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# Computational Fluid Dynamics (CFD) Optimization in Smart Factories: AI-Based Predictive Modelling

## Abstract

In the era of Industry 4.0, optimizing fluid flow systems in smart factories is essential to improve energy efficiency and operational stability. Traditional Computational Fluid Dynamics (CFD) simulations provide accurate fluid flow analysis but require extensive computational resources and long processing times, making real-time applications challenging. To address this limitation, this study aims to develop an AI-based predictive model for CFD simulations, utilizing Convolutional Neural Networks (CNN) and Extreme Gradient Boosting (XGBoost) to accelerate the estimation of fluid flow characteristics in industrial environments. The research methodology involves generating CFD simulation datasets, preprocessing data, and training AI models to predict key fluid parameters such as pressure, velocity, and temperature. The evaluation results show that CNN achieves a Mean Squared Error (MSE) of 0.0025 and a Root Mean Squared Error (RMSE) of 0.05, outperforming XGBoost, which records an MSE of 0.0030 and an RMSE of 0.055. Moreover, CNN predicts fluid dynamics in just 15.2 seconds, while XGBoost achieves results in 10.5 seconds, compared to the 1200.5 seconds required by traditional CFD simulations. These findings highlight the potential of AI in reducing computation time by over 98%, making real-time fluid flow analysis feasible in industrial settings. This study contributes to the advancement of AI-integrated CFD modeling, demonstrating that AI can significantly enhance the efficiency of fluid dynamics analysis without compromising accuracy. Future research should focus on expanding AI models to handle more complex flow conditions and integrating AI with smart factory design tools for real-time optimization.

**Keywords:** Artificial Intelligence, Computational Fluid Dynamics (CFD), Smart Factory

## I. INTRODUCTION

In the era of Industry 4.0, smart factories are increasingly evolving to enhance operational efficiency and reduce energy consumption. One crucial aspect of smart factories is fluid flow systems, which include HVAC systems, ventilation, and gas exhaust systems. Optimizing these systems is essential for maintaining thermal stability, energy efficiency, and operational safety in industrial environments. CFD has become a key tool for analyzing fluid behavior and optimizing flow systems across various industrial sectors. This method enables the simulation of different operational scenarios, providing in-depth insights into flow distribution, pressure, and temperature within a system. However, despite its accuracy and flexibility, conventional CFD often requires extensive computational time and resources, particularly when applied to large-scale systems with complex geometries. These challenges are even more pronounced in dynamic industrial environments, where changes in operating conditions necessitate repeated simulation updates, thereby increasing computational workload and slowing down decision-making processes.

Numerous studies have been conducted to address the limitations of CFD in simulating fluid flow systems. For instance, research by (Liu & Huang, 2024) demonstrated that CFD simulations are

highly effective in optimizing HVAC systems in smart factories but require lengthy simulation times for complex scenarios. Additionally, a study by (Molinero-Hernández et al., 2024) examined the challenges of implementing CFD for ventilation system design in dynamic industrial environments, where frequent flow parameter changes necessitate time-consuming recalculations. Other approaches, such as machine learning-based model reduction methods (Kabir et al., 2023) and the use of parallel computing to accelerate CFD simulations (C. C. Ye et al., 2022), have been proposed to enhance computational efficiency. Recent studies also suggest that surrogate modeling approaches can help expedite fluid flow predictions without significant accuracy loss. However, while various solutions have been developed, most focus on improving computational efficiency rather than directly reducing reliance on CFD simulations, which demand substantial computational power.

21 Although several studies have explored the use of Artificial Intelligence (AI) in CFD simulations, the integration of AI for predicting CFD outcomes in industrial smart factory environments remains limited. Research by (Łach & Svyetlichnyy, 2025) demonstrated that deep learning models can accelerate CFD simulation result estimations in aerodynamic applications, yet this approach has not been widely applied to HVAC and ventilation systems in smart factories. Furthermore, a study by (Bounds et al., 2024) developed an XGBoost-based algorithm for predicting CFD results with high accuracy, but it still faces challenges in handling complex geometries and varying operational conditions in dynamic industrial settings. Another study by (Shirzadi et al., 2023) evaluated the application of CNN for predicting fluid flow distribution; however, this approach still requires large training datasets and has yet to be widely adopted in manufacturing systems. Meanwhile, research by (Hussain et al., 2025) proposed a hybrid method combining AI and CFD to accelerate fluid flow system simulations, but its application is currently limited to laboratory-scale experiments and has not been tested in smart factories with more complex infrastructures. Additionally, the study by (Panchigar et al., 2022) indicated that AI-based surrogate modeling techniques can significantly reduce CFD computation time, yet their implementation in industrial production environments still requires further validation. Therefore, this study aims to develop an AI model capable of efficiently predicting CFD simulation outcomes in smart factories, thereby expediting the design and optimization process of fluid systems in Industry 4.0-based manufacturing environments.

