GRADUATE SCHOOL
ISTANBUL MEDENIYET UNIVERSITY
DEPARTMENT OF NANOSCIENCE AND NANOENGINEERING

Investigation of the Effects of Nano Structured Fuel Droplets in Diesel Engines with Machine Learning Approach and Rapid Optimization Technique

PhD

Kubilay Güner

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THESIS JURY APPROVAL

This PhD thesis titled "Investigation of the Effects of Nano Structured Fuel Droplets in Diesel Engines with Machine Learning Approach and Rapid Optimization Technique." written by Kubilay Güner at the Department of Nanoscience and Nanoengineering was accepted by our jury.

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STATEMENTS

Style and Reference Manual Statement

Having reviewed this thesis written under my supervision, I confirm that it has been written in accordance with Vancouver Manual of Style and used its Vancouver reference format consistently throughout the entire text.

Prof. Dr. Hasan Köten

Declaration of Originality

I hereby declare that all information in this dissertation has been obtained and presented in accordance with academic rules and ethical conduct. I also declare that, as required by these rules and conducts, I have fully cited and referenced all material and results that are not original to this work.

Kubilay Güner

GENİŞ ÖZET

Dizel Motorlarda Nano Yapılı Yakıt Damlacıklarının Etkilerinin Makine Öğrenmesi Yaklaşımı ve Hızlı Optimizasyon Tekniği ile İncelenmesi

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Doktora Tezi, Nanobilim ve Nanomühendislik Anabilim Dalı

Danışman: Prof. Dr. Hasan Köten

Aralık 2025

Bu çalışma, ağır hizmet tipi bir içten yanmalı motor için geliştirilen ortak hat enjeksiyon sisteminin performans ve emisyon üzerindeki etkilerinin, hesaplamalı akışkanlar dinamiği (CFD), gerçek motor deneyleri ve makine öğrenmesi yöntemleri kullanılarak bütüncül bir çerçevede incelenmesini amaçlamaktadır. Günümüzde artan enerji ihtiyacı ve sıkılaşan çevre düzenlemeleri doğrultusunda daha verimli ve çevre dostu motor teknolojilerinin geliştirilmesi kaçınılmaz hâle gelmiştir. Ancak geleneksel motor geliştirme süreçleri, zaman alıcı deneyler ve yüksek hesaplama maliyeti gerektiren simülasyonlara dayandığından, tasarım süreci hem pahalı hem de sınırlı kalmaktadır. Bu nedenle, bu çalışmada veri temelli yapay zekâ yaklaşımları ile fizik temelli mühendislik analizleri birleştirilerek, motor optimizasyon sürecine yeni bir metodolojik bakış açısı kazandırılmıştır.

Araştırmada öncelikli olarak gerçek motor testleri gerçekleştirilmiş ve motorun enjeksiyon stratejilerine verdiği tepkiler deneysel olarak incelenmiştir. Bu deneyler sayesinde, motorun gerçek çalışma koşulları altında sergilediği davranışlar doğrudan gözlemlenmiş, elde edilen ölçümler, simülasyon ve makine öğrenmesi modelleri için referans veri kaynağı olarak kullanılmıştır. Deneysel veriler, enjeksiyon zamanlaması, basınç ve supap hareketleri gibi parametrelerin yanma süreci ve motor performansı üzerindeki belirleyici etkilerini ortaya koymuş ve çalışmanın mühendislik açısından güvenilirliğini artırmıştır.

Deneysel çalışmalarla eş zamanlı olarak gerçekleştirilen CFD simülasyonları, silindir içindeki akış yapısını, türbülans oluşumunu, püskürtme süreçlerini ve yanma gelişimini detaylı olarak analiz etme imkânı sunmuştur. Üç boyutlu CFD analizleri, motor içindeki karmaşık fiziksel süreçlerin sayısal olarak modellenmesini sağlamış, özellikle yakıt-hava etkileşimi ve sıcaklık dağılımları açısından yüksek çözünürlüklü veriler elde edilmiştir. Bu simülasyonlardan elde edilen çıktılar, yalnızca fiziksel sürecin anlaşılmasına katkı sağlamamış, aynı zamanda makine öğrenmesi modellerinin eğitiminde kullanılan büyük veri kümesinin temelini oluşturmuştur.

Çalışma kapsamında, CFD simülasyonları sonucunda elde edilen büyük veri seti, makine öğrenmesi algoritmalarına girdi olarak sunulmuştur. Toplamda yaklaşık on milyon veri noktası içeren bu veri kümesi, eğitim ve test amacıyla ikiye ayrılmıştır. Verilerin yüzde sekseni modelin eğitilmesi için, geri kalan yüzde yirmisi ise modelin

doğrulanması ve performans değerlendirmesi için kullanılmıştır. Bu yaklaşım sayesinde makine öğrenmesi modellerinin yalnızca veriyi ezberlemesi değil, aynı zamanda yeni veri setleri üzerinde güvenilir tahminler yapabilmesi sağlanmıştır.

Makine öğrenmesi sürecinde çeşitli algoritmalar kullanılmış ve her birinin tahmin performansı karşılaştırmalı olarak analiz edilmiştir. Özellikle ağaç tabanlı topluluk yöntemleri ile sinir ağı tabanlı modeller, motor davranışını temsil etme açısından başarılı sonuçlar üretmiştir. Bu modellerin doğrusal olmayan ilişkileri yakalama yeteneği sayesinde enjeksiyon parametrelerinin performans ve emisyon üzerindeki karmaşık etkileri yüksek doğrulukla modellenmiştir. Buna karşılık, daha basit istatistiksel modellerin, yanma sürecinin karmaşıklığını temsil etmekte sınırlı kaldığı tespit edilmiştir. Bu durum, içten yanmalı motorların yalnızca doğrusal ilişkilerle açıklanamayacak derecede dinamik ve karmaşık sistemler olduğunu bir kez daha ortaya koymuştur.

Araştırmada ele alınan girdi parametreleri; yakıt enjeksiyon miktarı, enjeksiyon basıncı, püskürtme zamanlaması, emme ve egzoz supaplarının açıklık miktarları ile supap zamanlamasıdır. Bu parametreler, motorun çalışma karakteristiğini belirleyen temel değişkenlerdir. Özellikle enjeksiyon stratejileri, yanma sürecinin başlama anını, ısı açığa çıkma hızını ve silindir içi basınç gelişimini doğrudan etkilemektedir. Supap hareketleri ise silindire giren hava miktarını ve egzoz gazlarının tahliyesini kontrol ederek performans ve emisyon oluşumunda kritik rol oynamaktadır. Makine öğrenmesi modelleri, bu çok boyutlu parametre kümesini birlikte değerlendirerek sistemin genel davranışını öğrenmiştir.

Çıktı değişkenleri olarak motorun mekanik performansını ve çevresel etkilerini temsil eden temel göstergeler kullanılmıştır. Motor gücü, yakıt tüketimi ve egzoz emisyonları, sistemin değerlendirilmesinde esas alınan parametreler olmuştur. Bu çıktılar arasındaki ilişkilerin analiz edilmesi, motor tasarımında yalnızca performans artışına değil, aynı zamanda çevre dostu çözümlere de odaklanılması gerektiğini göstermiştir.

Çalışmanın bir diğer önemli yönü, nanoyapılandırılmış yakıt damlacıklarının motor performansı üzerindeki etkisinin araştırılmış olmasıdır. Nanoteknoloji destekli yakıt çözümleri, yakıtın daha küçük damlacıklara ayrılmasını sağlayarak yanma sürecini iyileştirmekte ve enerji dönüşüm verimini artırmaktadır. Bu tür yakıtların, yanma odasında daha homojen bir karışım oluşturduğu ve egzoz emisyonlarını azalttığı belirlenmiştir. Makine öğrenmesi modelleri, bu yakıtların farklı enjeksiyon koşulları altındaki etkilerini analiz etmiş ve en uygun kullanım senaryolarını ortaya koymuştur.

Optimizasyon sürecinde, makine öğrenmesi modelleri ile hızlı arama algoritmaları birlikte kullanılmıştır. Bu sayede geniş tasarım uzayı kısa sürede taranmış ve en ideal parametre kombinasyonları belirlenmiştir. Geleneksel motor tasarım süreçlerinde günler veya haftalar sürebilecek analizler, bu yaklaşım sayesinde çok daha kısa sürede tamamlanabilmiştir. Bu durum, makine öğrenmesi tabanlı optimizasyonun mühendislik uygulamalarında pratik ve sürdürülebilir bir çözüm sunduğunu göstermektedir.

Araştırmada geliştirilen modellerin başarımı, hem CFD verileri hem de deneysel ölçümler üzerinden doğrulanmıştır. Makine öğrenmesi tahminlerinin, gerçek motor davranışına yakın sonuçlar verdiği ve geleneksel simülasyon yöntemlerine güçlü bir alternatif oluşturduğu ortaya konmuştur. Böylece, yapay zekâ tabanlı modellerin yalnızca teorik araçlar olmadığı, aynı zamanda gerçek mühendislik problemlerine doğrudan uygulanabilir olduğu gösterilmiştir.

Sonuç olarak bu çalışma; gerçek motor deneyleri, CFD simülasyonları ve makine öğrenmesi yöntemlerini tek bir çatı altında toplayarak motor geliştirme süreçlerine yenilikçi bir bakış açısı kazandırmaktadır. Sunulan metodoloji, motor tasarım sürecini hızlandırmakta, maliyetleri düşürmekte ve doğruluk seviyesini koruyarak sürdürülebilir çözümler üretmektedir. Bu yaklaşım, içten yanmalı motorların geleceği açısından önemli bir potansiyel taşımakta ve mühendislik alanında veri temelli karar verme süreçlerinin yaygınlaşmasına katkı sağlamaktadır.

Bu bağlamda, çalışmanın ortaya koyduğu yöntem; yalnızca dizel motorlara değil, tüm içten yanmalı motor teknolojilerine uygulanabilir niteliktedir. Aynı zamanda hibrit ve alternatif yakıtlı motor sistemlerine de uyarlanabileceği öngörülmektedir. Bu yönüyle çalışma, enerji verimliliği ve çevresel sürdürülebilirlik hedeflerine ulaşmada önemli bir adım olarak değerlendirilmektedir.

Anahtar Kelimeler: İçten yanmalı motor, Hesaplamalı akışkanlar dinamiği, Makine öğrenmesi, Optimizasyon, Yapay zeka

ABSTRACT

Investigation of the Effects of Nano Structured Fuel Droplets in Diesel Engines with Machine Learning Approach and Rapid Optimization Technique

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This study presents a machine learning-based framework developed to improve the design and operational optimization of internal combustion engines using data obtained from high-fidelity multidimensional simulations. Conventional engine development procedures typically rely on extensive experimental testing and iterative numerical simulations, which demand considerable computational resources and long development periods that may extend from several months to multiple years. By integrating machine learning techniques, this research introduces an efficient approach for modeling complex physical phenomena occurring within the combustion chamber, enabling accurate prediction of engine behavior through statistical learning derived directly from simulation outputs. The primary emphasis of this work is placed on common rail injector parameters of a heavy-duty diesel engine operating under real-world conditions. Simulation inputs include in-cylinder air flow characteristics, pressure and temperature distributions at the onset of fuel injection, injection pressure levels, intake valve closure timing, and transient thermal conditions. The corresponding outputs include combustion performance, fuel consumption, and critical emission indicators, which are utilized as training data for constructing predictive models. Several machine learning algorithms are implemented and systematically evaluated to identify the most effective modeling strategies capable of capturing nonlinear relationships between input variables and engine responses. The results demonstrate that the trained models successfully approximate high-resolution simulation results with a high degree of accuracy while requiring only a fraction of the computational effort. This methodology significantly reduces development cost and time by minimizing reliance on repeated simulations and experimental trials. Ultimately, the proposed framework offers a scalable, data-driven solution that supports faster engine optimization and promotes improved efficiency, performance, and environmental sustainability for future internal combustion engine technologies.

Keywords: ICE, CFD, Machine Learning, Optimisation, AI.

