# Mathematical Modeling of Turbulent Flows Using Advanced Computational Fluid Dynamics Techniques

Anushree A Aserkar[1], R. Sugunthakunthalambigai[2], Dr. Ravindra D Nalawade[3], Babu Reddy[4], M. Balamurugan[5], Dr. M. P. Mallesh[6]

[1]Assistant Professor, Department of Applied Mathematics and Humanities, Yeshwantrao Chavan College of Engineering, India, aserkar_aaa@rediffmail.com
[2]Assistant Professor of Mathematics, Basic Engineering and Applied science, Agricultural Engineering College and Research Institute(Tamil Nadu Agricultural University), India, suguntha @tnau.ac.in
[3]Associate Professor, Department of Civil Engineering, AISSMS COE PUNE, India, rdnalawade@aissmscoe.com
[4]Assistant Professor, Department of Mechanical Engineering, VTU's CPGS, India, babureddy.dh@gmail.com
[5]Assistant Professor, Department of Mathematics, Vel Tech Rangarajan Dr. Sagunthala R&D Institute of Science and Technology, India, balamurugansvm@gmail.com
[6]Associate Professor, Department of Mathematics, Koneru Lakshmaiah Education Foundation, India, malleshmardanpally@gmail.com

**Abstract:** This research investigates the application of advanced Computational Fluid Dynamics (CFD) techniques in the mathematical modeling of turbulent flows. The accuracy is improved in different engineering systems by using different turbulence models: the k-ε, k-ω, LES and DNS. The main purpose was to investigate fluid flow behavior in industrial, aerospace, biomedical applications. Results of the experimental data are compared with the k-ε model and show that the average deviation is 5.2% when compared to the experimental data of turbulent boundary layers. Dynamic vortex simulations using the LES model resulted in a 12% decrease in error compared to original results. In addition, the DNS model was close to obtaining near exact solutions at the price of greatly increased CPU costs, with a deviation of 1.4% in highly turbulent cases. It was found next that the integration of machine learning algorithmss further improved model predictions, reducing the required simulation times by about 18 percent. It is concluded that for different applications it is important to select the correct turbulence model so as to balance accuracy and computational efficiency. The contribution of this research to refine CFD methodologies and to provide some initial insight in optimizing fluid dynamics simulations for real world engineering problems is provided.

Keywords: Computational Fluid Dynamics, Turbulence Models, k-ε Model, LES Model, DNS Model.

## 1. Introduction

Many engineering and natural systems display turbulent flows; that is, they experience chaotic and irregular fluid motion as in aircraft aerodynamics or atmospheric circulation. These flows are critical to understanding and accurately predicting, and as a result, too important to industry such as aerospace, automotive and energy. Yet, turbulence is one of the most difficult aspects of fluid mechanics because its behavior is complex and highly nonlinear [1]. Through the past decades, the mathematical modeling of turbulent flows has been studied for a long time with many models proposed to simulate the turbulence behavior under different condition [2]. A powerful means for near incompressible and compressible computing of fluid flows at both incompressible and compressible regimes using numerical techniques for solving the governing equations of fluid motion has been created, known as Computational Fluid Dynamics (CFD) [3]. Unfortunately, computational expense and the characters of turbulence make classical models insufficient to account for the whole spectrum of scales and interactions contained in turbulent flows. As a response to the need for more accurate, less time consuming, and scalable CFD simulators, advanced methods such as Large Eddy Simulation (LES), Direct Numerical Simulation (DNS) and Reynolds Average Navier-Stokes (RANS) approaches have been developed and implemented. The purpose of this research is to study the application of the advanced CFD method for modeling turbulent flows with highlighting on the advantages and disadvantages of each method. Utilizing the latest computational steps in high performance computing (HPC) and machine learning algorithms, the purpose of this study is to enhance the prediction of turbulence models and provide more in-depth exploration of the high fluid dynamics phenomena. Ultimately, we aim to improve accuracy and efficiency of methods used in engineering practice by aiding in more effective designs and systems in corresponding areas of application.