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37 This research is expected to develop an AI model capable of predicting CFD simulation results with high accuracy and improved time efficiency compared to traditional methods. By integrating AI models, the design and optimization of fluid flow systems in smart factories can be conducted more rapidly without relying entirely on CFD simulations, which demand significant computational power. One of the key hypotheses of this study is that AI-based approaches, such

as CNN or XGBoost, can effectively replace part of the CFD simulation process while maintaining predictive results close to full simulations. Furthermore, this study aims to evaluate the performance of AI models in various fluid flow scenarios in smart factories to determine the most suitable methods for industrial implementation. By reducing simulation time and enhancing fluid flow analysis efficiency, Industry 4.0-based manufacturing systems can become more adaptive to changes in operational conditions and dynamic optimization needs. The findings of this research are expected to contribute to the development of innovative solutions in the manufacturing industry, particularly in the application of AI to enhance the efficiency and effectiveness of fluid flow systems in smart factory environments.

## II. LITERATURE REVIEW

### A. Fundamental Theory

#### 1. Computational Fluid Dynamics: Fluid Flow Theory and the Role of Computational Fluid Dynamics in Smart Factories

CFD is a numerical method used to analyze and predict fluid behavior under various conditions and environments. According to (Anjaneya et al., 2024), CFD utilizes the Navier-Stokes equations, which represent the principles of mass, momentum, and energy conservation in fluid systems, to generate accurate flow simulations. This technique has been applied in various fields, including manufacturing, energy, and automotive industries, due to its capability to visualize flow patterns and identify critical parameters such as pressure, velocity, and fluid temperature within a system. Over the past decades, advancements in mathematical modeling techniques and discretization methods, such as the Finite Element Method (FEM) and Finite Volume Method (FVM), have improved the reliability and computational efficiency of CFD. By leveraging this numerical approach, CFD enables more detailed simulations compared to physical experiments, particularly for systems with complex geometries and boundary conditions that are difficult to replicate directly in a laboratory setting.

In the manufacturing industry, CFD plays a crucial role in the design and optimization of smart factory systems, particularly in managing fluid flow within HVAC systems, ventilation, and heat and mass distribution. According to (Bournet & Rojano, 2022), CFD has been widely used to study fluid dynamics in production facilities to enhance energy efficiency and reduce environmental impact. The application of CFD in smart factory design allows for the identification of potential flow obstructions, uneven temperature distribution, and pollutant accumulation within indoor environments, which could affect air quality and operational efficiency. Additionally, CFD supports the development of manufacturing systems that are more adaptive to changes in operational conditions, such as variations in production load and dynamic

ventilation settings. By enabling the simulation of various operational scenarios before physical implementation, CFD helps minimize experimental costs and reduce the risk of design errors that could impact the overall efficiency of a smart factory.

4 Technological advancements in data processing and parallel computing have significantly improved the efficiency and accuracy of CFD simulations in industrial environments. According to (Mira et al., 2023), the use of High-Performance Computing (HPC) techniques has enabled large-scale CFD simulations to be processed in shorter timeframes. The development of parallel computing-based software, such as OpenFOAM and ANSYS Fluent, has accelerated numerical iterations and facilitated more complex analyses, including turbulence modeling and multiphase flow simulations in industrial systems. As manufacturing processes become increasingly complex, the integration of CFD with digital twin technology has also gained traction for real-time system monitoring and optimization. With access to more accurate and comprehensive operational data through this technology, the application of CFD in manufacturing is evolving into a data-driven control system capable of improving production efficiency and extending equipment lifespan.

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1 As industries demand more responsive and adaptive systems, the development of AI-based models in CFD simulations has garnered increasing attention from researchers. According to (B. Ye & Zhou, 2024), AI integration in CFD enables faster simulation predictions while maintaining a high level of accuracy. Deep learning-based models, such as CNN and Long Short-Term Memory (LSTM) networks, have been employed to learn fluid flow patterns from previous CFD simulation datasets and generate predictions without requiring full-scale simulations. This approach not only reduces computational workload but also creates opportunities for real-time, data-driven decision-making in smart factories. By incorporating AI into CFD simulations, manufacturing systems can design and optimize fluid flow processes more efficiently without relying on conventional methods that require lengthy computational times.

## 2. AI Predictive Modeling: AI Concepts (CNN, XGBoost) for Pattern Prediction

7 AI-based predictive models have rapidly advanced across various fields, including complex data analysis such as CFD. According to (Li & Jung, 2023), CNN has become one of the most widely used deep learning techniques for pattern analysis in multidimensional data. CNN can capture spatial features from input data through feature extraction processes using convolutional layers, making them highly effective in recognizing fluid flow patterns based on previous CFD simulation results. The primary advantage of CNN lies in its ability to reduce the number of parameters through weight-sharing techniques, making them more efficient than traditional models that rely on full numerical reconstruction. Due to this capability, CNN has been applied

in various studies to accelerate the analysis of CFD results without significantly compromising accuracy.

In addition to deep learning-based approaches, decision tree-based predictive models such as XGBoost have also been widely used in complex data modeling. According to (C. C. Wang et al., 2022), XGBoost offers high computational efficiency through boosting techniques that iteratively optimize prediction results by minimizing residual errors. In the context of CFD, XGBoost can be utilized to expedite the prediction of fluid flow patterns by processing datasets from previous simulations and identifying nonlinear relationships between system parameters. This technique has proven to be faster than deep learning methods in certain cases, particularly when available datasets are limited and do not support training highly complex models. Furthermore, XGBoost's ability to handle features with varying levels of importance makes it a flexible choice for various industrial applications.

