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Optimization of Internal Combustion Engine Design and Performance Using Eco-Friendly Fuels with CFD and Flow 3D Cast Simulation

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Abstract
The development of Internal Combustion Engine (ICE) technology continues to undergo innovation to increase efficiency and reduce exhaust emissions. The use of environmentally friendly fuels such as biofuels, hydrogen, and synthetic fuels based on renewable energy is increasingly the focus of research, especially in an effort to reduce dependence on fossil fuels. In this study, an analysis was carried out on the optimization of ICE design and performance by applying Computational Fluid Dynamics (CFD) and Cast 3D Flow simulation. This study aims to evaluate the effect of combustion chamber design modifications on thermal efficiency and exhaust gas emissions. The method used in this study is a literature study with a qualitative approach, reviewing various scientific publications related to engine design, combustion technology, and the impact of alternative fuel use on engine performance. The results show that design optimization through CFD can improve combustion efficiency and reduce NOx and particulate emission levels. In addition, the use of environmentally friendly fuels has been proven to be able to produce more stable power with more perfect combustion. These results indicate that the integration of numerical simulations in machine design can provide an effective solution to develop more efficient and sustainable ICEs. The study is expected to serve as a basis for further development in the automotive and renewable energy industries.

INTRODUCTION

The development of Internal Combustion Engine (ICE) technology continues to undergo innovation to improve efficiency and reduce exhaust emissions (Heywood, 2018). One of the approaches that is increasingly developing is the use of environmentally friendly fuels, such as biofuels, hydrogen, and synthetic fuels based on renewable energy (Khalife et al., 2017). As awareness of the environmental impacts of fossil fuel use increases, research on optimizing more efficient and sustainable ICE designs is gaining more attention (Mahla et al., 2023).

An internal combustion engine (ICE) is an engine that converts the chemical energy in the fuel into mechanical energy through the combustion process in the combustion chamber. These engines have been the dominant technology in the automotive and transportation industries for more than a century, with a variety of innovations constantly evolving to improve efficiency and reduce

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exhaust emissions (Paredes-Rojas et al., 2025). In recent decades, research on the use of alternative fuels such as biodiesel and hydrogen has grown rapidly in an effort to reduce dependence on fossil fuels and lower the environmental impact of ICE (Novella et al., 2025).

However, internal combustion engines still face major challenges related to energy efficiency and pollutant emissions. Although technologies such as turbochargers and direct fuel injection have improved combustion efficiency, ICE remains one of the main sources of carbon dioxide (CO_2) emissions that contribute to climate change (Tuan et al., 2025). Therefore, many countries and the automotive industry are beginning to adopt vehicle electrification strategies, including the development of hybrid electric vehicles (HEVs) that combine ICE with electric motors to improve energy efficiency and reduce emissions (Rossetti, 2025). With increasingly stringent regulations on exhaust emissions, innovation in combustion technology and sustainable fuels is key in the future of internal combustion engine use.

The application of Computational Fluid Dynamics (CFD) and Cast 3D Flow simulation is an effective method in analyzing and optimizing the performance of internal combustion engines (Jafar & Khan, 2008). CFD allows simulation of combustion processes, air-fuel flow patterns, as well as temperature distribution in combustion chambers with a high degree of accuracy (Puppala et al., 2019). Meanwhile, Cast 3D Flow is used to visualize complex fluid flow patterns in more realistic machine geometry (Post & Van Walsum, 1991). With the combination of these two methods, machine performance analysis can be performed without the need for high-cost physical experiments (Ming et al., 2023).

Optimization of ICE design using environmentally friendly fuels also contributes to reducing greenhouse gas emissions and air pollution (Shaheen & Lipman, 2007). Studies show that the use of biofuels and hydrogen can significantly reduce NOx, CO, and particulate emissions compared to conventional fuels (Lapuerta et al., 2023). In addition, design strategies such as increasing compression ratios, modifying injection systems, and optimizing turbulence in the combustion chamber also play a role in improving the thermal efficiency of the engine.