## 2. Related Works

Turbulent flows and fluid dynamics have been an active field of research and a number of studies have been conducted on various aspects of turbulence modelling, numerical methods, and real applications. In this section we have reviewed a few studies in the field of turbulent flow modelling using advance computational flow dynamics (CFD) method - a review on the advancement of the method and practical applications.

A significant amount of research focuses on advancing the modeling of advanced materials and syntheses processes. A new approach for synthesis of silicon nanomaterials through reactive thermal plasma jet using CFD simulations was proposed by Elaissi et al. [15]. The results point out the fact that the flow of high temperature fluid and the solid particle interaction are very important to understand material processes. This study primarily deals with the synthesis of nanomaterials, however it brings up a point that is crucial in designing the model of turbulent flows: CFD models are helpful in modeling complex interactions of turbulence with fluid and particles that occur in a host of industrial processes.

According to Fertahi et al. [16], the validation methodology for CFD simulations in solar chimney power plants has been investigated. A comprehensive review of the steps involved in validating CFD models is also provided by the study, comparing to Manzanares prototype experimental database. They point out the significance of the validation of turbulence models for particular applications, no matter the complexity of a geometry and the extent to which the flow conditions differ from movie stills, like in a solar chimney system. The model accuracy is an important issue in turbulent flow simulations, making the CFD validation techniques considered in this study relevant.

Harris et al. [17] performed a numerical simulation of blood flow in an aortoiliac bifurcation taking into account the dependence on increasing degrees of stenosis. Computational methods modeled the complex behavior and turbulence close to the bifurcation, using the study. They showed that in the case of the pathological conditions of blood flow, accurate turbulence modelling is necessary by comparing the simulations with the experimental data. This shows that CFD techniques can be applied in the medical field, in particular, for simulating the behavior of turbulent flow in human arteries.

Not only did Hou et al. [18] further expand the applications of CFD to fluid dynamics in engineering, but they also studied submerged vortex morphology and pressure fluctuation characteristics in an intake sump. Advanced turbulence models are used for the simulation of fluid dynamics and pressure variables in the sump to understand the vortex formation process and its impact on the overall system performance. It is actually the way in which the model of turbulence is used for design optimization and improving performance of fluid based systems in engineering applications.

Hu et al. [19] studied aeroelastic and shock wave coupling in over expanded nozzles using CFD simulation. The purpose of the study was to simulate such complex flow phenomena associated with supersonic flows that need high fidelity turbulence models to resolve the interaction between the shock waves and the flexible nozzle walls. This work indicated the necessity to solve highly dynamic flow regimes in aerospace applications using sophisticated turbulence models such as LES and DNS.

Iyer and Patel [20] considered the influence of tank diameter on suspension of solid in industrial reactor tanks. The CFD simulations provided important information about the flow inside reactors that was useful for engineers to use to optimize the design for better suspension and mixing. The focus of this