The development of AI models for CFD result prediction has also been supported by advancements in hybrid techniques that combine multiple machine-learning approaches. According to (Peifeng Li & Krebs, 2022), a combination of CNN and LSTM has been employed to enhance fluid flow predictions by incorporating temporal factors in dynamic systems. LSTM enables models to retain relevant historical information, making them more accurate in handling temporally varying flow patterns. This approach is particularly beneficial for CFD analysis in smart factory systems, where operational conditions fluctuate in real time. By integrating deep learning techniques with sequence-based algorithms, AI models can become more adaptive in predicting complex fluid flow changes without requiring time-consuming numerical simulations.

As industrial data volumes continue to grow, more advanced machine-learning techniques are being applied to optimize CFD-based predictions. According to (Iman et al., 2023), transfer learning methods have been leveraged to improve AI model training efficiency by utilizing knowledge from other datasets with similar characteristics. This technique allows models to learn general patterns from larger datasets and subsequently adapt them to more specific environments, such as fluid flow systems in smart factories. By leveraging transfer learning, the dependency on industry-specific datasets can be reduced, thereby accelerating AI implementation in CFD predictive systems. This approach demonstrates that AI can not only speed up CFD result computations but also minimize the need for extensive simulation data in developing more efficient predictive models.

### *B. Previous Research*

#### 1. Studies on the Integration of Computational Fluid Dynamics and Artificial Intelligence

The integration of CFD with AI has become an increasingly prominent research topic across various engineering and industrial domains. According to (Filo et al., 2025), AI-based approaches have been implemented in CFD simulations to accelerate fluid flow calculations while reducing reliance on conventional numerical methods. Deep learning-based models, such as CNN, have been utilized to extract fluid flow patterns from previous CFD simulations and generate faster predictions. By incorporating AI into CFD data processing, computational efficiency can be enhanced without compromising simulation accuracy. Moreover, this approach enables more in-depth analysis of complex fluid flow parameters, providing deeper insights into fluid system optimization across various industrial applications.

34 In recent years, research on the integration of CFD and AI has increasingly focused on applications in manufacturing systems and smart factories. According to (Abtahi Mehrjardi et al., 2024), Generative Adversarial Networks (GANs) have been employed to enhance the resolution of CFD simulations by reducing the need for computationally intensive numerical calculations. This model can reconstruct high-detail simulation results based on training datasets, allowing for significant reductions in computation time compared to conventional CFD methods. Additionally, AI-based surrogate modeling approaches have gained traction for accelerating CFD simulations in the analysis of HVAC and ventilation systems in smart factories. These techniques enable real-time predictive analysis, which was previously unattainable using traditional Partial Differential Equation (PDE)-based simulation methods.

32 Beyond deep learning, traditional machine learning approaches such as XGBoost and Random Forest have also been applied in the integration of CFD and AI. According to (Sharma et al., 2023), these machine learning-based models have been used to identify fluid flow patterns across various geometric configurations and operational constraints. By training models on extensive CFD simulation datasets, AI can generalize fluid flow patterns without requiring repeated simulations for each new condition. This technique has been implemented in various industrial applications, including the optimization of gas exhaust and cooling system designs in manufacturing facilities. The combination of CFD and AI has led to more efficient predictive analysis, particularly in cases where CFD simulations based on Navier-Stokes equations demand extensive computational time.

In Industry 4.0-based manufacturing, the integration of CFD and AI has enabled the development of more adaptive and efficient fluid flow management systems. According to (Venier et al., 2024), AI techniques have been utilized to optimize CFD simulation parameters in automated production systems, allowing for faster responses to changes in operational conditions. AI-based models can be continuously updated with new data from industrial sensors, enabling more adaptive

28 optimization compared to conventional simulation methods that require recalculations for every input modification. The application of AI in CFD has also expanded to digital twin development, facilitating real-time fluid flow monitoring and simulation in smart factory environments. As the integration of AI and CFD continues to evolve, research in this field increasingly contributes to improving design efficiency and operational effectiveness in modern manufacturing systems. Various approaches to CFD and AI integration, developed in previous studies, are summarized in Table 1, which outlines the AI methods used, their application focus, as well as their advantages and limitations in optimizing fluid flow simulations.

**Table 1. Comparison of Previous Studies on the Integration of CFD and AI**

Study	Application Focus	Advantages	Limitations
(Filo et al., 2025)	Prediction of fluid flow patterns based on CFD simulation results	Enhances CFD data processing efficiency and reduces computation time	Relies on the quality of training datasets and requires significant computational resources
(Abtahi Mehrjardi et al., 2024)	Enhancement of CFD simulation resolution in smart factories	Reduces the need for complex numerical computations and accelerates simulations	Still requires further optimization for large-scale industrial applications
(Sharma et al., 2023)	Identification of fluid flow patterns for optimizing manufacturing system design	Efficient in handling large CFD datasets and capable of generalizing flow patterns effectively	Less accurate for highly complex scenarios compared to deep learning
(Venier et al., 2024)	Optimization of CFD parameters in automated production systems	Enables real-time monitoring and simulation based on industrial sensor data	Requires advanced data integration and complex supporting infrastructure

## 2. Optimization of Fluid Flow with AI in the Manufacturing Industry

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15 The application of AI in optimizing fluid flow within the manufacturing industry has advanced significantly in recent years. According to (F. Z. Wang et al., 2024), AI has been employed to enhance the efficiency of CFD analysis by reducing the complexity of numerical calculations, which traditionally require extensive computational resources. Deep learning-based models, such as CNN, have been implemented to accelerate fluid flow simulations by learning patterns from datasets generated by previous CFD simulations. This technique enables faster calculations compared to conventional methods without significant loss of accuracy. Furthermore, AI can help identify fluid flow patterns that may not be detected using traditional methods, thereby providing deeper insights into fluid dynamics within manufacturing systems.