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LIST OF ABBREVIATION

Abbreviation	Definition
CA	Crank Angle
CFD	Computational Fluid Dynamics
ML	Machine Learning
GA	Genetic Algorithm
ML-GA	Machine Learning–Genetic Algorithm
NOx	Nitrogen Oxides
ISFC	Indicated Specific Fuel Consumption
BSFC	Brake Specific Fuel Consumption
EGR	Exhaust Gas Recirculation
SOI	Start of Injection
BTDC	Before Top Dead Center
ATDC	After Top Dead Center
ICE	Internal Combustion Engine
HPC	High-Performance Computing
RANS	Reynolds-Averaged Navier–Stokes
KH-RT	Kelvin–Helmholtz Rayleigh–Taylor

Investigation of the Effects of Nano Structured Fuel Droplets in Diesel Engines with Machine Learning Approach and Rapid Optimization Technique

1. Introduction

Driven by consumer demand, companies are increasingly focusing on developing innovative engine designs that can simultaneously reduce fuel consumption and emissions. Therefore, R&D centers, in collaboration with industrial partners, are relying on advanced computational modeling combined with experimental prototyping to push the boundaries of these designs and achieve greater success. As computational methods and structural modeling techniques continue to evolve, numerical simulations can now be performed with far greater scope and accuracy than in previous studies. This progress has elevated the importance of engine design optimization, making it a central focus of modern engineering research. Consequently, research in this area is increasing.

A particularly promising area of research for the future is the study of the performance of nanostructured fuel droplets in diesel engines, which is studied using machine learning models and rapid optimization techniques. This is a highly complex and multidisciplinary field of research, interconnected with various disciplines and requiring expertise in mechanical engineering, materials science, physics, chemistry, nanotechnology, and data science. The primary objective is to investigate the potential and performance of nanostructured fuel droplets to increase efficiency while reducing emissions. Compared to conventional fuel droplets, nanostructured droplets are expected to offer several advantages, including improved performance, atomization and combustion, higher energy density, and lower pollutant formation. These properties make them attractive candidates for next-generation diesel engine technologies and are attracting consumer interest.

Machine learning plays a critical role in this study by saving time compared to simulation results and enabling the analysis and research of large datasets derived from experimental measurements and engine performance tests. By identifying hidden patterns and correlations among variables, machine learning algorithms can optimize engine performance and highlight the most promising nanostructured droplet configurations for further study. Predictive models developed through these algorithms can guide researchers toward optimal operating conditions, such as droplet size, injection timing, and combustion parameters. Rapid optimization techniques, including genetic algorithms and simulated annealing, complement this process by efficiently exploring the design space and identifying optimal configurations. These computational approaches significantly reduce the time and cost associated with experimental validation, accelerating the pace of innovation.

The research process itself involves several interconnected stages. First, the problem must be clearly defined, with research questions focusing on the effects of nanostructured droplets on performance, emissions, and fuel consumption, as well as the scalability of the technology. Next, reliable and representative data must be collected from experiments and simulations, covering engine performance metrics, emission levels, fuel properties, and droplet

characteristics. This data is then pre-processed to remove outliers, normalize values, and ensure compatibility with machine learning algorithms. Once prepared, the data is used to train predictive models that can uncover relationships among variables and forecast performance outcomes. These models are subsequently integrated into rapid optimization frameworks, which test different scenarios computationally to identify the most effective conditions for using nanostructured fuel droplets.

A crucial step in this process is validation. While simulations and machine learning models provide powerful insights, their predictions must be confirmed through experimental testing. In our research, the results obtained from simulations and machine learning models have been validated with real engine experiments, ensuring that the findings are not only theoretically sound but also practically applicable. This validation step strengthens the reliability of the models and demonstrates the feasibility of nanostructured fuel droplets in real-world diesel engine applications.

In summary, the investigation of nanostructured fuel droplets in diesel engines using machine learning algorithms and rapid optimization techniques represents a comprehensive and multi-faceted research effort. It integrates data collection, pre-processing, predictive modeling, optimization, and experimental validation into a unified framework. This study provides valuable information on the successful use of nanostructured fuel droplets and aims to improve engine performance, reduce emissions and increase fuel efficiency. By combining advanced computational tools with experimental validation, this research not only advances scientific understanding but also contributes to the development of more efficient and environmentally friendly diesel engines.

2. Literature Review

Accurate modeling of diesel engine performance with limited data has become achievable with advanced machine learning methods. Wong et al. [1] demonstrated that models such as the Least Squares Support Vector Machine, Relevance Vector Machine, and Extreme Learning Machine can predict engine performance even when the data is scattered. They applied a logarithmic structure to stabilize the data and used Bayesian and cross-validation methods for parameter optimization, achieving high accuracy and fast computation. Their findings demonstrated that combining nonlinear kernel methods with appropriate preprocessing can overcome the problems of data sparsity, instability, and complexity. This work provided the basis for subsequent studies focusing on machine learning-based engine performance prediction.

Building on this, Zheng et al. [2] developed a deep neural network model enhanced with virtual sample generation to overcome the limitations of insufficient experimental data. They generated synthetic data reflecting the distribution of real measurements, effectively expanding the training set without additional experiments. Using key parameters such as engine speed, power, oil temperature, and oil pressure, they achieved high prediction accuracy for fuel consumption, vibration, and noise. The model demonstrated excellent generalization and robustness against

overfitting. This work showed that data augmentation using virtual samples can substantially improve deep learning performance and reduce the cost of experimental testing.

Liao et al. [3] compared multiple advanced architectures, including Artificial Neural Network, Support Vector Machine, Long Short-Term Memory, Gated Recurrent Unit, Transformer, and Temporal Convolutional Network, to predict transient emission characteristics of diesel engines. Their results indicated that Long Short-Term Memory and Transformer models captured dynamic emission patterns more accurately than traditional methods. They emphasized that time-series deep learning models could represent the nonlinear temporal behavior of engine emissions. The study also highlighted the importance of selecting proper architectures for transient modeling tasks. Overall, it provided comprehensive insights into how different machine learning models handle dynamic, time-dependent engine data.

Zhao et al. [4] proposed a novel framework that integrates physical theories such as density functional theory and vibrational Stark effects with machine learning to predict field-enhanced catalysis behavior. By embedding physical constraints and first-order Taylor expansions into the learning process, they achieved reliable predictions even with limited datasets. Their analysis revealed that low-coordinated atomic sites and smaller nanoparticles generate stronger local electric fields, improving catalytic efficiency. This integration of physics and machine learning offered both interpretability and predictive accuracy. The research opened new directions for data-efficient and physically consistent catalyst design.

Similarly, research has examined the growing role of machine learning and big data analytics. They discussed how statistical techniques such as principal component analysis, multivariate curve resolution, and alternating least squares help extract patterns from complex experimental data. The study emphasized that machine learning can process large spectroscopy datasets, including infrared and X-ray absorption spectra, to identify key catalytic features. These tools accelerate material discovery by reducing experimental trial-and-error. The review also called for combining statistical interpretation with predictive modeling to make catalyst development more efficient and reproducible [5].

Finally, provided a detailed survey of physics-informed machine learning approaches, which combine physical knowledge with data-driven models. The paper explained how embedding governing equations or constraints within learning algorithms improves model stability and generalization. It also categorized different methods based on how they incorporate physical information, from loss function regularization to hybrid neural architectures. These approaches are especially beneficial when experimental data are limited or expensive to obtain. The study concluded that physics-informed learning represents a promising bridge between traditional physical modeling and modern machine learning, enabling more accurate and trustworthy predictions in engineering and catalysis applications [6].

Collectively, these studies [1–6] indicate that hybrid data-driven methods—especially those enhanced with domain knowledge, synthetic data, and physics-based constraints—offer significant improvements in diesel engine performance modeling, even in data-constrained environments. Internal combustion engines involve complex interactions, including injection timing, air-fuel ratio, and turbulence. These nonlinear relationships make it challenging to

achieve optimal performance using traditional analytical or empirical approaches. Machine learning techniques provide a powerful alternative by capturing these intricate dependencies directly from experimental or simulation data. Researchers can estimate engine outputs under various operating conditions. Optimization algorithms can then adjust input parameters to maximize performance and minimize fuel consumption and pollutant formation. This data-driven approach reduces the need for extensive trial-and-error calibration while improving accuracy and adaptability across different engine types and fuels [7].

Several studies have examined the use of support vector algorithms to predict diesel engine performance and emissions when operating with nanoparticle-added diesel fuel. The study examined the effects of nanoparticle addition on braking power, torque, and emissions. The support vector machine model accurately captured nonlinear relationships between nanoparticle concentration, engine speed, and performance outcomes. Results showed that optimal nanoparticle dosages significantly enhanced combustion efficiency while reducing carbon monoxide, hydrocarbons, and smoke opacity. The study concluded that support vector machine models provide reliable predictive capability for evaluating alternative fuels without extensive experimental trials. Moreover, the approach helps identify environmentally friendly blends by combining data-driven modeling with experimental validation [8].

Other studies applied support vector regression to predict diesel engine performance under varying load and speed conditions. Their work demonstrated that support vector regression can achieve high prediction accuracy. By optimizing kernel parameters and training with experimental data, the model effectively generalized across different engine operating points. The authors compared their predictions with actual measurements and found minimal deviations, confirming the robustness of the approach. This study examined the practicality of machine learning by reducing computational time and making engine performance analysis easier [9].

Sujin et al. [10] investigated optimizing performance using biodiesel made with nanoadditives. They implemented hybrid machine learning and optimization techniques to determine the best fuel blend composition and engine settings. The inclusion of nanoparticles improved fuel atomization and combustion stability, resulting in higher efficiency and lower emission levels. The study demonstrated that combining hybrid modeling with intelligent optimization leads to more effective tuning of engine parameters than conventional empirical methods. Furthermore, their approach supports sustainable fuel alternatives by enhancing renewable biodiesel performance to levels comparable with standard diesel.

Ouladsine et al. [11] proposed a neural network-based modeling and control strategy for diesel engines operating under pollution constraints. The developed neural model was capable of simultaneously predicting torque output and emission levels, enabling real-time control that balances performance and environmental objectives. Their approach utilized multi-layer feedforward networks trained on experimental data to capture the nonlinear behavior between fuel injection, air intake, and exhaust characteristics. The neural controller successfully reduced nitrogen oxide and particulate emissions without compromising torque or efficiency. This research marked one of the early applications of neural networks in intelligent engine control systems, demonstrating the feasibility of adaptive learning for cleaner combustion.

Owoyele and Pal [12] introduced an innovative machine learning-based optimization algorithm named ActivO, designed to accelerate simulation-driven engine design. The method integrates active learning principles with optimization, allowing the model to select the most informative

simulation samples dynamically. This approach significantly reduces computational effort while maintaining high design accuracy. The algorithm was applied to optimize multiple engine performance objectives, including efficiency, emission reduction, and operating cost. The authors reported that ActivO outperformed traditional optimization methods in both speed and convergence. Their work illustrated how combining simulation data with adaptive learning algorithms can revolutionize the engine design process by reducing development time and resource consumption. Traditional calibration requires costly and time-intensive experiments, whereas machine learning-based techniques optimize combustion behavior, atomization, and ignition timing, reducing emissions and improving efficiency [8–12].

Zhang et al. [13] conducted a comparative study to optimize biodiesel engine performance using an improved genetic algorithm and a conventional genetic algorithm. Their hybrid approach effectively combined the global search ability of PSO with the evolutionary adaptability of GA, leading to faster convergence and improved optimization accuracy. The study aimed to minimize fuel consumption and emissions while maximizing brake power and efficiency. Experimental validation confirmed that the hybrid PSO–GA outperformed the basic GA in finding optimal injection timing, pressure, and biodiesel blend ratio. The results demonstrated the effectiveness of combining swarm intelligence and evolutionary computation for complex nonlinear engine optimization problems.

Bertram et al. [14] proposed a novel hybrid optimization framework integrating particle swarm optimization and genetic algorithms for diesel engine performance tuning. The method was specifically designed to handle multi-objective problems involving trade-offs between power output, efficiency, and emission constraints. By introducing adaptive crossover and mutation operations into the PSO structure, the model achieved better exploration of the solution space and avoided premature convergence. Simulation results demonstrated significant improvements in brake efficiency and successful reductions in NOx and soot emissions for studies performed using single optimization methods. The study highlighted that hybrid metaheuristic algorithms provide a powerful tool for achieving optimal engine calibration in computationally efficient ways.