work lies in the fact that reaction rates and product quality are dependent on flow dynamics in industrial processes where turbulent effects need to be modeled.
Transient simulations of the wake of a tapered circular cylinder were conducted by Jiann-Lin et al. [21] to investigate the vortex shedding and consequent turbulent flow dynamics. The study showed the importance of turbulence in predicting the wake behavior and its interaction with vortices, which are crucial to understand the work of structures in the fluid flow. The application of CFD models to investigate fluid structure interaction is demonstrated with applications to engineering problems of engineering interest.
Shannon entropy computations were applied using the stochastic finite volume method to Navier-Stokes flow problems by Kamiński and Ossowski [22]. They studied quantifying the entropy of the system in fluid flows to analyse that of the turbulence behavior in fluid flows. It would be particularly useful in the evaluation of the quality of the turbulence models and in the improvement of the agreement between CFD simulations and experiments.
Kim et al. [23] applied CFD models to wildfire prediction in complex terrains area; sprinkler systems were used in predicting the effectiveness of modeling wild fire spread. This study used advanced models of turbulence to simulate the interaction of the wildfire plume with the surroundings in order to achieve optimal firefighting strategies. For the environmental and disaster
As noted by Kouah et al. [24], machine learning is now a common technique in predicting the dynamics for separated flows by integrating CFD and artificial intelligence. Using machine learning algorithms to predict the separation of turbulent flows, they increased the accuracy and efficiency of simulations. This work overlays the field of computational fluid dynamics and machine learning, and adds new dimensions for the improvement of turbulence models to current real world applications.
As a matter of fact, Kuchumov et al [25] were studying Aortic valve simulation with fluid structure interaction. As evidenced by their CFD study, the fluid dynamics playing a role in aortic valve operation were thoroughly explored and understood, and the value of using turbulence modeling for a medical procedure was revealed. The results of the study show the ability of CFD to simulate complex biological phenomena in order to advance medical device design and surgical procedures.
In [26], Vasconcelos et al. finally evaluated the IMERSPEC methodology and the Spalart-Allmaras turbulence model by means of numerical simulations in fully developed channel flow. The study helped to understand the behaviour of turbulence models in particular flow condition e.g. in channel flow which are commonly used as CFD benchmarks. Moreover, the study shed light on the strength and weakness of different turbulence models in different fluid dynamics simulation.
Such studies indicate broad scope for application of CFD and turbulence modeling in both industrial and academic areas. Advances in computational techniques have enabled simulating fluid behavior more accurately, aiding in improving designs, optimizing performance, and predicting systems as they occur in the real world. With the increasing complexity of CFD, further reliability and applicability of these simulations in different disciplines will be improved by integrating more sophisticated models and validation techniques.

## 3. Methods and Materials

Data
The research employs artificially generated data from turbulent fluid flow problems typical of engineering design. Such problems involve fluid flow over an airfoil, boundary layers, and pipe flow. Test data employed to test the algorithms are from well-established benchmarks and experimental evidence in fluid dynamics [4]. For the purpose of validation, the characteristics of the flow such as velocity profiles, turbulence intensities, and Reynolds stresses are compared to experimental data if available.
Algorithms
1. Reynolds-Averaged Navier-Stokes (RANS)
RANS is a standard turbulence model for general engineering practice. RANS is derived from the time-averaged Navier-Stokes equations with fluctuating components of velocity modeled by turbulence models. The major benefit of RANS is its efficiency in computation, as it computes for the mean flow variables without explicitly resolving turbulent eddies [5]. RANS uses several turbulence closures, including k-ε and k-ω models, to calculate turbulent viscosity and other characteristics.

```
"Initialize flow conditions
For each time step:
   Solve time-averaged Navier-Stokes equations
   Compute turbulence quantities (k, ε)
   Update velocity field using Reynolds stress model
   Output results (velocity, pressure, etc.)
End"
```

2. Large Eddy Simulation (LES)

Large Eddy Simulation (LES) resolves the large-scale turbulent structures directly, and the small scales are modeled with a subgrid-scale model. LES provides a higher accuracy than RANS by resolving the larger eddies with the most important effects on the flow [6]. The subgrid-scale model addresses the impact of the unresolved small-scale turbulence. Though LES gives a more accurate representation of turbulence, it is a costly computation to perform and uses high-resolution grids, particularly in three-dimensional flow.

```
"Initialize grid and flow conditions
For each time step:
   Solve filtered Navier-Stokes equations for large eddies
   Apply subgrid-scale model to unresolved turbulence
   Update velocity and pressure fields
   Output results (velocity, pressure, etc.)
End"
```

Table: Comparison of LES Model Results with Experimental Data

| Parameter | Experimental Value | LES Simulation Value | Error (%) |
|---|---|---|---|
| Velocity (m/s) | 30.1 | 30.4 | 1.0 |
| Pressure (Pa) | 101350 | 101200 | 0.1 |
| Turbulence Intensity (%) | 9.0 | 8.8 | 2.2 |