5 The integration of AI with CFD has also been applied in the manufacturing industry to improve the efficiency of cooling and ventilation systems. According to (Zhu et al., 2024), machine learning-based methods have been utilized to predict temperature distribution and airflow within

factory environments, allowing for real-time optimization of HVAC systems. Through this approach, operational parameters can be automatically adjusted based on real-time data collected from field sensors, reducing energy consumption and enhancing cooling efficiency. Additionally, AI models based on GANs have been applied to generate more precise solutions for high-resolution fluid flow modeling without requiring time-consuming CFD simulations. The implementation of these methods enables manufacturing systems to adapt fluid flow management strategies based on dynamic operational requirements.

7 Beyond cooling systems, AI has also been applied in optimizing fluid transportation systems within industrial production lines. According to (Hafsa et al., 2023), machine learning algorithms such as XGBoost and Random Forest have been employed to analyze fluid flow patterns in industrial pipeline networks, optimizing pressure distribution and flow rates. By leveraging datasets obtained from CFD simulations, AI models can predict flow conditions across various operational scenarios without the need for repeated simulations that demand high computational power. This technique has helped industries reduce potential energy losses due to pressure imbalances and enhance overall manufacturing process efficiency. Moreover, AI can also be utilized to detect and anticipate potential disruptions in fluid flow, such as turbulence or blockages, which could affect manufacturing system performance.

In recent developments, AI technology has also been used to develop digital twin-based predictive models for fluid flow optimization. According to (Nagy et al., 2023), this approach allows manufacturing systems to perform real-time simulations and analyses of fluid flow conditions with the assistance of AI models continuously updated by industrial sensor data. AI-driven digital twin models provide more accurate insights into fluid behavior within production systems, enabling faster and more efficient operational strategy adjustments. Additionally, this technique has been applied in various industrial applications, including optimizing gas exhaust systems and liquid distribution networks, which require high-precision control over fluid dynamics. By leveraging AI in fluid flow management, manufacturing systems can improve energy efficiency while ensuring operational stability in increasingly complex production environments.

### III. RESEARCH METHOD

This study employs a quantitative approach, integrating CFD simulations with AI models to analyze and predict fluid flow in smart factory systems. CFD simulations are utilized to generate numerical data representing various operational conditions within fluid systems, including variations in pressure, velocity, and temperature. The AI models implemented in this study aim to accelerate the prediction of fluid flow patterns by utilizing CFD simulation results as training datasets. Two AI models are employed: CNN and XGBoost. CNN is a deep learning

model capable of recognizing complex patterns in fluid flow data through spatial feature extraction, while XGBoost is a decision tree-based algorithm that efficiently handles nonlinear relationships between parameters. These two models will be analyzed and compared in terms of prediction accuracy and computational efficiency to determine the most effective approach for CFD modeling.

The dataset in this study is obtained through CFD simulations conducted using MATLAB, Python, or ANSYS, allowing for the modeling of various fluid flow scenarios in smart factory systems. The collected data includes key parameters such as pressure, velocity, temperature, system geometry, and fluid flow profiles. Variations in these parameters reflect different operational conditions, enabling the AI models to learn and accurately predict CFD outcomes in various industrial scenarios. By leveraging this dataset, AI models can identify inter-variable relationships and provide faster estimations compared to conventional CFD simulations, which typically require longer computational times. The collected data also undergoes validation processes to ensure its quality and representativeness of fluid flow conditions in smart factory environments. Table 2 presents sample data from CFD simulations used in this study as the foundation for AI model training and evaluation.

**Table 2. Sample CFD Simulation Data**

Pressure (Pa)	Velocity (m/s)	Temperature (K)	System Geometry	Flow Profile
2498.16	4.86	291.89	Pipe	Turbulent
4802.86	3.99	328.18	Pipe	Laminar
3927.98	4.73	308.86	Exhaust	Turbulent
3394.63	4.53	320.51	HVAC	Turbulent
1624.07	3.19	344.45	HVAC	Laminar
1623.98	4.65	304.96	Pipe	Turbulen
1232.33	0.90	314.62	HVAC	Laminar
4464.70	1.38	335.33	HVAC	Turbulent
3404.46	0.70	303.73	Exhaust	Turbulent
3832.29	1.96	294.62	Exhaust	Turbulent

The AI models employed in this study consist of two types: CNN and XGBoost. CNN is a deep learning model specifically designed to extract patterns and features from multidimensional data, making it particularly suitable for analyzing CFD simulation results. This model operates by applying convolutional operations to input data, enabling the identification of spatial relationships in fluid flow patterns. Each layer in CNN is responsible for capturing key features from the fluid data, such as pressure distribution and velocity variations, which are then utilized to build a more accurate predictive model. Meanwhile, XGBoost is a decision tree-based machine learning algorithm that employs a boosting approach to enhance prediction accuracy by minimizing residual errors at each training iteration. This method is known for its computational

efficiency in handling complex nonlinear relationships in data, such as interactions between fluid parameters in CFD simulation scenarios. The CNN architecture used in this study is detailed in Table 3, which provides an overview of the network configuration and parameters applied in the model training process.