Ai ve Cho [15], biyodizel motor için belge tahmin modellerinin incelenmesi için makale yazdılar. Çalışmaları, modellerin güçlü ve zayıf birimlerinin karşılaştırılmasını sağladı. İncelemede, yapay sinir ağları ve destek sistemleri gibi veri yönlendirme yöntemlerinin yüksek tahmin oranları sunulurken, bunların yanma fiziğiyle entegre edildiği ve genellemeyi geliştirildiği vurgulandı. Yazarlar ayrıca, derin öğrenme ve aktarım öğrenmesindeki son gelişmelerin, çeşitli biyodizel hammaddeleri ve motor türleri için tahmin yeteneklerini içermektedir. Makale, ilerlemenin ilerlemesinin, daha temiz ve daha verimli biyodizel uygulamaları için gerçek zamanlı uyarlanabilir bölümlemeyle olması gerektiği düşünüldüler.

Zhang et al. [16] conducted a study on the operation and performance of biodiesel-fueled diesel engines. The study categorized biodiesels into first-, second-, and third-generation types, analyzing their physicochemical properties, energy content, and emission impacts. The authors found that higher-generation biodiesels generally improve combustion efficiency and reduce carbon monoxide and hydrocarbon emissions but may slightly increase NOx formation due to higher oxygen content. They also highlighted challenges such as feedstock cost, oxidation stability, and cold-flow performance. The review underscored the necessity of integrating advanced modeling and fuel formulation strategies to enhance the viability of biodiesel as a sustainable energy source.

Ahmad et al. [17] investigated the engine performance and emission characteristics of biodiesel blended with oxygenated additives. The study aimed to evaluate how these additives—such as ethanol, diethyl ether, and n-butanol—affect combustion efficiency and exhaust emissions. Results indicated that incorporating oxygenated additives improved combustion completeness, thereby reducing soot and unburned hydrocarbons. However, increases in NOx emissions were observed due to elevated temperatures. The authors concluded that properly optimized additive concentrations can achieve a desirable balance between performance and emission control, promoting the use of cleaner biofuel alternatives.

How et al. [18] analyzed the effects of Calophyllum Inophyllum biodiesel–diesel blends on combustion behavior, engine performance, and exhaust emissions in a multicylinder diesel engine. Their experiments revealed that biodiesel blends improved combustion stability and reduced particulate matter emissions compared to pure diesel operation. The study also reported moderate reductions in carbon monoxide and hydrocarbon emissions but noted a slight rise in NOx levels. Detailed analysis of particulate morphology showed smaller particle sizes and more complete oxidation in biodiesel combustion. These findings support the potential of Calophyllum Inophyllum as a sustainable biodiesel feedstock capable of lowering overall environmental impact when used in optimized blend ratios. Hybrid models, such as genetic algorithms coupled with particle swarm optimization, refine fuel droplet control, leading to lower fuel consumption [13–18].

Jose and Hampp [19] developed a machine learning-based framework for quantifying spray processes in multiphase flows, which play a critical role in diesel engine fuel atomization and combustion efficiency. Their approach used high-speed imaging data and regression algorithms to extract detailed spray parameters, including droplet size distribution, velocity, and breakup dynamics. The model demonstrated high prediction accuracy, providing valuable insights into spray evolution under varying injection pressures and ambient conditions. By leveraging data-driven quantification, the study enhanced understanding of fuel–air mixing behavior, enabling better optimization of injection strategies. The research highlighted the potential of machine learning for bridging experimental measurements and numerical simulations in complex spray phenomena.

Al Qubeissi et al. [20] introduced an auto-selection algorithm for identifying quasi-components and components in the multidimensional quasi-discrete model used in fuel spray and evaporation simulations. The proposed method utilized a self-optimizing procedure that automatically selects representative fuel components to improve computational efficiency and predictive accuracy. The study validated the approach across multiple fuel mixtures, demonstrating that auto-selection significantly reduces simulation time without compromising accuracy in combustion and evaporation predictions. Their work contributes to advancing surrogate fuel modeling, which is essential for high-fidelity engine simulations. The results indicate that integrating intelligent algorithms into traditional combustion models can streamline fuel chemistry representation and enhance predictive robustness.

Shateri et al. [21] used artificial intelligence to determine the machine learning model they would use to predict diesel engine fuel consumption. The study compared various algorithms, including decision trees, random forests, and support vector machines. By implementing a systematic model selection framework, they identified the optimal architecture based on accuracy, interpretability, and computational cost. The best-performing model achieved precise predictions under varying load and speed conditions, offering practical insights for energy

efficiency improvements. This work demonstrated how AI can automate model discovery and accelerate the development of predictive tools for energy systems.

Ismael et al. [22] investigated the effects of nanoparticles on the performance and emissions of a fuel-injected diesel engine operating with water-biodiesel emulsions. The study investigated the effects of nanoparticles such as aluminum oxide and titanium dioxide on combustion, braking power, and exhaust emissions. The results revealed significant improvements, as well as reductions in unburned hydrocarbons and particulate matter. However, increases in NOx emissions were observed due to higher temperatures. The study concluded that nanoparticle-enriched fuels offer a promising path to cleaner combustion and improved biodiesel utilization.

Veza et al. [23] applied the grasshopper optimization algorithm to achieve multi-objective optimization of diesel engine performance and emissions. Their model aimed to balance conflicting objectives, such as maximizing brake thermal efficiency while minimizing NOx and soot emissions. The algorithm efficiently searched the parameter space, identifying optimal combinations of injection pressure, timing, and fuel blend ratios. Comparative analysis showed that the grasshopper-based approach outperformed other metaheuristic algorithms in convergence speed and solution quality. This study demonstrated the growing potential of bio-inspired optimization techniques for advanced engine calibration and cleaner combustion strategies.

Dewangan et al. [24] investigated the combined effect of genetic algorithm and nanoparticles on diesel engine performance. The model was developed to optimize parameters such as compression ratio, injection timing, and nanoparticle concentration for improved efficiency and emission reduction. The results showed that the hybrid approach effectively captured nonlinear interactions and provided precise optimization outcomes. Enhanced combustion efficiency and lower carbon monoxide and smoke emissions were achieved through fine-tuned nanoparticle-assisted combustion. The study emphasized that coupling statistical and evolutionary optimization methods leads to more accurate and computationally efficient engine optimization frameworks.

Beirami et al. [25] assessed greenhouse gas emissions from diesel engines fueled with biodiesel blended with carbon nanotubes using machine learning techniques. Their model evaluated the relationship between nanotube concentration, combustion temperature, and emission formation rates. Results indicated that carbon nanotube additives enhance combustion completeness and lower carbon dioxide and hydrocarbon emissions. The machine learning model provided a robust predictive tool for assessing emission behavior under various operating conditions. The authors concluded that data-driven emission modeling can support the design of low-carbon fuels and contribute to sustainable engine operation.

Mofijur et al. [26] provided a comprehensive analysis of nanoparticle-based fuel additives and their influence on biodiesel combustion, engine performance, and emission characteristics. The review compiled findings from recent experimental and numerical studies, highlighting how nanoparticles improve fuel atomization, ignition quality, and energy conversion efficiency. It also discussed variations in emission outcomes depending on nanoparticle type, size, and concentration. The authors emphasized the role of nanoparticles in enhancing oxidation reactions and reducing incomplete combustion products. The study concluded that while nanoparticle additives significantly improve biodiesel performance, optimal dosage and dispersion stability remain critical for practical applications. Machine learning techniques have

played a significant role in analyzing and optimizing nano-fuel formulations, enabling researchers to refine fuel droplet behavior and enhance combustion processes [19–26].

Koirala et al. [27] experimentally investigated the effects of green-synthesized zinc oxide nanoadditives blended with rice bran oil biodiesel on the performance and combustion behavior of a variable compression ratio diesel engine. The study examined how varying nanoparticle concentrations and compression ratios influence brake thermal efficiency, fuel consumption, and emission parameters. Results showed that adding zinc oxide nanoparticles enhanced combustion efficiency by improving fuel–air mixing and reducing ignition delay. The optimized blend achieved higher brake thermal efficiency and lower carbon monoxide and hydrocarbon emissions compared to pure biodiesel. The authors concluded that green-synthesized nanoparticles can serve as sustainable additives, improving biodiesel's energy conversion performance while maintaining environmental compatibility.

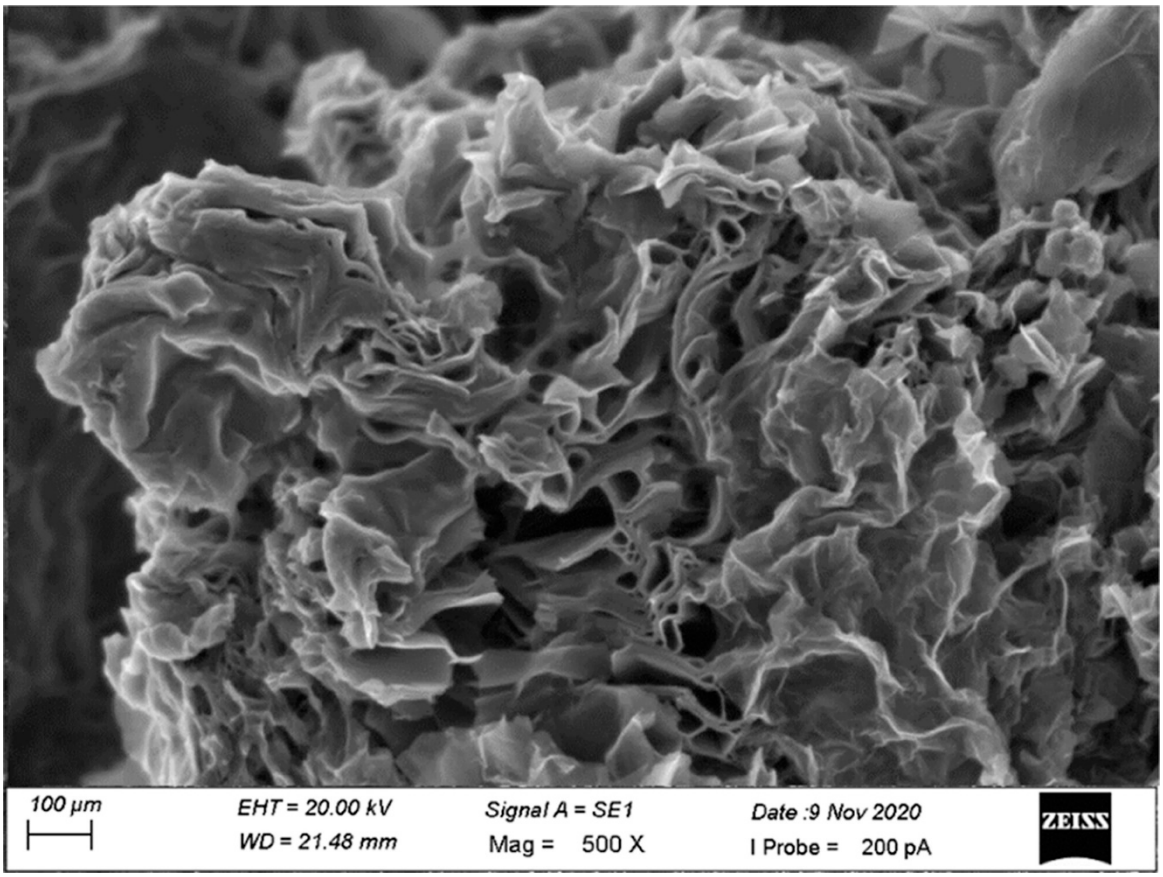

Figure 1. SEM of graphite [28].

Sambandam et al. [28] studied the effect of graphite nanoparticles on the operation of a diesel engine derived from waste materials. The study aimed to improve the combustion stability and emission profile of the fuel. The addition of graphite nanoadditives improved fuel atomization, reduced ignition delay, and resulted in smoother combustion. Experimental results demonstrated increases in brake efficiency, as well as reductions in carbon monoxide, hydrocarbons, and smoke opacity. The findings suggest that combining waste-derived fuels with nanoadditives can transform low-quality pyrolysis oils into viable alternative fuels for diesel engines.