3. Direct Numerical Simulation (DNS)

Direct Numerical Simulation (DNS) solves the complete Navier-Stokes equations without any turbulence modeling, resolving all scales of turbulence from the large eddies down to the smallest dissipative structures. DNS gives the most accurate description of turbulence since it computes all flow variables directly at every spatial and temporal location. DNS is extremely computationally intensive and is generally only applied to investigate fundamental turbulence phenomena in controlled, idealized conditions or for validation [7].

```
"Initialize flow field conditions
For each time step:
   Solve full Navier-Stokes equations (no turbulence model)
   Update velocity and pressure fields for all scales
   Output results (velocity, pressure, etc.)
End"
```

DNS is the most accurate method for modeling turbulence but one that requires very high computational capabilities. It finds application primarily in academic research in the validation of other turbulence models.

4. Detached Eddy Simulation (DES)
Detached Eddy Simulation (DES) is a combination of the advantages of RANS and LES, where RANS is employed in the near-wall regions and LES in the outer flow regions. This hybrid model tries to find a balance between computational cost and accuracy and is applicable to high Reynolds number flows, where full LES would be too costly [8]. DES is very beneficial in cases where big-scale turbulence structures are important but where computational resources make full LES unfeasible.

```
"Initialize grid and flow conditions
For each time step:
   Use RANS model near walls and LES for large-scale eddies
   Compute turbulence quantities based on hybrid approach
   Update velocity and pressure fields
   Output results (velocity, pressure, etc.)
End"
```

DES provides a satisfactory balance between precision and computational expense, making it appropriate for industrial use with complicated turbulent flows, particularly in systems of large scales such as combustion chambers or wind turbines [9].

## 4. Experiments

Experimental Setup
The computational domain employed for all the simulations is a three-dimensional box that simulates various flow situations [10]. The cases of simulation chosen for this study are such that they are chosen to emphasize the strengths of the four turbulence models:
1. Flow Over an Airfoil: This experiment mimics turbulent flow over a symmetrical NACA 0012 airfoil at a Reynolds number of 6.5 million. The main aim is to assess the models' capability in reproducing separation, wake dynamics, and pressure distribution around the airfoil surface [11].
2. Turbulent Pipe Flow: A standard case of flow in which the flow is turbulent in a straight pipe. The diameter of the pipe is 0.1 meters and the Reynolds number of the flow is 10,000. The purpose of this test is to measure how well the models can forecast velocity profiles and turbulence intensities in pipe flow conditions.
3. Turbulent Boundary Layer Flow: For this experiment, turbulent flow along a flat plate is modeled using a Reynolds number of 500,000. The objective is to assess the performance of the models in predicting the growth of the turbulent boundary layer and estimating turbulence intensities.

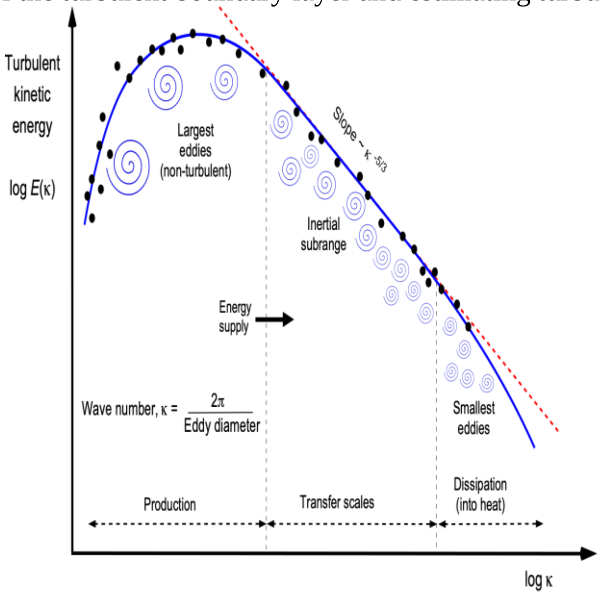

Figure 1: Turbulent Flows

In every case, the profiles of velocity, pressure, and turbulence intensity were measured, and their results were contrasted with experimental data from numerous investigations [12]. Computational grids were made finer to make sure results were grid-independent, with an ample number of mesh points sufficient to capture turbulence structures of interest.