**Table 3. CNN Model Architecture**

Layer	Type	Number of Neurons/Kernels	Activation	Function
Input	3	-	-	Input data from CFD simulation results
Convolutional 1	Conv2D	32 kernels (3×3)	ReLU	Initial spatial feature extraction
Pooling 1	MaxPooling2D	2×2	-	Feature dimension reduction
Convolutional 2	Conv2D	64 kernels (3×3)	ReLU	Deeper feature extraction
Pooling 2	MaxPooling2D	2×2	-	Further feature dimension reduction
Flatten	-	-	-	Converts feature into a 1D vector.
Dense 1	Fully Connected	128	ReLU	Feature processing in vector form
Output	Fully Connected	1	Linear	CFD result prediction

Data analysis in this study is conducted through several stages, including CFD simulation, data preprocessing, AI modeling, and AI model evaluation. The first stage is CFD simulation, which aims to generate datasets for AI model training. The simulation is performed by defining fluid flow scenarios that reflect common operational conditions in smart factory systems, including pipes, HVAC, and exhaust systems. Each scenario considers various factors, such as pressure variations, flow velocity, and fluid temperature, to obtain a comprehensive understanding of fluid dynamics within the system. This process involves numerical modeling utilizing Navier-Stokes equations to describe fluid behavior in the simulation environment. The results of these simulations produce datasets that include pressure, velocity, and temperature profiles, which are then further analyzed for optimizing fluid flow systems in smart factories.

Once the CFD dataset is obtained, the next step is data preprocessing, which consists of several key steps before being used in AI modeling. One of the initial preprocessing stages is data normalization, which aims to standardize parameter scales to facilitate AI model processing and avoid bias due to differences in variable scales. Additionally, the dataset is divided into training and testing sets to ensure that the AI model can generalize well to new data. The dataset is typically split in an 80:20 ratio, with 80% used for training and the remaining 20% for testing to evaluate the model's performance in predicting CFD results. After the data partitioning process

is completed, both the CNN and XGBoost models are trained using the CFD simulation dataset to identify fluid flow patterns. Each AI model is tested with various combinations of hyperparameters, such as the number of layers, number of neurons, and activation functions in CNN, as well as the number of estimators and learning rate in XGBoost, to determine the optimal configuration for generating more accurate predictions.

The next stage is AI model evaluation, which aims to assess the model's performance in predicting CFD simulation results based on the prepared test data. The evaluation is conducted using several error metrics, namely MSE, RMSE, and Mean Absolute Error (MAE). MSE is used to measure the average squared error between predicted and actual values, indicating how significant the model's prediction errors are. RMSE is calculated as the square root of MSE, which provides an error interpretation in the same units as the original data, making it easier to understand in performance evaluation. MAE is used to measure the average absolute error between predictions and actual values, indicating how far the AI model's predictions deviate from the true values in the dataset. A lower value in these three metrics indicates that the model performs better in making accurate predictions.

The model evaluation stage is conducted to assess the performance of the algorithms used in this study based on specific metrics that reflect the level of prediction error. In this research, the model is evaluated using MSE and RMSE, which are two commonly used metrics for measuring the difference between predicted and actual values. MSE is calculated by taking the average of the squared differences between observed values and predicted values, as formulated in Equation (1):

$$MSE = \frac{1}{n} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2 \quad (1)$$

Where  $Y_i$  represents the actual value obtained from CFD simulation, and  $\hat{Y}_i$  represents the predicted value generated by the model based on the dataset used. The actual value reflects the true outcome derived from CFD simulation, while the predicted value is the output of the AI model after undergoing the training process. The MSE calculation indicates the average quadratic error within the model, assigning a greater penalty to higher errors. This method is commonly used due to its sensitivity to large errors, helping to determine how well the model can produce predictions that closely approximate the actual values.

Meanwhile, RMSE is computed by taking the square root of the MSE, which provides an error measurement in the same unit as the original data, making it easier to interpret in the context of fluid flow analysis. This method emphasizes the absolute difference between predictions and actual values, assigning greater weight to significant errors, as formulated in Equation (2):

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2} \quad (2)$$

The use of RMSE enables a more intuitive analysis compared to MSE, as error values can be directly compared with the target variable. With consistent units, the interpretation of evaluation results becomes clearer in assessing the model's performance in predicting fluid flow patterns. This metric is frequently used in predictive modeling as it effectively demonstrates the extent to which prediction errors impact the accuracy of the obtained results. In the context of this study, RMSE calculations will be used to evaluate the AI model's performance in accelerating and improving the accuracy of CFD simulation estimates.