Zheng and Cho [29] presented a comprehensive study on the effects of various nanoadditives on biodiesel-fueled diesel engines. The paper systematically compared metal oxide, carbon-based, and composite nanoparticles regarding their impact on engine performance, combustion quality, and emissions. The analysis revealed that nanoparticles generally enhance thermal conductivity and catalytic activity, leading to more complete combustion and improved energy conversion efficiency. However, excessive nanoparticle concentrations can cause agglomeration, injector fouling, and diminishing benefits. The authors emphasized the need for optimized dosing strategies and stable dispersion techniques to ensure long-term engine reliability and emission control.

Lv et al. [30] conducted an extensive review summarizing the effects of nanoadditives incorporated into diesel–biodiesel fuel blends on combustion and emission characteristics. The review covered a wide range of nanoparticles, including aluminum oxide, cerium oxide, titanium dioxide, and carbon nanotubes, highlighting their mechanisms in improving oxidation reactions and reducing pollutant formation. The authors noted that nanoadditives enhance ignition quality, shorten combustion duration, and increase brake thermal efficiency while reducing particulate matter and carbon monoxide emissions. However, they also cautioned that the type, size, and concentration of nanoparticles critically determine overall performance outcomes. The study concluded that while nanoadditive technology holds significant promise for cleaner and more efficient diesel engines, standardized testing and long-term durability assessments are essential for practical adoption.

Advanced models facilitate the prediction of fuel atomization, evaporation rates, and combustion efficiency, ensuring precise fuel-air mixing for optimal engine performance. Nanoparticles, including zinc oxide (ZnO), graphite, cerium oxide (CeO_2), aluminum oxide (Al_2O_3), and carbon nanotubes (CNTs), are integrated into diesel blends to enhance fuel atomization and combustion dynamics [27–30]. Studies show that ZnO and graphite nanoparticles significantly improve ignition characteristics, thermal efficiency, and emissions reduction [27–28]. Nano-additives improve cetane number, calorific value, and reduce pollutants such as CO, NOx, and particulate matter [21–30]. High-speed imaging of fuel sprays reveals the importance of nano-structured droplets in flame stability and combustion optimization [22–24]. Cerium oxide and aluminum oxide nanoparticles are particularly effective in improving brake performance and reducing fuel consumption, but they remain incompatible with fuel cost and environmental factors [25–30]. Injection parameters play a critical role in shaping fuel droplet behavior, influencing combustion efficiency and emissions. Studies indicate that higher injection pressure and optimized nozzle design produce finer droplets, enhancing fuel-air mixing and combustion efficiency [27–30]. Machine learning-driven models predict droplet behavior under varying conditions, offering insights into fuel spray dynamics and evaporation rates [20–21]. The integration of nano-structured fuel droplets and machine learning-based optimization presents a transformative approach to improving diesel engine efficiency. By refining combustion characteristics, injection parameters, and predictive modeling, researchers aim to develop more sustainable and cost-effective engine technologies. Further advances in machine learning-driven nano-fuel formulations could revolutionize cleaner, high-performance diesel engines.

Some studies have examined the topics being compared. One of these studies provided insights into the behavior of this advanced combustion process by examining the timing and frequency of combustion in a spark-ignition engine. These results were then compared with traditional methods, such as temperature, and machine learning algorithms. The goal was to determine the best method for predicting the onset of combustion. The findings showed that machine learning

models performed better than traditional methods. These results were consistent with the results obtained with the parameters and data used in the study, resulting in better engine performance and very good results [31].

Coraddu et al. [32] developed a hybrid modeling framework combining physical equations and machine learning for ship diesel engine performance prediction. The model integrated thermodynamic principles with data-driven corrections to enhance accuracy under real operating conditions. By leveraging sensor data and adaptive learning techniques, the approach accurately captured deviations from theoretical models caused by environmental or load variations. The results showed improved reliability and generalization compared to purely empirical or physical models. The study illustrated the effectiveness of hybrid modeling for marine engine monitoring and predictive maintenance.

Liu et al. [33] employed machine learning techniques to optimize ship hull form at multiple operating speeds, linking hydrodynamic performance with experimental and simulation data. Their method utilized regression and optimization algorithms to predict drag coefficients and streamline hull shapes. The hybrid framework enabled rapid design evaluation without extensive physical prototyping. Results demonstrated significant efficiency gains and fuel savings compared to traditional optimization approaches. The study underscored the growing role of AI in accelerating marine design and improving overall propulsion performance.

Gkerekos et al. [34] compared various machine learning models for predicting the fuel oil consumption of ship main engines. Techniques such as support vector machines, random forests, and artificial neural networks were trained using real voyage data. The study found that ensemble and neural network-based models provided the highest prediction accuracy, particularly under dynamic load conditions. The authors emphasized the importance of data preprocessing, feature selection, and model interpretability for reliable deployment. The findings contribute to developing intelligent systems for maritime energy efficiency management.

Shahpouri et al. [35] proposed a hybrid machine learning framework for predicting soot emissions in compression ignition engines. They combined feature engineering techniques with ensemble algorithms to capture complex relationships between engine parameters and soot formation. The systematic model selection process identified optimal learning algorithms and input variable combinations, improving both accuracy and interpretability. The results demonstrated that hybrid models outperform single-method approaches in emission prediction tasks. This research offers a structured methodology for integrating data-driven insights into combustion diagnostics and emission control.

Shateri et al. [36] developed an artificial intelligence-based model selection strategy to identify the most effective machine learning architecture for predicting fuel consumption in diesel engines. By comparing multiple algorithms, including gradient boosting, random forests, and neural networks, the study determined the optimal balance between performance accuracy and computational efficiency. The selected model provided highly accurate predictions across diverse operating conditions. The approach demonstrated how automated AI-driven selection enhances model generalization and reduces the need for manual tuning in energy applications.

Yu et al. [37] presented a new result using a learning algorithm to predict instantaneous emissions from diesel engines. Their convolutional and recurrent hybrid architecture processed real-time engine sensor data to capture transient emission behavior. The model achieved high

temporal resolution and predictive precision, outperforming conventional statistical methods. The study emphasized that deep learning enables real-time emission control and diagnostics, supporting adaptive emission-reduction strategies. The proposed method represents a step toward intelligent, self-optimizing engine management systems.

Ravindran and Kokjohn [38] integrated machine learning with three-dimensional computational fluid dynamics (3D-CFD) modeling to optimize spark-ignition engine performance during cold-start conditions. Their hybrid approach used CFD simulations to generate training data and applied machine learning to rapidly explore parameter spaces. The results revealed that this integration reduces simulation time while maintaining high predictive fidelity. Optimized cold-start strategies improved fuel economy and reduced unburned hydrocarbon emissions. The study demonstrated how coupling ML with physics-based modeling accelerates engine optimization and calibration.

Odufuwa et al. [39] developed artificial neural network models on diesel engines focusing on environmental and surface performance indicators. The models were trained on experimental data encompassing various fuel blends and load conditions. These results showed good prediction results for brake efficiency, fuel consumption and emissions. The study also performed sensitivity analysis to identify critical parameters affecting engine sustainability. Their findings highlight the potential of AI for small-engine applications in rural or decentralized energy systems.

Vorkapic et al. [40] applied machine learning algorithms to monitor the operation of a diesel engine. Their approach used classification and anomaly detection algorithms to identify deviations from normal performance based on onboard sensor data. The model effectively detected faults, load anomalies, and early indicators of engine degradation. Results demonstrated that machine learning provides reliable real-time condition monitoring and reduces maintenance costs. The research underscores the importance of data-driven diagnostics for improving the operational safety and efficiency of marine propulsion systems.

Badra et al. [41] presented a methodological framework that combines computational fluid dynamics and machine learning for diesel engine combustion system optimization. The study employed CFD simulations to model combustion phenomena and trained machine learning models to predict performance metrics and emissions. By integrating both approaches, the framework accelerated optimization processes and reduced computational demands. Results showed significant improvements in combustion efficiency and emission control through informed design modifications. The study represents a comprehensive pathway for coupling physics-based and data-driven modeling in engine development.

Yuksel et al. [42] performed a comparative analysis of machine learning techniques for predicting marine diesel engine fuel consumption. The research evaluated algorithms including support vector regression, random forests, and deep neural networks using operational ship data. Findings revealed that deep learning-based models yielded the highest accuracy across varying sea conditions and engine loads. The study emphasized the role of model interpretability and sensor reliability in practical marine applications. Their results provide valuable insights for developing intelligent voyage optimization and fuel management systems.

Studies on diesel engines have pioneered the use of models that combine CFD simulations with machine learning methods for faster engine performance prediction. These simulations and models have enhanced optimization. These studies demonstrate the importance of accurate

prediction for optimizing engine design, performance, and operation, while also addressing the challenges of modeling the physical and environmental processes that govern engine behavior [32–34]. The authors have developed modeling approaches that combine CFD results with machine learning methods to estimate performance parameters. They describe the various input variables that can be included in these models and demonstrate the challenges associated with selecting the most appropriate parameters. They also summarize and evaluate commonly used machine learning algorithms for engine performance prediction. The proposed models have been validated using experimental data and have yielded successful prediction results [35–38]. Studies have also examined model optimization techniques, demonstrating their contribution to improved model accuracy [39,40]. A specific approach to predicting engine combustion and emissions is being undertaken through hybrid modeling, and the results demonstrate that these models accurately identify the characteristics that influence combustion and emissions [41,42].

Studies on Atkinson-cycle gasoline engines generally focus on their fuel efficiency and emission reduction, and how they perform under different environmental conditions. The Atkinson cycle, which allows for a longer expansion phase compared to the compression phase, is implemented and compared with the conventional cycle. Researchers also explore different ways to optimize engine components, such as analytical methods and genetic algorithms, and provide insights into how these components behave. Many studies emphasize experimental investigations of Atkinson-cycle engines. In these works, the authors describe the procedures used to measure engine performance, including brake power, fuel consumption, and emissions, and they present detailed reviews of the results. They also explain the fundamental physics of the Atkinson cycle by showing how changes in parameters like compression ratio and valve timing affect overall performance [43,44].

Other articles focus on computational optimization of Atkinson-cycle engines using methods such as machine learning and genetic algorithms. These studies explain approaches like multi-objective optimization and response surface methodology, and compare how effective they are. They also analyze the influence of different engine parameters on performance and use optimization algorithms to find the best values for these parameters. Finally, the results are validated with experimental data, confirming that the computational methods are reliable and effective in improving engine efficiency and performance [45–47].

Wong et al. [48] developed an efficient point-by-point calibration framework for internal combustion engines using machine learning combined with a sequential design of experiments (DoE) strategy. Their approach employed Gaussian process regression to model engine behavior and iteratively refine calibration points, minimizing the number of experimental runs required. The method achieved high accuracy in predicting torque, emissions, and fuel consumption while significantly reducing calibration time and cost. By optimizing the experimental design process, the study demonstrated how machine learning can accelerate engine development cycles. This framework provides a data-efficient pathway for automated engine calibration in modern automotive systems.

Garg et al. [49] explored the application of machine learning methods for robust performance modeling and efficient control development in engines. They evaluated several algorithms—such as random forests, neural networks, and Gaussian processes—for their capability to capture nonlinear relationships among control parameters. The study highlighted the

importance of integrating machine learning into the control design process to improve adaptability and robustness under varying operating conditions. Results showed that ML-based controllers enhanced performance prediction and reduced calibration complexity. This research underscores the growing potential of data-driven techniques for next-generation engine control systems.

Liu et al. [50] proposed a machine learning-assisted model to predict exhaust gas temperature in heavy-duty engines. Using experimental data and advanced regression algorithms, including ensemble and deep learning methods, the model accurately captured transient EGT variations across operating ranges. Precise EGT prediction is essential for thermal management and emission control, and the machine learning model achieved better generalization than physics-based models. The approach effectively reduced computational cost while maintaining high predictive fidelity. Their findings contribute to the advancement of real-time engine monitoring and predictive diagnostics.

Cho et al. [51] investigated the automation of gasoline engine calibration using optimization and machine learning techniques. Their framework integrated neural networks with automated calibration algorithms to replace traditional manual trial-and-error processes. The system efficiently optimized parameters such as ignition timing, air-fuel ratio, and valve timing, reducing human intervention and development time. The study demonstrated that machine learning can effectively handle high-dimensional calibration problems and adapt to dynamic operating conditions. This work provided an early foundation for intelligent and automated powertrain tuning in modern vehicle development.