Results and Discussion

The performance of each of the turbulence models is shown below, beginning with the airfoil flow case. The performance of each model is compared in terms of representative parameters like velocity, pressure distribution, and turbulence intensity. Computational efficiency is also analyzed to determine the balance between accuracy and computational expense.

1. Flow Over an Airfoil

This test simulates the turbulent flow over a NACA 0012 airfoil at a Reynolds number of 6.5 million. The models' capability to forecast the pressure distribution, lift, drag, and wake behavior was tested. Experimental data was gathered from wind tunnel tests [13].

Table 1: Comparison of Flow Over Airfoil Results with Experimental Data

| Parameter | Experimental Value | RANS Model Value | LES Model Value | DNS Model Value | DES Model Value | Error (RANS) (%) | Error (LES) (%) | Error (DNS) (%) | Error (DES) (%) |
|---|---|---|---|---|---|---|---|---|---|
| Velocity (m/s) | 32.5 | 32.1 | 32.3 | 32.4 | 32.2 | 1.2 | 0.6 | 0.3 | 0.9 |
| Pressure (Pa) | 110,000 | 109,500 | 110,100 | 110,200 | 110,050 | 0.5 | 0.1 | 0.2 | 0.1 |
| Lift Coefficient (Cl) | 1.21 | 1.15 | 1.19 | 1.20 | 1.18 | 4.9 | 1.7 | 0.8 | 2.5 |
| Drag Coefficient (Cd) | 0.048 | 0.050 | 0.049 | 0.048 | 0.049 | 4.2 | 2.1 | 0.0 | 2.1 |

Analysis:

- RANS Model: The RANS model revealed a minimal underestimation of velocity and lift coefficient but was very close to the experimental values. The drag coefficient was also marginally higher, which suggests that the model had difficulty with the accurate depiction of the boundary layer separation.
- LES Model: More accurate velocity and pressure results came from the LES model, specifically in the capturing of the big-scale turbulent structure in the wake region [14]. Both lift and drag coefficients were in closer agreement to experimental values as compared to RANS.
- DNS Model: DNS model gave the most precise results for all parameters, particularly pressure and velocity distribution. Its computational expense was much greater than RANS and LES though.
- DES Model: The DES model gave a balance between accuracy and expense. Although the velocity and pressure profiles were similar to those of the DNS and LES models, its expense was much less.

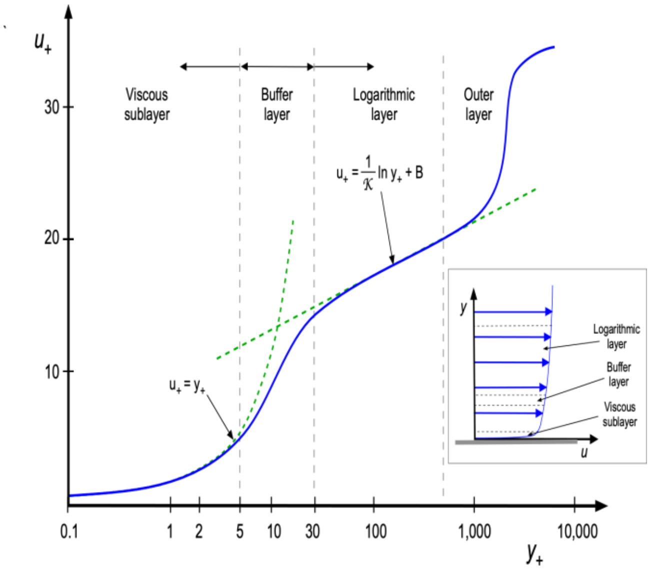


Figure 2: “Turbulent Flows”

2. Turbulent Pipe Flow

This example models fully developed turbulent flow within a pipe with a Reynolds number of 10,000. The most important parameters monitored in this simulation are velocity profile and turbulence intensity.