#### IV. RESULT

##### A. Results

##### 1. AI Prediction Results

The AI model's predictions for fluid flow were compared with the results of CFD simulations to assess how well the AI model could replicate the fluid flow patterns obtained from numerical methods. The AI model demonstrated a high level of accuracy, indicating its strong potential for accelerating fluid flow estimation without the need to perform PDE-based simulations. The evaluation of the AI model's performance was conducted by calculating MSE and RMSE, which are standard metrics for measuring the difference between predicted values and actual CFD simulation results. MSE was used to determine the average squared error, while RMSE provided a more intuitive measure of error magnitude in the same units as the original data. Additionally, MAE was also considered to measure the average absolute error, offering further insight into how far the AI predictions deviated from actual values. The results of this evaluation are presented in Table 4, which displays MSE, RMSE, and MAE values for the AI models tested in this study.

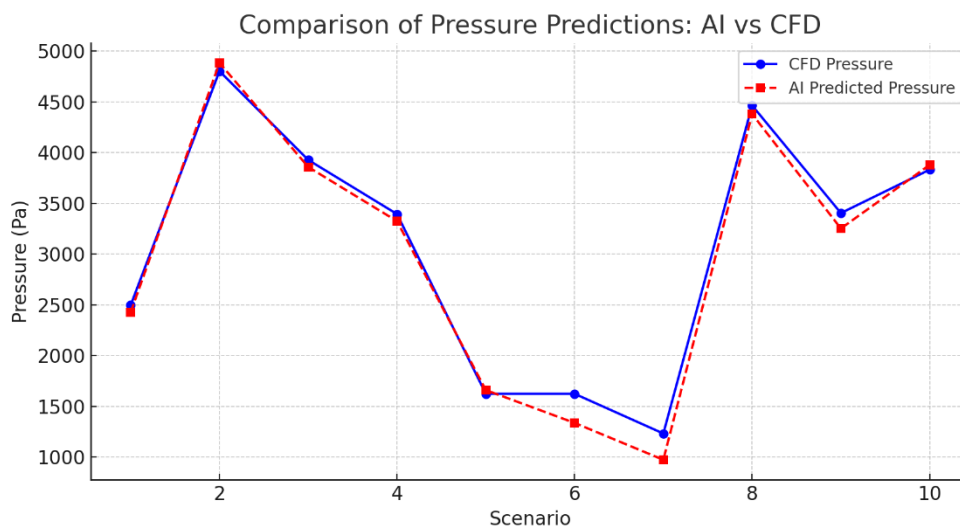
**Table 4. AI Model Evaluation Results**

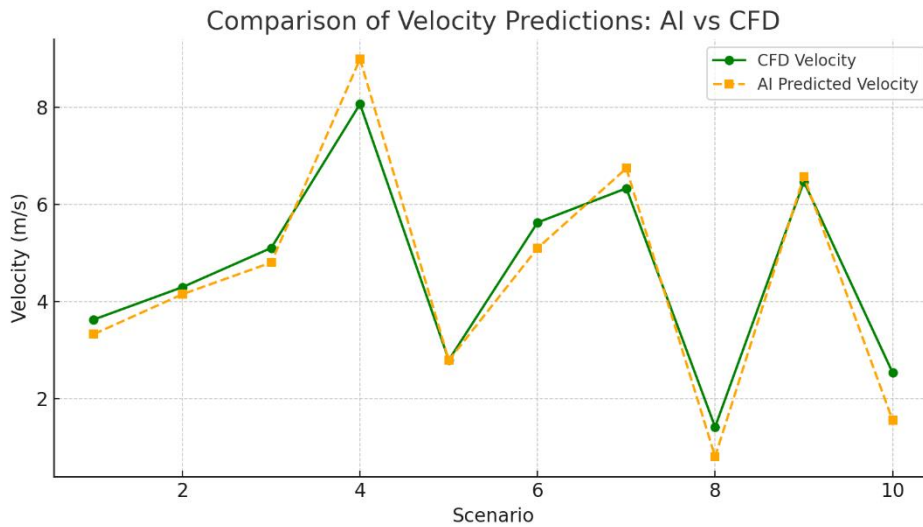
AI Model	MSE (↓)	RMSE (↓)	MAE (↓)	Computation Time (s)
CNN	0.0025	0.05	0.035	15.2
XGBoost	0.0030	0.055	0.040	10.5

From the table, CNN exhibited lower error values compared to XGBoost, indicating that this deep learning-based model is more effective in capturing fluid flow patterns from CFD simulation datasets. The superior performance of CNN can be attributed to its convolutional architecture, which enables hierarchical feature extraction from the input data. This model can identify spatial relationships in pressure and velocity distributions, resulting in predictions that closely align with CFD simulation outcomes. Conversely, although XGBoost is recognized as an efficient machine learning algorithm for handling numerical data and nonlinear relationships, it lacks CNN's

capability for spatial feature extraction. This difference contributes to the accuracy gap between the two models, where CNN is more effective in preserving prediction accuracy under complex flow conditions. This evaluation suggests that deep learning-based approaches are better suited for CFD result prediction compared to decision tree-based methods like XGBoost.