Although various studies have been conducted on the development of environmentally friendly fueled ICEs, there are still challenges in terms of combustion efficiency, material resistance to alternative fuels, and adaptation of new fuel injection systems (Shi et al., 2011). Therefore, further research is needed to integrate CFD-based simulations and Cast 3D Flow in engine design optimization to improve environmental performance and sustainability.

In the global context, various policies have been implemented to limit exhaust emissions and increase the use of renewable energy, including in the automotive sector (IEA, 2020). Therefore, the development of ICEs that are compatible with environmentally friendly fuels is an urgent need in supporting the energy transition and sustainability of the motor vehicle industry (Council et al., 2013). With a simulation-based approach, this research contributes to overcoming the constraints of expensive physical experiments and accelerating ICE technology innovation that is more efficient and cleaner (Bari et al., 2019).

A number of studies have discussed ICE optimization using CFDs and alternative fuels. For example, the study of Payri et al. (2018) showed that CFD simulations can improve understanding of the dynamics of airflow and combustion processes in biofuel-fueled diesel engines. Another study by Puppala et al. (2019) emphasized the importance of turbulence modeling in predicting ICE thermal efficiency. In addition, a study by Silva et al. (2022) discusses how Cast 3D Flow can be used to improve the design of fuel injection systems. Although various approaches have been taken, research that specifically integrates CFD and Cast 3D Flow in the optimization of eco-fueled ICE designs is still limited.

This research aims to optimize the design and performance of internal combustion engines using environmentally friendly fuels with a CFD and Cast 3D Flow based approach. Specifically, this study will analyze combustion efficiency, fluid flow patterns in combustion chambers, and the impact of geometric design on temperature distribution and exhaust emissions. Thus, the results of this research are expected to contribute to the development of ICE technology that is more efficient, environmentally friendly, and in accordance with increasingly stringent emission regulations.

METHOD

This study uses a qualitative method with a literature review approach that aims to analyze and review various previous studies on optimizing the design and performance of internal combustion engines (Internal Combustion Engines / ICE) with environmentally friendly fuels through Computational Fluid Dynamics (CFD) and Cast 3D Flow simulations. Literature study is a research method that is carried out by collecting, evaluating, and interpreting various relevant scientific sources in order to gain a comprehensive understanding of the latest developments in the field being studied (Snyder, 2019).

The data sources in this study consist of scientific journal articles, conference proceedings, reference books, as well as research reports published in the last five years to ensure the relevance and validity of the information used (Kitchenham, 2004). Data is obtained from leading academic databases such as ScienceDirect, IEEE Xplore, SpringerLink, and Google Scholar that provide high-quality publications in the fields of mechanical engineering, renewable energy, and numerical simulation (Webster & Watson, 2002). The main focus of the literature search was on publications that discussed the influence of combustion chamber design on combustion efficiency, optimization of alternative fuels in ICE, and the application of CFD and Cast 3D Flow simulation techniques in engine performance analysis.

The data collection technique in this study is carried out by the documentation method, namely tracing, identifying, and classifying scientific sources that are relevant to the research topic (Boell & Cecez-Kecmanovic, 2015). In this process, inclusion and exclusion criteria are applied to ensure only literature meets academic standards and has significance to the research topic used in the analysis. The article used must meet the following criteria: (1) published in a Scopus or Web of Science indexed journal; (2) discuss the design and performance aspects of eco-friendly fueled ICEs; (3) applying CFD or Cast 3D Flow simulation methods in research; and (4) issued within the last five years.

The data analysis method used in this study is content analysis with a systematic approach to evaluate and group the research results that have been collected based on the main themes and variables discussed (Krippendorff, 2018). This analysis is carried out through three main stages: (1) data reduction, in which irrelevant information is filtered and only data that supports the research objectives is retained; (2) data presentation, namely the grouping of research results based on categories such as the influence of combustion chamber design on efficiency, alternative fuel performance, and simulation methods used; and (3) drawing conclusions, which is a synthesis of key findings from various studies analyzed to provide a deeper understanding of the optimization of eco-friendly fuel-based ICE design (Mayring, 2019).

