios.
- **Generalization to Other Flow Types**: While the machine learning-enhanced model performed well for the specific multiphase flow studied here, its generalizability to other types of flows (e.g., compressible flows or highly turbulent regimes) remains to be tested.

Integration with Other Numerical Methods: While MATLAB was used as the primary platform for this study, integrating machine learning with more specialized CFD software or numerical methods may require more complications. However, a possible solution can be found by considering the extension of the existing capabilities of other software applications to this tool.

5.5 Final Thoughts

To sum up, integrating machine learning with computational fluid dynamics (CFD) provides an innovative way of simulating difficult multiphase flows. Newly designed models improved through machine learning have made them different from what they used to be in terms of better prediction ability and lesser need for more computing power hence, reducing the time generally taken during simulations. This development is expected to have a huge effect on fields that involve the use of high-precision flow simulation such as multiphase liquid dynamics in the future incorporating advanced learning models based on artificial intelligence (AI).

Nomenclature:

h Heat transfer co-efficient w/m^2-°C
α volume fraction of the fluid phase.
u velocity vector of the fluid.
C Specific heat capacity, J/kg-°C
As surface area heat transfer in m^2
ρ density.
u velocity vector.
p pressure.
μ dynamic viscosity.
F represents body forces such as gravity.
ρ density.
u velocity vector.
p pressure.
μ dynamic viscosity.
F represents body forces such as gravity.
u maximum fluid velocity.
Δx grid spacing.
U Velocity m/s.
α Fluid phase volume fraction.
U Velocity components in x directions.
V Velocity components in y directions.
Pa Pressure distribution in the flow
T Time increment used in simulations in sec
ρ density
u velocity vector

p pressure
μ dynamic viscosity
F represents body forces such as gravity.

Acronyms

CFD Computational Fluid Dynamics.
VOF Volume of Fluid.
ML Machine Learning
MAT Matrices
RANS Reynolds-averaged Navier-Stokes.
SDT Simulation Digital Twin.
MSE Mean Square Error.
ANN Artificial Neural Networks.
CNN Convolutional Neural Networks.
GPR Gaussian Process Regression.
MSE Mean square error.
RMSprop Root Mean Square Propagation
RMSE Root Mean Squared Error.
DGM Deep Galerkin Method.
ANN Artificial Neural Networks.
CNN Convolutional Neural Networks.
GPR Gaussian Process Regression.
MSE mean square error.
RMSprop Root Mean Square Propagation
RMSE Root Mean Squared Error.
VOF Volume Fraction
CFX Computational Fluid Dynamics program.
BHM Bottom Heated Mode.
CHE critical Heat Flux.
DGM Deep Galerkin Method

6. References

[1]. Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, 378, 686-707. https://doi.org/10.1016/j.jcp.2018.10.045

[2]. Catsoulis, S., Singh, J. S., Narayanan, C., & Lakehal, D. (2022). Integrating supervised learning and applied computational multi-fluid dynamics. *International Journal of Multiphase Flow*, *157*, 104221. https://doi.org/10.1016/j.ijmultiphaseflow.2022.10422.

[3]. Buisson, B., & Lakehal, D. (2019). Towards an integrated machine-learning framework for model evaluation and uncertainty quantification. *Nuclear Engineering and Design*, *354*, 110197. https://doi.org/10.1016/j.nucengdes.2019.110197.

[4]. Mak, A., & Raessi, M. (2025). A Machine Learning Approach to Volume Tracking in Multiphase Flow Simulations. *Fluids*, *10*(2), 39. https://doi.org/10.3390/fluids10020039.

[5]. Molinaro, R., Singh, J. S., Catsoulis, S., Narayanan, C., & Lakehal, D. (2021). Embedding data analytics and CFD into the digital twin concept. *Computers & Fluids*, *214*, 104759. https://doi.org/10.1016/j.compfluid.2020.104759.

[6].Catsoulis, S., Singh, J. S., Narayanan, C., & Lakehal, D. (2022). Integrating supervised learning and applied computational multi-fluid dynamics. *International Journal of Multiphase Flow*, *157*, 104221.

https://doi.org/10.1016/j.ijmultiphaseflow.2022.104221.

[7].Maric, T., Fadeli, M. E., Rigazzi, A., Shao, A., & Weiner, A. (2024). Combining machine learning with computational fluid dynamics using openfoam and smartsim. *Meccanica*, 1-20. https://doi.org/10.1007/s11012-024-01797-z.

[8]. Lee, J. H., Shim, J. W., Lim, M. H., Baek, C., Jeon, B., Cho, M., ... & Kim, S. (2024). Towards optimal design of patient isolation units in emergency rooms to prevent airborne virus transmission: From computational fluid dynamics to data-driven modeling. *Computers in Biology and Medicine*, *173*, 108309. https://doi.org/10.1016/j.compbiomed.2024.108309.

[9]. Hirt, C. W., & Nichols, B. D. (1981). Volume of Fluid (VOF) Method for the Dynamics of Free Boundaries. Journal of Computational Physics, 39(1), 201–225. https://doi.org/10.1016/0021-9991(81)90145-5

[10]. Brunton, S. L., Noack, B. R., & Koumoutsakos, P. (2020). Machine Learning for Fluid Mechanics. Annual Review of Fluid Mechanics, 52, 477–508. https://doi.org/10.1146/annurev-fluid-010719-060214

[11]. Duraisamy, K., Iaccarino, G., & Xiao, H. (2019). Turbulence Modelling in the Age of Data. Annual Review of Fluid Mechanics, 51, 357–377. https://doi.org/10.1146/annurev-fluid-010518-040547.

[12]. Maulik, R., & San, O. (2017). A neural network approach for the blind deconvolution of turbulent flows. Journal of Fluid Mechanics, 831, 151-181. https://doi.org/10.1017/jfm.2017.637.

[13].Sirignano, J., & Spiliopoulos, K. (2018). DGM: A Deep Learning Algorithm for Solving Partial Differential Equations. Journal of Computational Physics, 375, 1339–1364. https://doi.org/10.1016/j.jcp.2018.08.029.

[14]. Pilliod Jr, J. E., & Puckett, E. G. (2004). Second-order accurate volume-of-fluid algorithms for tracking material interfaces. *Journal of Computational Physics*, *199*(2), 465-502. https://doi.org/10.1016/j.jcp.2003.12.023.

[15]. Sirignano, J., & Spiliopoulos, K. (2018). DGM: A Deep Learning Algorithm for Solving Partial Differential Equations. Journal of Computational Physics, 375, 1339–1364. https://doi.org/10.1016/j.jcp.2018.08.029.

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