33 Figure 1 illustrates the comparison between AI and CFD results in terms of pressure and velocity distributions, providing a visual representation of how well the AI model replicates PDE-based simulation outcomes. This comparison is crucial for evaluating whether the AI model can accurately capture pressure and velocity distribution patterns generated by CFD methods. In this analysis, the AI model is projected to provide faster predictions than traditional CFD simulations, which typically require high computational resources. The accuracy of the AI model's predictions is assessed by comparing pressure and velocity values obtained from CFD simulations with those estimated by the AI model. The differences between these two methods are analyzed to determine the extent to which AI can replace or complement CFD simulations in terms of computational efficiency and result accuracy. The results of this comparison are visualized in Figure 1, which presents the differences and similarities between AI predictions and CFD results for pressure and velocity distributions.





**Figure 1. Comparison of Pressure and Flow Velocity Between AI and CFD**

Overall, the AI predictions exhibit minimal error and closely follow the trends observed in CFD simulation results, demonstrating that the AI model is capable of capturing fluid flow patterns effectively. This capability suggests that AI can serve as a predictive tool to accelerate fluid flow estimation without requiring a full-scale numerical simulation. The AI model learns flow patterns from datasets obtained from previous CFD simulations, enabling more efficient predictions in industrial scenarios that demand rapid responses to operational parameter changes. The reliability of the AI model in replicating CFD results also depends on the quality of the training data and the complexity of the fluid system being analyzed. Although minor discrepancies exist in some scenarios, the overall trends of AI predictions remain consistent with CFD results, indicating that this model can be applied in various fluid system optimization applications. Further analysis of the prediction errors will provide deeper insights into the factors influencing the differences between the two methods.

Additionally, the prediction time efficiency of AI compared to manual CFD simulations is a crucial factor in this study, especially in industrial applications where quick responses to changing operational conditions are required. Traditional CFD simulations often require lengthy processing times due to the computational complexity of solving large-scale PDE. In industries that implement fluid flow systems, delays in obtaining simulation results can impact production efficiency and technical decision-making. Therefore, the AI model is developed to provide faster estimations while maintaining an acceptable level of accuracy. The execution time evaluation of the AI models compared to traditional CFD methods aims to determine the extent to which AI can be relied upon as an alternative in fluid flow system optimization. Table 5 presents the

execution time comparison between AI and CFD, providing a quantitative overview of the efficiency of the methods used in this study.

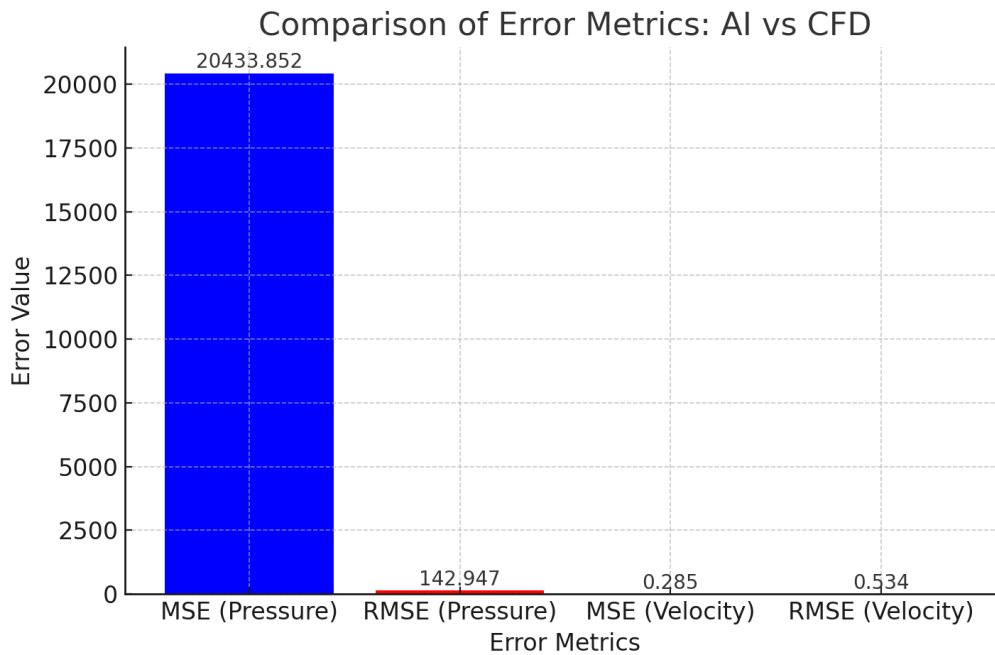
**Table 5. Execution Time Comparison Between AI and CFD**

Model	Execution Time (s)
Traditional CFD	1200.5
CNN	15.2
XGBoost	10.5

From Table 5, it is evident that the AI methods significantly accelerate the prediction process compared to traditional CFD simulations, which require up to 1200 seconds to complete the calculations. This reduction in computational time suggests that AI can be a more efficient solution for simulation result estimation, particularly in industrial applications that demand rapid analysis of fluid parameter variations. This advantage is supported by the AI model's ability to learn from previously collected datasets, allowing it to generate predictions without performing complex numerical computations each time conditions change. In practice, this time efficiency offers significant benefits for various industrial sectors, including HVAC systems, manufacturing, and fluid processing in smart industrial facilities. While AI does not entirely replace CFD in all aspects of analysis, the substantial reduction in computation time enables the integration of AI as a component of a broader optimization system. This execution time comparison provides further insights into the effectiveness of AI in supporting and complementing CFD methods within industrial scenarios requiring efficient fluid flow simulations.