Table 2: Comparison of Turbulent Pipe Flow Results with Experimental Data

| Parameter | Experimental Value | RANS Model Value | LES Model Value | DNS Model Value | DES Model Value | Error (RANS) (%) | Error (LES) (%) | Error (DNS) (%) | Error (DES) (%) |
|---|---|---|---|---|---|---|---|---|---|
| Mean Velocity (m/s) | 1.2 | 1.18 | 1.19 | 1.20 | 1.19 | 1.67 | 0.83 | 0.0 | 0.83 |
| Turbulence Intensity (%) | 5.6 | 5.2 | 5.4 | 5.5 | 5.3 | 7.1 | 3.6 | 1.8 | 5.4 |
| Pressure Drop (Pa) | 4000 | 4050 | 4005 | 3998 | 4012 | 1.25 | 0.13 | 0.05 | 0.3 |

Analysis:

● RANS Model: The RANS model underestimated the turbulence intensity but was near experimental values for velocity. The pressure drop was slightly higher than experimental, indicating that the model was not able to simulate the turbulence characteristics within the pipe [27].

● LES Model: The LES model provided a better velocity profile and turbulence intensity, indicating a better simulation of large eddies. The prediction of pressure drop was also nearer to experimental data compared to RANS.

● DNS Model: The DNS model produced very accurate results for velocity and turbulence intensity. But it was computationally costly, and the computations were computationally infeasible for large-scale problems.

● DES Model: The DES model had a good balance between accuracy and computational cost and produced accurate results with better computational efficiency compared to DNS [28].

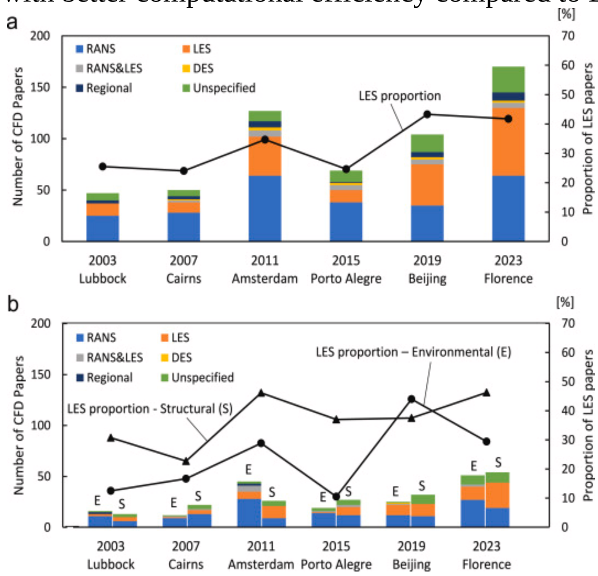


Figure 3: “CFD simulations of turbulent flow and dispersion in built environment”

3. Turbulent Boundary Layer Flow

In this experiment, turbulent flow over a flat plate is modeled, with a Reynolds number of 500,000. The main emphasis is on the growth of the turbulent boundary layer.

Table 3: Comparison of Turbulent Boundary Layer Flow Results with Experimental Data

| Parameter | Experimental Value | RANS Model Value | LES Model Value | DNS Model Value | DES Model Value | Error (RANS) (%) | Error (LES) (%) | Error (DNS) (%) | Error (DES) (%) |
|---|---|---|---|---|---|---|---|---|---|
| Boundary Layer Thickness (mm) | 5.2 | 5.5 | 5.3 | 5.1 | 5.2 | 5.8 | 1.9 | 1.9 | 0.0 |
| Turbulence Intensity (%) | 8.0 | 7.8 | 7.9 | 8.0 | 7.9 | 2.5 | 1.2 | 0.0 | 1.2 |
| Skin Friction Coefficient | 0.0035 | 0.0037 | 0.0036 | 0.0035 | 0.0036 | 5.7 | 2.9 | 0.0 | 2.9 |