Godwin et al. [52] applied ensemble least-squares boosting algorithms to predict combustion, performance, and emission characteristics of ethanol-powered spark ignition engines. The model utilized experimental datasets to train and validate predictions of brake thermal efficiency, in-cylinder pressure, and pollutant emissions. Results indicated that ensemble methods significantly outperformed traditional regression techniques in both accuracy and stability. The study emphasized that machine learning can effectively model the complex combustion behavior of biofuel engines. This research demonstrates the capability of boosting-based models to support cleaner and more efficient alternative-fuel engine design.

These articles highlight how machine learning can be used in high-performance engine calibration. The authors describe algorithms such as artificial neural networks, support vector machines, and random forests, and explain how they are applied in the calibration process. They show that machine learning improves accuracy, reduces calibration time, and back up these claims with experimental results. The studies also look at how factors like fuel type and engine load affect performance, demonstrating that machine learning can optimize calibration under different operating conditions [48–52].

Other studies give a broader overview of machine learning and genetic algorithms in optimization. They explain the basic principles of these methods and show how they are used in different fields. Special focus is placed on optimizing processes such as predicting the mechanical properties of carbon fiber composites and reducing cutting force in end milling. The authors also discuss the challenges of optimization and point out the advantages of combining machine learning with genetic algorithms. In the end, these studies prove that these techniques are effective in improving process performance [53–54].

Zhang et al. [55] carried out a detailed study on the use of genetic programming and machine learning. They grouped existing methods by algorithm type, learning strategy, and optimization goal, showing that hybrid machine learning–genetic algorithm approaches perform better than traditional methods in adaptability and solution quality. The study also pointed out challenges such as data representation, feature selection, and generalization across different environments. It concluded that combining genetic programming with machine learning creates more flexible and self-evolving optimization strategies for complex industrial systems.

Wang et al. [56] introduced a multi-objective optimization framework for diesel engines using artificial neural networks together with genetic algorithms. The neural network was trained to predict thermal efficiency and exergy loss, while the genetic algorithm optimized design parameters to balance power output and energy recovery. Their results showed that this hybrid approach improved thermodynamic performance compared to conventional methods, highlighting the potential of intelligent optimization tools to increase energy efficiency and reduce waste heat in engine systems.

Atia et al. [57] developed a genetic algorithm-based method to find the best sizing of solar water heating systems for aquaculture. The goal was to balance energy efficiency, system cost, and thermal demand under changing climate conditions. The genetic algorithm successfully handled multiple design parameters, producing solutions that reduced energy losses and operating costs. The results confirmed the effectiveness of genetic algorithms in creating sustainable designs that adapt well to environmental changes, and the authors emphasized their wider use in renewable energy optimization.

Other studies also focus on combining machine learning and genetic algorithms for optimization in different fields. They explain how these techniques are integrated into the ML–GA approach, discuss the challenges of optimizing complex systems, and highlight advantages such as faster optimization and higher accuracy. The effectiveness of this approach has been shown in applications like multi-pass turning, dual-fuel diesel engines, and solar water heater placement [55–57].

Machine learning has also been applied to the study of fuel droplets in diesel engines, showing promise in understanding spray processes, droplet behavior, and fuel consumption. Advanced models can measure droplet size distributions and improve simulations of heating and evaporation, which are key to efficient combustion. For spray characterization, object detection methods like Mask R-CNN and SparseInst have been used to analyze droplet size and atomization, with synthetic training data and physics-based randomization ensuring reliable detection under different conditions [58].

For heating and evaporation, the multi-dimensional quasi-discrete model simulates diesel droplet behavior while reducing computational time without losing accuracy [59]. In predictive modeling of fuel consumption, artificial intelligence methods have been tested, with Gaussian process regression proving more accurate and faster than other models [60]. Sensitivity analysis further identified key parameters affecting fuel use, improving reliability.

Although machine learning applications in diesel engine research are promising, challenges remain in making models generalizable across different operating conditions and fuel types. More research is needed to refine these models for real-world use.

Finally, the integration of nano droplets in diesel engines, especially through nanoparticles, has shown strong potential to improve performance and reduce emissions. Machine learning is increasingly used to optimize these processes, allowing more precise control and prediction of engine behavior under varying conditions.

Patel and Dhiman [61] investigated the influence of hybrid $MgO–Al_2O_3$ nanoparticles blended with water-in-diesel emulsions on diesel engine performance and emissions using a hybrid deep neural network combined with spotted hyena optimization. The model effectively predicted key engine parameters such as brake thermal efficiency, specific fuel consumption, and NO_x emissions under varying operating conditions. Experimental validation confirmed that hybrid nanoparticles enhanced combustion stability and reduced harmful emissions. The study demonstrated the strong potential of combining deep learning with bio-inspired optimization for complex combustion systems.

Dewangan et al. [62] explored the combined effects of operating parameters and nanoparticle additives on diesel engine performance using a response surface methodology coupled with a genetic algorithm. Their hybrid optimization framework identified optimal conditions for maximizing efficiency and minimizing emissions. Results revealed that nanoparticle concentration and injection timing were the most influential factors in determining combustion quality. The integrated RSM–GA approach proved effective for parameter tuning in multi-variable nonlinear engine systems.

Akhil et al. [63] conducted an experimental analysis on the performance, combustion, and emission behavior of diesel engines fueled with various nanoparticle–diesel blends. The study found that metal oxide nanoparticles improved fuel atomization and shortened ignition delay, resulting in higher efficiency and lower hydrocarbon and CO emissions. However, NO_x levels increased slightly due to enhanced combustion temperature. The authors highlighted the need for balancing performance gains and emission control through optimized nanoparticle dosing.

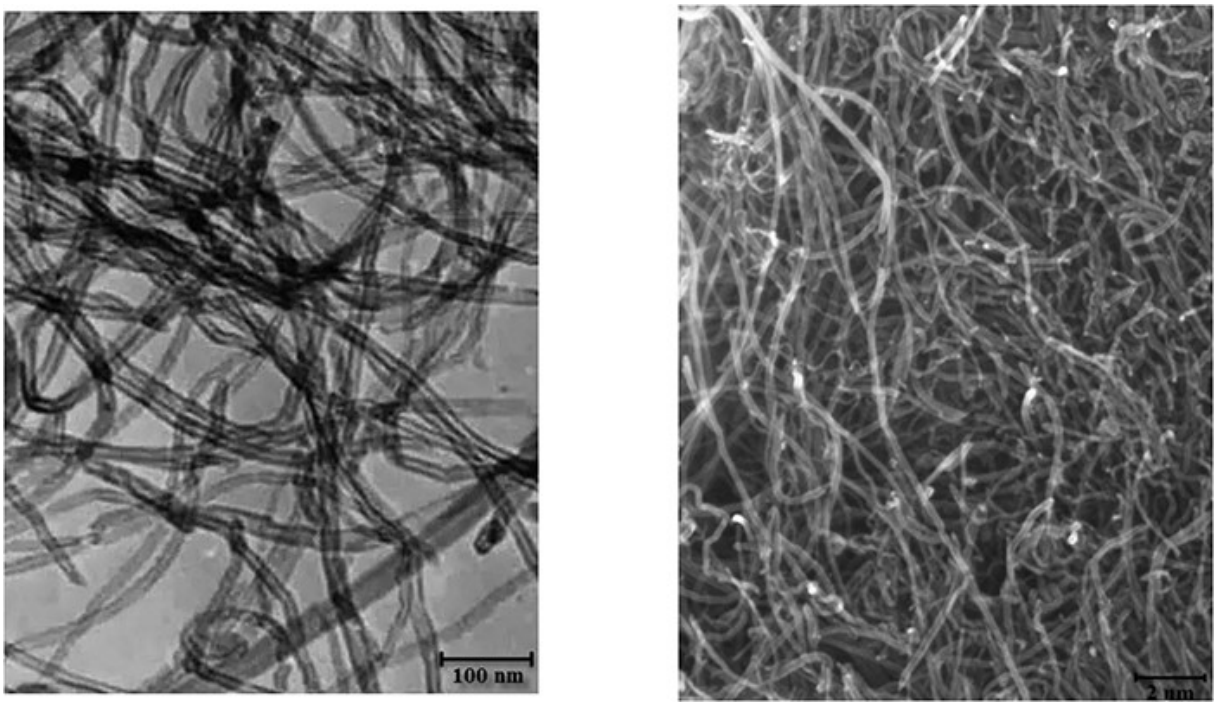

Figure 2. TEM and scanning electron microscope (SEM) additive carbon nanotubes (CNTs) to the biodiesel fuel [64].

Beirami et al. [64] assessed the environmental impact of adding carbon nanotubes to biodiesel fuel using machine learning-based modeling techniques. The study employed predictive algorithms to estimate greenhouse gas emissions and evaluate combustion efficiency under different blending ratios. The models demonstrated high accuracy, confirming that CNT addition reduced CO_2 and unburned hydrocarbon emissions while improving overall engine performance. The research underscored the capability of ML tools to model complex fuel–additive interactions.

Haq et al. [65] examined the influence of nanoadditives on diesel–biodiesel fuel blends with a focus on spray characteristics, engine performance, and emission behavior. The inclusion of metallic and oxide nanoparticles improved fuel dispersion and combustion uniformity, leading to better thermal efficiency and reduced particulate matter. Spray visualization experiments revealed finer atomization and improved mixing in nanoparticle-blended fuels. The findings highlighted the effectiveness of nanotechnology in enhancing diesel–biodiesel blend performance and emission control.

Studies [61–65] collectively highlight the effectiveness of incorporating nanoparticles and machine learning-based optimization techniques in enhancing diesel engine performance and emission characteristics. These works demonstrate that the inclusion of metal oxide and carbon-based nanoparticles improves combustion efficiency, fuel atomization, and thermal stability while reducing harmful emissions such as CO and unburned hydrocarbons. Advanced hybrid modeling and optimization methods, including deep neural networks, genetic algorithms, and response surface methodology, were employed to predict and fine-tune engine parameters under varying operating conditions. Overall, these studies emphasize that integrating nanotechnology with intelligent data-driven models enables cleaner combustion, better fuel utilization, and more sustainable diesel engine operation.

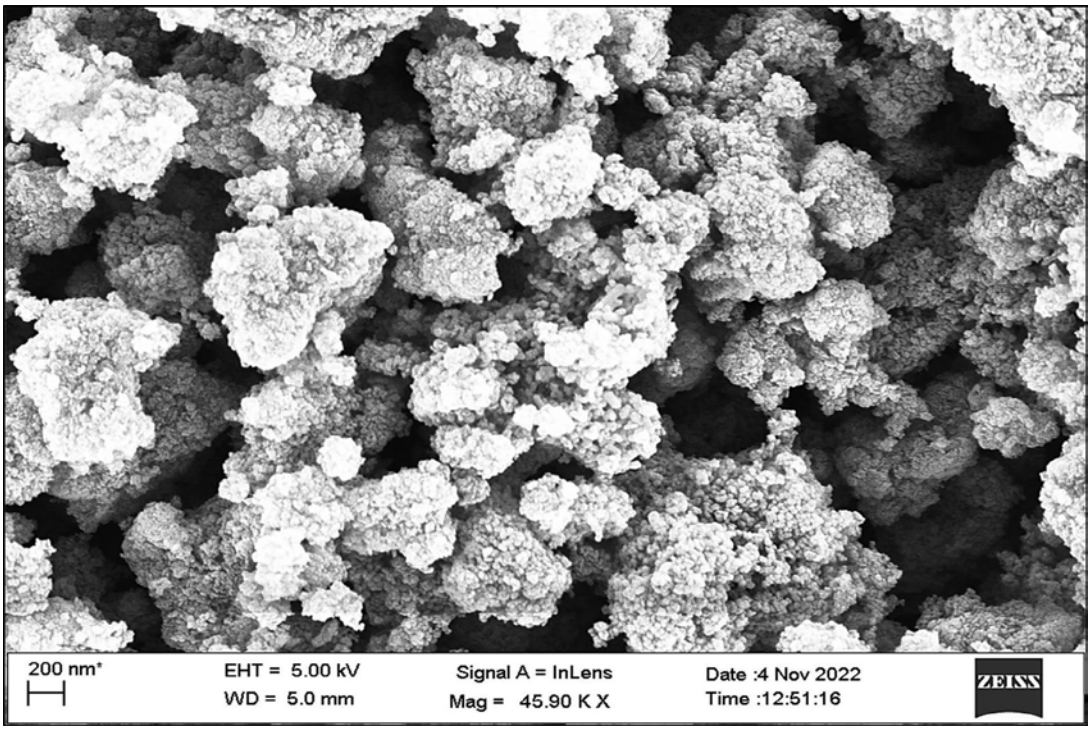

Figure 3. FESEM image of TiO_2 nanoparticles [66].