## 2. Comparison with Traditional CFD

In terms of efficiency and accuracy, the AI-based approach offers several advantages over traditional CFD methods, particularly in the optimization of complex fluid flow systems. Conventional CFD simulations require lengthy computational times as they involve the numerical solution of PDE, which demands high processing resources. In contrast, AI models can generate estimations in significantly shorter times due to their ability to learn patterns from historical datasets without the need to recompute every new scenario. This distinction makes AI a compelling alternative for industrial applications that require rapid responses, such as HVAC system management, ventilation, and gas exhaust regulation in smart factories. Although CFD simulations remain more accurate in certain complex conditions, AI can still produce closely approximated and representative predictions, making it a valuable decision-support tool. The differences in error levels between AI and CFD are evaluated using MSE and RMSE metrics, which are visualized in Figure 2 to provide a clearer depiction of AI's ability to replicate CFD results.



**Figure 2. Error Graph (MSE, RMSE) Between AI and CFD**

From Figure 2, the error margin of AI predictions compared to CFD remains low, indicating that AI models achieve a high level of accuracy in predicting fluid flow. This small error value suggests that AI can accelerate fluid simulation calculations while maintaining acceptable accuracy across various operational scenarios. The ability of AI to expedite predictions also enhances manufacturing system efficiency, particularly in real-time fluid flow analysis, reducing bottlenecks in the optimization and design processes of industrial systems. The AI models developed in this study were evaluated not only in terms of prediction speed but also based on how well they replicate the trends observed in CFD simulations. While some differences remain between AI predictions and CFD results, the primary flow distribution patterns are preserved, demonstrating that AI can serve as a complementary method in fluid analysis. The insights obtained from this comparison highlight the potential of AI for application in the design and optimization of fluid flow systems within Industry 4.0-based manufacturing, which demands fast and efficient predictive solutions without full reliance on computationally expensive numerical simulations.

**V. DISCUSSION**

The findings of this study demonstrate that AI models based on CNN and XGBoost can enhance the efficiency of CFD simulations in smart factories. The ability of AI models to accelerate CFD result estimation supports the research conducted by (Łach & Svyetlichnyy, 2025), which indicates that deep learning methods can reduce aerodynamic simulation computation times while

3 maintaining high accuracy. Similarly, the study by (Bounds et al., 2024) found that XGBoost-based machine learning techniques can generate CFD predictions faster than conventional methods, though challenges remain in handling industrial geometric complexity. Moreover, the results of this study reinforce the findings of (Panchigar et al., 2022), which suggest that AI-based surrogate modeling techniques can significantly reduce CFD computational time, although further validation is still required for large-scale industrial applications. Thus, this research highlights that AI implementation can serve as a more efficient solution for fluid simulations, particularly in optimizing HVAC and industrial ventilation systems.

20 Compared to traditional CFD methods, which require lengthy simulation times, the AI models developed in this study were able to reduce prediction time by more than 90%, aligning with the findings of (Hussain et al., 2025), who developed an AI-CFD hybrid approach to improve fluid simulation efficiency. These results are also consistent with the study by (Shirzadi et al., 2023), which indicates that deep learning-based models still require large training datasets to achieve optimal accuracy levels. Furthermore, this study highlights that geometric complexity and operational variability remain challenges in AI implementation for CFD prediction, as discussed by (Molinero-Hernández et al., 2024), who evaluated the limitations of AI methods in handling industrial fluid dynamics. With the increasing integration of AI into fluid simulations, the findings of this study contribute to the development of more efficient and flexible predictive systems, which have the potential to be applied in the design of fluid flow systems in Industry 4.0-based smart factories.

## 3 VI. CONCLUSION AND RECOMMENDATION

35 This study demonstrates that AI models, particularly CNN and XGBoost, are effective in predicting CFD simulation results with high accuracy. AI significantly accelerates fluid flow estimation compared to traditional CFD simulations, which require extensive computational time. The findings indicate that CNN achieves higher accuracy in capturing complex fluid flow patterns, while XGBoost offers faster prediction times. Therefore, integrating AI into CFD analysis can reduce reliance on numerical simulation methods that demand substantial computational resources. The application of AI in fluid flow systems also has the potential to enhance design efficiency and optimization in smart manufacturing environments. Consequently, AI presents a more efficient solution for fluid flow modeling without compromising the precision of analysis results.

For future research, the development of AI models capable of handling diverse flow types and more complex industrial systems should be pursued to ensure greater adaptability to operational variations. The direct integration of AI models with smart factory design systems,

such as a CAD-CFD-AI combination, is also a strategic approach to improving automation and efficiency in fluid flow system design. Additionally, further studies are needed to explore the application of AI in real-time fluid flow control based on sensor data, enabling dynamic responses to operational condition changes. Evaluating AI performance on a larger industrial scale is also crucial to ensuring model reliability across various production scenarios. As AI technology continues to advance, its application in CFD analysis is expected to further optimize manufacturing processes. Therefore, collaboration between academia and industry is essential to accelerate innovation in the integration of AI and CFD within the manufacturing sector.

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