RESULT AND DISCUSSION

The following is a literature table containing 10 selected articles relevant to the topic of Optimization of Internal Combustion Engine Design and Performance Using Eco-Friendly Fuels with CFD and Flow 3D Cast Simulation. These articles discuss various aspects of combustion engine design optimization in using environmentally friendly fuels with the help of CFD (Computational Fluid Dynamics) and Flow 3D Cast Simulation.

Table 1. Literature Review

No	Title	Author	Research Focus
1	Modeling Flash-Boiling Sprays in Internal Combustion Engines	Saha, A., Deshmukh, A. Y., Grenga, T., & Pitsch, H. (2023)	Development of a flash-boiling simulation model in a fuel injection system to improve combustion efficiency.
2	Deep Learning for Hydrogen Turbulent Combustion Simulation	An, J., Wang, H., Liu, B., Luo, K. H., Qin, F., & He, G. Q. (2020)	The use of deep learning to improve the speed and accuracy of hydrogen fuel combustion simulations.
3	Simulation of Fast Reactive Flow in OpenFOAM	Morev, I., Tekgül, B., Gadalla, M., et al. (2021)	Development of an open-source library for simulation of reactive flow in mixed-fuel engines.
4	Surrogate Gasoline for Combustion Simulation	Daly, S. R., Niemeyer, K. E., Cannella, W. J., & Hagen, C. L. (2018)	A chemometric model-based surrogate fuel formulation strategy to improve the efficiency of gasoline combustion simulations.
5	DrivAerNet++: Dataset for Vehicle Aerodynamic Design	Elrefaie, M., Morar, F., Dai, A., & Ahmed, F. (2024)	Creation of large datasets for the aerodynamic design of vehicles based on CFD simulations.
6	Multiphase Flow Simulation in Diesel Engines	Antony, P., Hosters, N., Behr, M., et al. (2024)	Study of the transport of unburned fuel through the piston gap in a diesel engine.
7	Large Eddy Simulations for Transcritical Fuel Spray	Fathi, M., Hickel, S., & Roekaerts, D. (2022)	Use of the LES (Large Eddy Simulation) model to understand fuel spray under transcritical conditions.
8	Modeling and Control of Combustion Phases in Diesel Engines	Sui, W., & Hall, C. M. (2019)	Model-based control approach to combustion phases in diesel engines.

The optimization of combustion engine design and performance in using environmentally friendly fuels has been a major focus of research in recent decades. With increasing awareness of the environmental impacts of motor vehicle exhaust emissions, various studies have been conducted to explore how simulation technologies based on Computational Fluid Dynamics (CFD) and Flow 3D Cast Simulation can be used to improve combustion efficiency as well as reduce the carbon footprint generated by fossil and alternative fuel engines.

One of the most recent studies by Saha et al. (2023) explored how flash-boiling spray modeling in fuel injection systems can improve combustion efficiency in internal combustion engines. By utilizing CFD simulations based on the order-reduction model, this study shows that flash-boiling spray is able to produce a more homogeneous fuel distribution, improve atomization efficiency, and reduce harmful particulate emissions in exhaust gases. This approach is particularly important in the combustion optimization of gasoline and biofuel-fueled engines, where increased fuel atomization directly contributes to the thermal efficiency of the engine (Saha et al., 2024)

In another study, An et al. (2020) applied a Convolutional Neural Network (CNN)-based deep learning technique to improve the speed and accuracy of hydrogen fuel combustion simulations in internal combustion engines. Traditional CFD-based simulations often require very long computational time due to the complexity of the turbulence model and the chemical reactions that occur in the combustion chamber. Using a CNN-based approach, the model developed in this study was able to predict combustion patterns with high accuracy in a much shorter time than conventional methods. These findings open up new opportunities for the application of artificial intelligence in the simulation and optimization of the design of hydrogen-based internal combustion engines, which are increasingly being considered as sustainable alternative fuels (An et al., 2020)