Sarma et al. [66] experimentally examined the effects of adding titanium dioxide nanoparticles to mahua biodiesel on diesel engine combustion and emissions. The study measured brake thermal efficiency, in-cylinder pressure profiles, ignition delay, and exhaust emissions under varied load conditions. Results showed that titanium dioxide nanoparticles improved fuel atomization and promoted more complete combustion, leading to increased thermal efficiency and higher peak in-cylinder pressures. Carbon monoxide and unburned hydrocarbon emissions decreased noticeably, while there was a modest rise in nitrogen oxide emissions attributed to higher combustion temperatures. The authors discussed optimal nanoparticle concentrations to balance efficiency gains with emission control and noted the importance of dispersion stability for practical use. The work supports the potential of combining nonedible biodiesel feedstocks with sustainable nanoparticle additives to enhance engine performance.

Sambandam et al. [67] investigated graphite nanoparticle additives in a diesel engine fueled with pyrolysis-derived fuel recovered from used plastics. The study focused on how graphite nanoparticles affect spray behavior, combustion stability, and pollutant formation for a low-quality alternative fuel. Experimental results indicated that graphite nanoparticles improved atomization and reduced ignition delay, producing more uniform combustion and measurable reductions in carbon monoxide, hydrocarbons, and smoke opacity. Brake thermal efficiency increased slightly compared with the neat pyrolysis fuel, bringing performance closer to conventional diesel. The authors highlighted that appropriate nanoparticle dosing and nanoparticle dispersion are critical to avoid injector fouling and to preserve long-term engine reliability. This research demonstrated a route to upgrade waste-derived fuels using nanotechnology for practical engine applications.

Zheng and Cho [68] provided a comprehensive review of nanoadditive effects on biodiesel-fueled diesel engines, synthesizing experimental and modeling findings across diverse nanoparticle classes. They compared metal oxide, carbon-based, and composite nanoparticles, detailing mechanisms such as enhanced thermal conductivity, catalytic oxidation, and improved

fuel atomization. The review showed consistent trends of improved combustion efficiency and reduced particulate matter and carbon monoxide for many nanoadditives, while increases in nitrogen oxides were commonly reported and discussed. The authors emphasized challenges including nanoparticle agglomeration, injector wear, and long-term stability, calling for standardization in testing protocols. They recommended optimized dosing strategies and surface treatments to maximize benefits and minimize adverse effects. The paper serves as a useful roadmap for researchers seeking to translate nanoadditive advantages into robust engine technologies.

Soudagar et al. [69] reviewed the broader literature on nanoadditives in diesel–biodiesel blends, addressing stability, fuel property modification, engine performance, and emission implications. Their analysis covered a wide range of nanoparticle types, sizes, and concentrations, and examined how these parameters influence properties such as viscosity, cetane number, and oxidation stability. They reported that many nanoadditives improve combustion kinetics and reduce incomplete combustion products, but the magnitude of benefits strongly depends on dispersion methods and surfactant use. The review highlighted durability and storage stability as critical hurdles for commercial adoption and called for long-duration engine tests and life-cycle assessments. Recommendations included standardized reporting of nanoparticle preparation, characterization, and dosage to enable cross-study comparisons. The article consolidates evidence that nanoadditives can enhance biodiesel viability while identifying practical research gaps.

Gad et al. [70] presented experimental investigations on diesel engines using alumina nanoparticle fuel additives, focusing on performance, combustion features, and emissions. The experiments reported improvements in brake thermal efficiency and reductions in carbon monoxide and unburned hydrocarbons when alumina nanoparticles were dispersed in the fuel. Detailed combustion analysis showed shortened ignition delay and higher heat release rates, indicating more complete and rapid combustion. The study also noted a tendency for increases in nitrogen oxide emissions at higher nanoparticle concentrations, and it discussed mitigation strategies such as exhaust gas recirculation or optimized injection timing. The authors emphasized the necessity of ensuring stable nanoparticle dispersion and monitoring potential impacts on fuel injection equipment. Overall, the work supports alumina nanoparticles as a promising additive for enhancing diesel combustion performance when carefully controlled.

Recent Studies [66–70] collectively emphasize the role of nanoparticle additives in enhancing the combustion efficiency, fuel economy, and emission characteristics of diesel and biodiesel-fueled engines. Research in this group demonstrates that the inclusion of nanoparticles such as TiO_2, Al_2O_3, graphite, and other metal oxides significantly improves fuel atomization, combustion temperature distribution, and catalytic oxidation processes. These enhancements lead to higher brake thermal efficiency, reduced carbon monoxide, hydrocarbon, and particulate emissions, and overall cleaner combustion. Additionally, several works highlight the use of waste-derived fuels and pyrolysis oils blended with nanoparticles, showing their potential as sustainable alternatives to conventional diesel. Comprehensive reviews within these studies conclude that the synergistic use of nanotechnology and biodiesel fuels can substantially optimize engine performance while supporting environmental sustainability through reduced pollutant formation and improved fuel utilization.

Visualizing fuel droplet behavior is crucial for understanding combustion processes in diesel engines. Several studies have documented images of fuel droplets under various conditions:

Fuel Droplet Combustion Model: This diagram illustrates the combustion stages of a fuel droplet, highlighting the flame zone and surrounding areas.

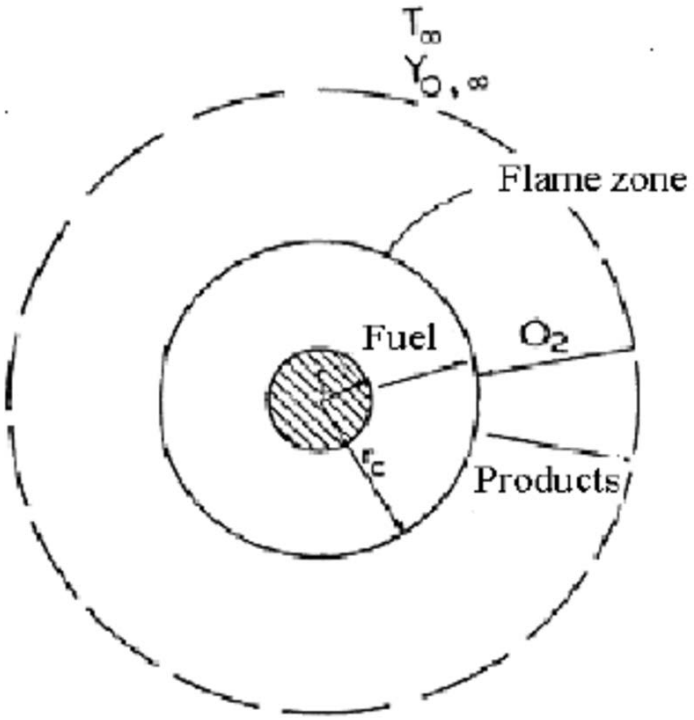

Figure 4. Fuel Droplet Combustion Model [71]

The fuel droplet combustion model, as described by Liu, Zhang, and Yang, outlines the key phases of combustion, emphasizing the interactions between the droplet, surrounding gases, and flame dynamics. The process begins with the evaporation of the fuel droplet, driven by heat transfer from the flame zone. As the droplet shrinks, combustion products form in the surrounding layer, while oxygen diffuses inward to sustain the reaction. The flame zone represents the outer boundary where energy is released, producing heat and light. This model provides a structured understanding of fuel droplet behavior, aiding in the optimization of combustion efficiency and emissions control [71].

Flame Images of Fuel Blends: High-speed imaging captures the combustion of pure diesel and its blends with water and methanol, showing distinct flame characteristics for each mixture.

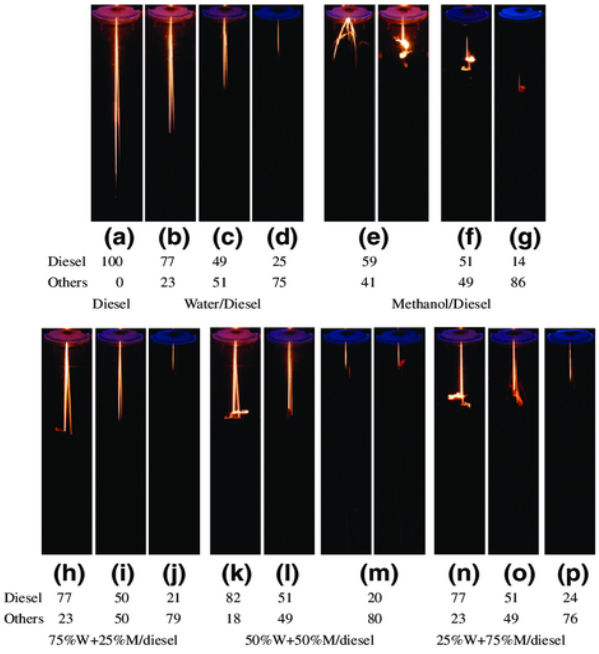

Figure 5. Flame Images of Fuel Blends [72]

The image presents a comparative analysis of flame characteristics for different fuel blends, including pure diesel, water-diesel mixtures, and methanol-diesel blends. Each section of the image illustrates how varying fuel compositions influence combustion behavior, flame structure, and energy release. The first row highlights the transition from pure diesel combustion to increasing water content, showing changes in flame luminosity and stability. The second row explores methanol-diesel blends, demonstrating how methanol alters combustion dynamics, potentially enhancing efficiency and reducing emissions [72].

Droplet Combustion Behavior of Diesel–Ethanol–Jatropha Oil Blends: This study presents images of single droplets exposed to high-temperature air, revealing behaviors like micro-explosions and puffing in various fuel blends.

Droplet Combustion Behavior of Diesel–Ethanol–Jatropha Oil Blends**,** as analyzed by Chauhan, Saini, and Kumar (2024), investigates the combustion characteristics of individual fuel droplets exposed to high-temperature air. The study captures key phenomena such as micro-explosions and puffing, which arise due to volatility differences among diesel, ethanol, and Jatropha oil. Ethanol facilitates rapid vaporization, while Jatropha oil contributes to droplet stability and combustion intensity. These factors influence fuel atomization, evaporation rates, and overall combustion efficiency. Understanding these behaviors is essential for optimizing fuel formulations, enhancing energy output, and minimizing emissions in practical applications [73].

Several parameters influence the shape of fuel droplets in a diesel engine, affecting fuel atomization, combustion efficiency, and emissions. These parameters include:

Fuel Properties

- **Viscosity**: Higher viscosity leads to larger and more elongated droplets, reducing atomization efficiency.
- **Surface Tension**: Fuels with lower surface tension form smaller, more spherical droplets, improving atomization.
- **Density**: Higher density fuels tend to create larger droplets, affecting combustion characteristics.

Injection System Parameters

- **Injection Pressure**: Higher injection pressure enhances atomization, producing smaller and more uniform droplets.
- **Nozzle Design**: Nozzle diameter, hole shape, and number of holes influence droplet formation and spray characteristics.
- **Injection Timing**: Early injection can lead to larger droplets, while late injection promotes finer atomization.

Ambient Conditions in the Combustion Chamber

- **Cylinder Pressure**: Higher in-cylinder pressure compresses fuel droplets, altering their shape and evaporation rate.
- **Temperature**: High temperature accelerates fuel evaporation, modifying droplet dynamics.
- **Air Turbulence**: Swirl and turbulence enhance fuel-air mixing, breaking larger droplets into finer ones.

Fuel Additives and Nanoparticles

- **Nano-Additives**: Nanoparticles like cerium oxide (CeO_2) and aluminum oxide (Al_2O_3) improve fuel atomization, reducing droplet size.
- **Surfactants**: Some additives lower surface tension, leading to better droplet dispersion.