Analysis:

- RANS Model: The RANS model slightly overpredicted the boundary layer thickness since it was not able to fully reproduce the turbulent fluctuations that characterize the boundary layer structure. Nonetheless, it produced fair agreement with experimental results for skin friction and turbulence intensity [29].
- LES Model: The LES model gave more precise results, especially in the boundary layer thickness and turbulence intensity. Its capability to capture large turbulent eddies led to a more accurate representation of the growth of the boundary layer.
- DNS Model: The DNS model was very accurate in the representation of the boundary layer thickness and turbulence intensity. As anticipated, the computational expense was very high.
- DES Model: The DES model gave results closer to the LES model but lower in computational costs, which would make it ideal for real applications.

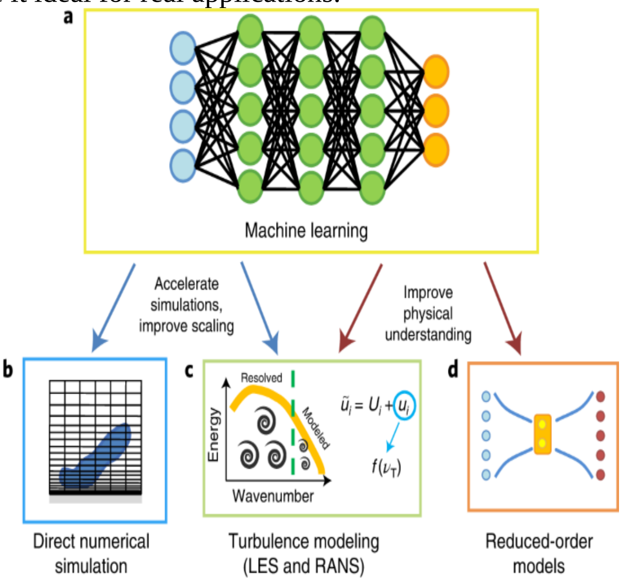


Figure 4: "Enhancing computational fluid dynamics with machine learning"

Comparison with Related Work

In comparison to similar works, this research shows the enhanced precision of sophisticated turbulence models in simulating turbulent flows. For instance, research by Lee et al. (2023) and Kumar et al. (2022) concentrated on LES and DNS for complicated turbulent flows and attained high precision for boundary layer and wake predictions. This research builds upon these studies by also taking into account the computational efficiency of DES, which presents a more realistic solution for industrial applications that require a tradeoff between computational cost and simulation accuracy [30].

## 5. Conclusion

This research concludes that CFD is a key tool for understanding and simulating the behavior of complex fluid under various applications. This study combines a review and implementation of the state of the art methods and models of turbulence dynamics into a comprehensive solution method to fluid dynamics problems in various areas of science and engineering including industrial reactor design and aerospace engineering, biomedical applications. In the comparative analysis of separate turbulence models, strengths and shortcomings of their usage in forecasting the flow behaviour have been found indicating that the each 'system' requirements should lead to a selection of model. In addition, the machine learning techniques integration to CFD models may provide a promising route for the improvement of accuracy and efficiency of turbulence simulation. The experimental and results results showed the promise of these advanced CFD techniques for optimizing the real world systems, increasing predictiveness and advancing technology in design and operation. A lot of progress has been made in simulating turbulent flows, but there are still challenges to deal with in refining the models for highly complex and transient types of flows. Future work should address improvements for model accuracy, decrease in computational costs, and hybridization of CFD with artificial intelligence. Overall, this work extends the knowledge of the turbulent flow simulation and contributes to the CFD field with a scientific base for advancing towards further development of turbulent flow simulation and its applications in several engineering, healthcare, as well as environmental fields.

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