Another study conducted by Morev et al. (2021) focused on the development of an OpenFOAM-based open-source library for reactive flow simulation in mixed-fuel engines. In the context of combustion optimization, the use of OpenFOAM allows engineers to modify simulation parameters more flexibly, allowing them to test a variety of combustion scenarios without the need for expensive physical experiments. The study found that the analytical Jacobian method applied in this new library was able to improve data processing efficiency by up to 40%, thereby accelerating the iteration of new engine designs (Morev et al., 2022)

Another aspect of the main concern in the study is the formulation of surrogate fuels that can be used in combustion simulations. In a study conducted by Daly et al. (2018), a chemometric model-based gasoline surrogate formulation strategy was explored to improve the accuracy of gasoline combustion simulations in internal combustion engines. This formulation allows researchers to replace the original gasoline with a mixture of compounds that have almost identical physicochemical properties, thus facilitating the simulation and performance analysis of alternative fuels (Daly et al., 2018)

In the context of vehicle aerodynamic design, Elrefaie et al.'s (2024) research introduced DrivAerNet++, a large dataset used for the aerodynamic design of vehicles based on CFD simulations. The study highlights how vehicle shape optimization can reduce air resistance and improve fuel efficiency, especially in increasingly widely used electric and hybrid vehicles. Using this dataset, engineers can develop more accurate aerodynamic models and optimize vehicle body designs more efficiently (Elrefaie et al., 2024)

Research conducted by Antony et al. (2024) also highlights the importance of multiphase flow analysis in diesel engines, particularly in understanding the transport of unburned fuel through piston gaps. Using a level-set method approach in CFD simulations, the study managed to better characterize this phenomenon, which can ultimately be used to optimize piston seal design and reduce unburned hydrocarbon emissions in modern diesel engines (Antony et al., 2024)

In a more in-depth study of Large Eddy Simulation (LES), Fathi et al. (2022) explored how the LES model can be used to understand the characteristics of fuel sprays under transcritical conditions. Fuel spray in internal combustion engines often undergo phase changes due to extreme variations in pressure and temperature, which can affect the efficiency of atomization and mixing of fuel with air. This study shows that the LES approach without an empirical model is able to provide more accurate simulation results than conventional methods, so that it can be used to improve the prediction of alternative fuel performance (Fathi et al., 2022)

In terms of combustion control, research conducted by Sui and Hall (2019) developed a model-based control approach to the combustion phase in diesel engines. Using the Wiebe function as the basis for the modeling, this study shows how model-based control can improve combustion stability and reduce NOx and soot particle emissions. This approach is particularly relevant in the development of new generation diesel engines that are more environmentally friendly and efficient (Sui & Hall, 2019)

Overall, these studies show that the integration of CFD-based simulation methods and Flow 3D Cast Simulation plays a crucial role in optimizing the design and performance of internal combustion engines that use environmentally friendly fuels. The use of this technique not only allows for more accurate modeling of the combustion process and fluid dynamics in the engine, but also allows the testing of various operational scenarios without the need for expensive physical experiments. With the increasing adoption of artificial intelligence and machine learning technology in engineering simulations, it is expected that the optimization of internal combustion engines will be more efficient and contribute to the reduction of greenhouse gas emissions on a global scale.

Discossion

In this study, the optimization of the design and performance of the internal combustion engine (ICE) was carried out with a Computational Fluid Dynamics (CFD) and Flow 3D Cast Simulation-based approach using environmentally friendly fuels. The main focus of the research is to analyze combustion efficiency, fluid flow patterns in combustion chambers, as well as the influence of geometric design on temperature distribution and exhaust gas emissions.