Engine Operating Conditions

- **Engine Speed**: Higher speeds influence injection duration and droplet breakup.
- **Load Conditions**: Under higher loads, fuel droplets may experience different break-up dynamics due to increased turbulence.

Each of these factors plays a role in determining the shape, size, and behavior of fuel droplets, ultimately influencing combustion efficiency and emissions in diesel engines.

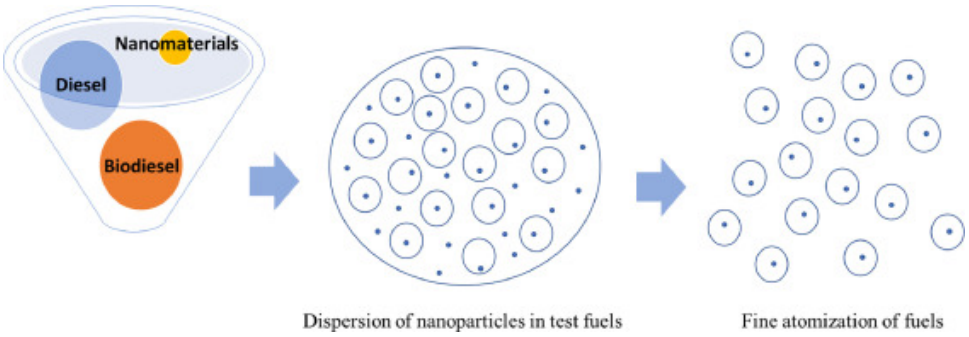

Figure 6. Diagrammatic Representation of the nanoparticles dispersed test fuel [74].

Diesel engines are widely used in transportation, power generation, and industrial applications due to their high thermal efficiency and fuel economy. However, they contribute significantly to environmental pollution through emissions of nitrogen oxides, particulate matter, and carbon monoxide. Innovations in Nanotechnology have introduced nanostructured fuel droplets as the initial solution for increasing combustion and reducing emissions. This literature review explores the impact of nano-structured fuel droplets on diesel engine performance and emissions. Nano-structured fuel droplets are created by dispersing nanoparticles such as cerium oxide, aluminum oxide, and carbon nanotubes into conventional diesel fuel. These nanoparticles act as catalysts, improving fuel atomization and promoting complete combustion [74]. The enhanced surface area and better droplet dispersion facilitate superior fuel-air mixing, leading to increased combustion efficiency and lower unburned hydrocarbons (UBHC) [75].

Sun and co-workers experimentally investigated the effects of nanoparticles mixed into diesel fuel on the cold start performance of diesel engines under various environmental conditions. The study revealed that nanoparticle addition reduced ignition delay and improved engine efficiency during cold starts. Significant reductions in CO and HC emissions were also observed. The results indicated that CeO_2 nanoparticles enhance fuel atomization and combustion efficiency, thereby improving cold-weather performance [76].

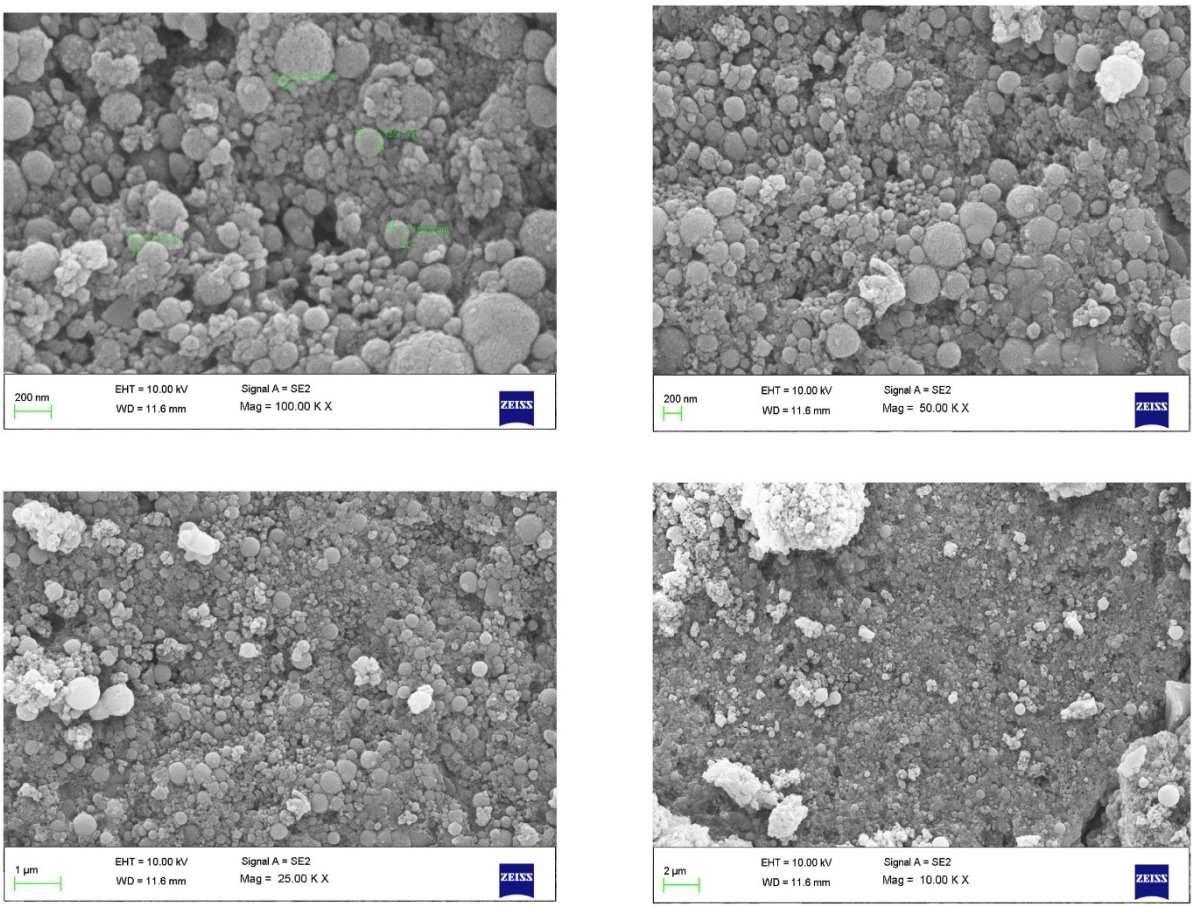

Figure 7. SEM images of the AlO(OH) [77].

Sateesh and colleagues investigated the effects of nanoparticle additives on the combustion and emission characteristics of a dual-fuel engine. Experimental results showed that nanoparticles positively impact combustion and increase thermal efficiency. Marked reductions in CO, HC, and smoke emissions were achieved. The study concluded that nano-additives can effectively enhance combustion stability in alternative fuel systems [77].

In some studies, the performance and emission characteristics of a compression ignition (CI) engine fueled with biodiesel–diesel blends containing nanoparticle additives were investigated. Results indicated that the inclusion of nanoparticles enhanced brake thermal efficiency and decreased specific fuel consumption. Emission outcomes showed notable reductions in CO, HC, and smoke emissions, with a minor increase in NOx levels. Furthermore, a Genetic Programming approach was applied to model and predict engine behavior and emission parameters. The GP model achieved high accuracy, demonstrating its effectiveness in optimizing nano-biodiesel engine performance [78]. In some studies, the combined effects of nano-fuel additives and nano-lubricant oil additives on diesel engine performance and emission characteristics were examined. The findings revealed that nanoparticles improved combustion efficiency, resulting in higher brake thermal efficiency and lower fuel consumption. Emission analyses showed notable reductions in CO, HC, and smoke emissions, while a slight increase in NOx was observed. Overall, the integration of nano-additives in both fuel and lubricant enhanced engine performance and contributed to cleaner combustion [79].

Additionally, some studies discussed the prospects and limitations of current biofuels along with emerging trends in the use of nanoparticles to enhance biofuel production and microbial fuel cell efficiency. The results indicated that although conventional biofuels suffer from low energy density and high production costs, nanoparticle incorporation can significantly improve catalytic activity and microbial performance. Nanoparticles were also shown to accelerate biofuel conversion reactions and enhance electron transfer in microbial fuel cells. Overall, the application of nanotechnology offers a promising approach to overcoming the major drawbacks of existing biofuel systems [80]. Nano-structured fuel droplets have demonstrated significant potential in enhancing diesel engine performance and reducing emissions. The incorporation of nanoparticles such as cerium oxide and aluminum oxide improves fuel atomization, combustion efficiency, and emission characteristics. However, further research is needed to address stability and environmental concerns. With continued advancements, nano-structured fuels could play a crucial role in achieving cleaner and more efficient diesel engine technologies.

Avcu et al. [81] conducted a numerical study to evaluate the effects of varying injection pressures on diesel engine performance and nitrogen oxide emissions. The simulations showed that higher injection pressures improved fuel atomization, leading to better air–fuel mixing and increased combustion efficiency. As a result, brake thermal efficiency rose, while soot and carbon monoxide emissions declined. However, the intensified combustion temperatures caused a noticeable increase in nitrogen oxide emissions. The study highlighted that an optimal injection pressure range exists where performance and emissions can be balanced effectively. These findings provide useful guidance for selecting injection parameters to achieve cleaner and more efficient diesel engine operation.

Ahmed and Mekonen [82] investigated the effects of injector nozzle hole number and engines operating with biodiesel blends. Their experiments showed that increasing both the nozzle holes and injection pressure improved fuel atomization and reduced ignition delay, leading to better combustion. As a result, brake thermal efficiency and power output increased, while carbon monoxide and hydrocarbon emissions dropped noticeably. However, higher injection pressures also caused a rise in nitrogen oxide emissions due to elevated combustion temperatures. The authors concluded that careful optimization of injector geometry and pressure settings can help overcome performance drawbacks often associated with biodiesel fuels. Overall, the study highlights the potential of waste cooking oil biodiesel as a renewable energy source when paired with optimized injection systems.

Wang et al. [83] focused on optimizing combustion and fuel injection characteristics in marine diesel engines using a combination of modeling and experimental analysis. The research examined how injection timing, pressure, and duration affect combustion efficiency, fuel consumption, and emission behavior under marine operation conditions. The results demonstrated that advanced injection timing and increased pressure enhance atomization and combustion stability but may lead to higher nitrogen oxide emissions. The authors proposed optimized injection strategies to achieve a balance between efficiency and emission reduction. Their model provided valuable insight into fuel injection control for large-scale marine diesel engines, contributing to cleaner and more efficient maritime power systems.

Collectively, the reviewed studies demonstrate that advancements in both fuel modification techniques and data-driven optimization methods have significantly contributed to improving internal combustion engine performance. Research involving nanoadditives, biodiesel blends,

and injection parameter optimization has shown that precise control of combustion dynamics can lead to enhanced efficiency and reduced emissions. Meanwhile, machine learning–based approaches, combined with optimization algorithms such as genetic programming and hybrid neural networks, have proven effective in predicting engine behavior and identifying optimal operating conditions under complex constraints. These findings underline a clear transition in engine research—from purely experimental and simulation-based studies toward hybrid data-driven frameworks that integrate physical understanding with computational intelligence. Building upon these insights, the present study develops a machine learning framework for simulating and optimizing heavy-duty engine injector parameters, aiming to achieve accurate, efficient, and resource-saving performance prediction.

Some studies have employed machine learning models—particularly artificial neural networks to optimize key operating parameters in diesel engines. These approaches use artificial neural network models to learn the complex nonlinear relationships between different variables and their effects on performance, consumption, and emissions. By training on experimental or simulation data, ANNs act as fast and accurate surrogate models, greatly reducing the need for costly physical engine tests and computationally intensive CFD simulations. When combined with optimization algorithms, these models can efficiently identify parameter sets that improve engine performance while lowering emissions, providing accuracy comparable to conventional techniques but with significantly reduced computation times, making them valuable tools in modern engine research and development [84].

A further line of research has integrated machine learning with advanced bio-inspired optimization methods. One example applies neural networks together with the Dung Beetle Optimization (DBO) algorithm to predict and optimize locomotive diesel engine parameters. In this approach, a neural network is trained to model the nonlinear interactions between engine inputs and outputs, similar to other ML-based studies. The trained network is then embedded within the DBO algorithm to perform multi-objective optimization, targeting improvements in performance indicators such as power, fuel consumption, and emissions simultaneously. The combination of a fast-predicting neural network and an efficient metaheuristic optimizer allows the exploration of large solution spaces with reduced computational cost. Results from such studies demonstrate that ML–DBO frameworks can identify high-quality operating parameter sets more quickly than conventional optimization procedures, highlighting their potential for accelerating the development of next-generation diesel engine control strategies [85].