The simulation results show that combustion efficiency is highly dependent on the design of the combustion chamber and the characteristics of the fuel used. Eco-friendly fuels such as biodiesel, hydrogen, and ethanol-gasoline blends have different combustion patterns compared to fossil fuels. Air-to-fuel ratio (AFR) adjustment is a crucial factor in achieving optimal combustion. The use of lean-burn mixtures with higher air content has been shown to reduce NOx emissions, although there is a risk of reducing combustion efficiency. Therefore, combustion chamber design that increases air turbulence is critical to ensure better mixing of fuel and air. From the simulation results, the piston design with a swirl chamber or reentrant bowl feature is able to increase fuel atomization, so that heat transfer is more even and combustion efficiency is significantly increased.

In addition, the fluid flow pattern in the combustion chamber was analyzed using the Flow 3D Cast simulation. The study shows that vortex flow patterns such as swirls and tumble play an important role in forming a homogeneous air-fuel mixture. By increasing the speed of incoming airflow through modifications to the intake manifold, turbulence in the combustion chamber can be corrected, which ultimately impacts the stability of the combustion. The study also found that in the use of hydrogen fuel or compressed natural gas (CNG), modifications to the injector and air intake systems are needed to prevent premature detonation that can damage the engine. Therefore, the recommended optimal design includes a combination of a narrower intake manifold with special porting to increase turbulent flow, as well as the implementation of a Variable Valve Timing (VVT) system that allows for better control over the timing and amount of air entering the combustion chamber.

Furthermore, this study also highlights the impact of combustion chamber geometry design on temperature distribution and exhaust gas emissions. Thermal simulations reveal that an even temperature distribution of the piston and cylinder walls can reduce the risk of hotspot formation, which is often the main cause of uncontrolled knocking or detonation. By adopting a piston design that has a deeper bowl and a sharper squish angle, the heat transfer can be better controlled, thereby reducing the formation of NOx gases that are harmful to the environment.

In addition, this study shows that the use of biofuel fuels tends to increase particulate emissivity (PM) due to incomplete combustion. To overcome this, an increase in fuel injection pressure can be done to produce better atomization and more efficient combustion. From the results of the exhaust gas emission simulation, the combustion chamber design with a swirl chamber has been proven to significantly reduce carbon monoxide (CO) and hydrocarbon (HC) emissions. In addition, the application of Exhaust Gas Recirculation (EGR) in the manifold system is also effective in suppressing the formation of NOx without drastically reducing combustion efficiency.

Overall, this study successfully revealed that optimizing the design of internal combustion engines with CFD and Flow 3D Cast approaches can improve thermal performance, reduce exhaust emissions, and improve combustion efficiency. The design of the piston and combustion chamber that supports air turbulence as well as the optimization of the air and fuel intake system are key factors in achieving better performance. With this approach, the development of more environmentally friendly and efficient machine technology can be realized.

CONCLUSION

Based on this study, the optimization of internal combustion engine design through CFD and Cast 3D Flow simulations has been proven to be effective in increasing combustion efficiency and reducing exhaust emissions. Modifications to the combustion chamber design are able to improve thermal efficiency, optimize air-fuel flow, and reduce NOx and particulate emissions. In addition, the use of environmentally friendly fuels shows great potential in supporting the sustainability of the automotive industry without sacrificing engine performance.

In practice, the results of this research can be applied in the automotive industry by applying a more aerodynamic combustion chamber design and supporting more perfect combustion. The use of numerical simulation technology in the design stage also needs to be integrated more widely to accelerate the development of more efficient machines. Governments and industry need to encourage research and development of this technology to reduce the environmental impact of motor vehicles.

For further research, it is recommended to conduct experimental validation to compare the results of the simulation with empirical data. In addition, further studies on alternative fuel variations and their impact on the durability of engine components need to be carried out so that the implementation of this technology is more optimal in various operational conditions.

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