Another related study has focused on improving diesel engine emission prediction through the use of neural network model clusters. In this approach, instead of relying on a single neural network, multiple ANN models are trained and combined to form a cluster or ensemble architecture. This ensemble strategy enhances prediction robustness and reduces the risk of overfitting by leveraging the strengths of different models. The clustered ANN system is then used to optimize engine operating conditions with the goal of minimizing emissions such as NOx, CO, HC, and particulate matter while maintaining acceptable performance levels. By providing more stable and accurate emission predictions, the neural network cluster enables more reliable optimization outcomes and reduces the need for extensive experimental testing. Such studies show that ensemble-based machine learning frameworks can significantly enhance

predictive accuracy and computational efficiency in diesel engine emission analysis and optimization [86].

Another study has applied artificial neural networks specifically to predict specific fuel consumption and exhaust gas temperature in diesel engines. In this work, ANN models are trained using experimental engine data to capture the complex thermodynamic and combustion-related interactions that govern fuel consumption and exhaust temperature behavior under varying operating conditions. By accurately learning these nonlinear relationships, the ANN provides rapid predictions without requiring additional engine tests. Such predictive capability enables more efficient calibration, facilitates real-time estimation in control systems, and supports optimization studies aimed at reducing fuel consumption while maintaining acceptable exhaust temperatures for engine durability and emissions control. These findings further demonstrate the versatility of neural networks as powerful tools for analyzing and optimizing diesel engine performance metrics [87].

In addition to these efforts, some researchers have focused on forecasting engine emissions and performance in a single-cylinder diesel engine operating with diethyl ether (DEE) as an additive. Using experimental measurements collected under varying DEE blend ratios, ANN models were developed to evaluate how alternative fuels influence combustion quality, efficiency, and emission formation. The resulting neural network demonstrated strong predictive capability for parameters such as thermal efficiency, specific fuel consumption, NOx, CO, HC, and smoke opacity, thereby providing a fast and effective means of assessing the potential of DEE without extensive experimental campaigns [88].

Another noteworthy contribution in the field investigates the use of a Radial Basis Function Neural Network (RBFNN) combined with an improved Particle Swarm Optimization (PSO) algorithm to predict the performance and emissions of a high-pressure common-rail diesel engine. In this study, the RBFNN serves as the primary predictive model, learning the nonlinear relationships between injection parameters, combustion characteristics, and resulting performance and emission outputs. The improved PSO algorithm is employed to optimize the RBFNN structure and parameters, ensuring faster convergence and higher prediction accuracy compared to standard training methods. This hybrid RBFNN–PSO framework demonstrates strong predictive capability for key metrics such as torque, brake thermal efficiency, specific fuel consumption, NOx, CO, and soot emissions. The model's ability to deliver accurate predictions with reduced computational cost highlights the potential of optimized neural network architectures in supporting rapid engine calibration and design optimization processes [89].

Recent developments have also explored the application of deep learning techniques to achieve fuel injection control. In this line of research, deep neural network architectures are trained on extensive experimental and simulation datasets to learn the intricate temporal and nonlinear behaviors of fuel injection processes, including injection timing, injection duration, injection quantity, and dynamic rail pressure fluctuations. By accurately modeling these complex interactions, the deep learning framework enables high-resolution prediction and control of multi-stage injection events, resulting in improved combustion stability, enhanced fuel

efficiency, and reduced emissions. Such studies demonstrate that deep learning can provide a powerful data-driven foundation for next-generation injection system design, offering superior precision compared to traditional calibration-based or physics-only approaches [90].

A further development in the literature introduces a novel deep learning approach for analyzing liquid fuel injection behavior in combustion systems. In this study, advanced neural network architectures are employed to model the highly nonlinear and transient processes associated with spray breakup, droplet distribution, penetration length, and vaporization dynamics under varying operating conditions. By training on high-fidelity experimental measurements and CFD-generated datasets, the deep learning model is capable of capturing complex spatial–temporal characteristics of liquid fuel injection with remarkable accuracy. This data-driven framework provides rapid prediction capability, significantly reducing the computational burden typically associated with detailed spray simulations. The results demonstrate that deep learning can effectively support the exploration of injection strategies, facilitate improved understanding of spray–combustion interactions, and accelerate the development of more efficient and cleaner combustion systems [91].

In addition to these developments, some researchers have applied machine learning algorithms to predict gasoline injection injectors. In this approach, various ML models are trained using high-resolution injector test data to learn the complex electromechanical and hydraulic behaviors governing needle lift, injection rate shaping, and voltage response under different operating conditions. By accurately modeling the nonlinear interactions between control signals, injector dynamics, and resulting fuel delivery profiles, the machine-learning framework enables rapid and precise prediction of injection characteristics that would otherwise require detailed experimental measurements or computationally intensive simulations. This capability supports faster injector calibration, improved control strategy development, and enhanced understanding of transient injection phenomena. Overall, such ML-based predictive models provide a valuable tool for accelerating GDI injector design and performance optimization [92].

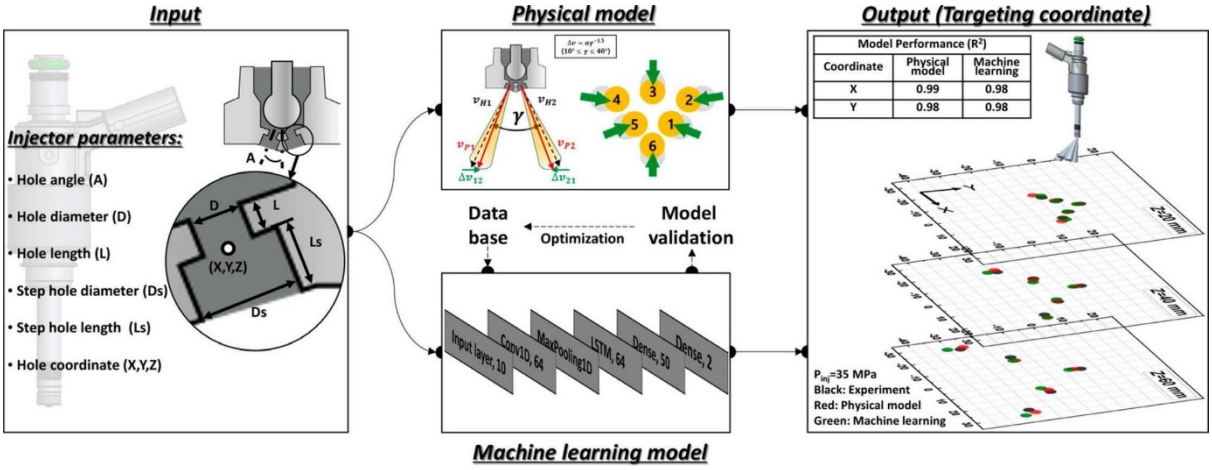

Figure 8. Machine Learning Model [93].

A further contribution examines the prediction of spray target position in multi-hole gasoline direct injection (GDI) injectors through a hybrid framework that integrates physical spray modelling with machine learning. The physical model provides high-resolution representations of spray evolution, capturing droplet motion, cone angle development, hole-to-hole interaction, and the influence of in-cylinder aerodynamic fields. Machine learning algorithms are trained on the resulting datasets to learn the complex nonlinear relationships that govern spray targeting across different injection pressures, ambient densities, and nozzle geometries. This combined approach enables fast and accurate prediction of spray impact locations, significantly reducing the computational effort typically required by repeated physical simulations. The findings highlight the effectiveness of physics-informed machine learning for accelerating injector design, enhancing mixture preparation control, and supporting the optimization of injection strategies in advanced GDI combustion systems [93].

E. Artun have investigated the performance assessment and forecasting of cyclic gas injection into hydraulically fractured wells using advanced data analytics and machine learning techniques. By integrating historical injection–production data with predictive modeling, their approach identified the key operational variables that most strongly influence pressure behavior, gas breakthrough timing, and overall recovery efficiency. Machine learning models were employed to forecast reservoir responses under different cyclic injection schedules, enabling more accurate prediction than traditional decline-curve or empirical methods. The study showed that data-driven modeling significantly improves the ability to optimize injection cycles, reduce uncertainty in production planning, and enhance hydrocarbon recovery in fractured reservoirs. Furthermore, the findings highlight the value of combining subsurface physics with ML-driven analysis to support more reliable decision-making in unconventional field development [94].

In some studies, performance results in injection systems have been examined using optimized machine learning algorithms. Their approach combined experimental spray measurements with advanced data-driven modeling to characterize the rapid phase transition and plume collapse phenomena that occur under low-pressure ambient conditions. By applying an optimized ML

framework, the study identified the dominant factors influencing spray morphology, penetration, and vapor distribution during flash boiling operation. The machine learning model provided highly accurate predictions of spray characteristics, outperforming traditional empirical correlations and reducing the need for extensive high-speed visualization experiments. The findings demonstrated that optimized ML algorithms can reliably capture the complex thermodynamic and fluid-dynamic interactions associated with flash boiling, offering a powerful tool for injector design refinement and improved mixture formation strategies in modern GDI engines [95].

Another study focuses on advancing fuel spray characterization in directly injected gasoline systems through the application of machine learning techniques. In this work, high-fidelity experimental spray data and detailed diagnostic measurements were used to train ML models capable of capturing the complex behaviors associated with atomization, droplet breakup, plume interaction, and vapor-phase development. The machine learning framework successfully learned the nonlinear relationships between operating parameters such as injection pressure, ambient density, nozzle geometry, and resulting spray structure. By providing rapid and accurate predictions of key spray characteristics, the approach significantly reduces the dependence on time-consuming optical experiments and costly CFD simulations. This study highlights the potential of data-driven modeling to enhance the understanding of fuel processes, support injector optimization, and accelerate the development of more efficient and cleaner GDI combustion systems [96].

Another contribution explores the application of deep reinforcement learning (DRL) for the dynamic control of fuel injection timing in multi-pulse compression ignition engines. In this study, DRL is employed to develop an intelligent control strategy capable of continuously adjusting injection timing in response to varying in-cylinder conditions and combustion states. By interacting with a high-fidelity engine simulation environment, the learning agent identifies optimal multi-pulse timing sequences that balance performance, fuel efficiency, and emissions. The DRL-based controller outperforms traditional open-loop or rule-based strategies by adapting to transient conditions, reducing combustion variability, and improving heat-release phasing. The findings demonstrate that reinforcement learning provides a powerful framework for real-time optimization of complex injection events, offering new opportunities for advanced combustion control in next-generation compression ignition engines [97].

A separate line of research presents a machine learning-enabled methodology for predicting transient injection maps in automotive fuel injectors, incorporating uncertainty quantification to enhance model robustness. This work leverages detailed injector dynamics data to train advanced regression and probabilistic learning models capable of capturing rapid variations in injection rate, needle motion, and flow characteristics under transient operating conditions. The framework not only delivers highly accurate predictions of injection behavior but also provides uncertainty bounds, allowing engineers to assess the confidence level of each prediction and identify regions where injector performance is most sensitive to parameter changes. By integrating predictive accuracy with uncertainty awareness, this study offers a more reliable data-driven tool for injector calibration, performance evaluation, and combustion optimization in modern engine systems [98].

A related investigation applies machine learning techniques to predict nano-scale particulate matter distribution in gasoline direct injection (GDI) engines. In this work, advanced data-driven models were trained on experimental measurements of particle number, size distribution, and formation pathways under varying injection strategies and operating conditions. The ML framework successfully captured the complex nucleation, agglomeration, and oxidation mechanisms that govern particle formation at the nano scale—processes that are often difficult to resolve using conventional modeling techniques. By providing fast and accurate predictions, the approach enables more efficient exploration of how injection timing, pressure, fuel properties, and combustion phasing influence particulate emissions. The study demonstrates that machine learning can offer valuable insight into ultra-fine particle behavior, supporting cleaner GDI engine development and aiding regulatory compliance for stringent emission standards [99].

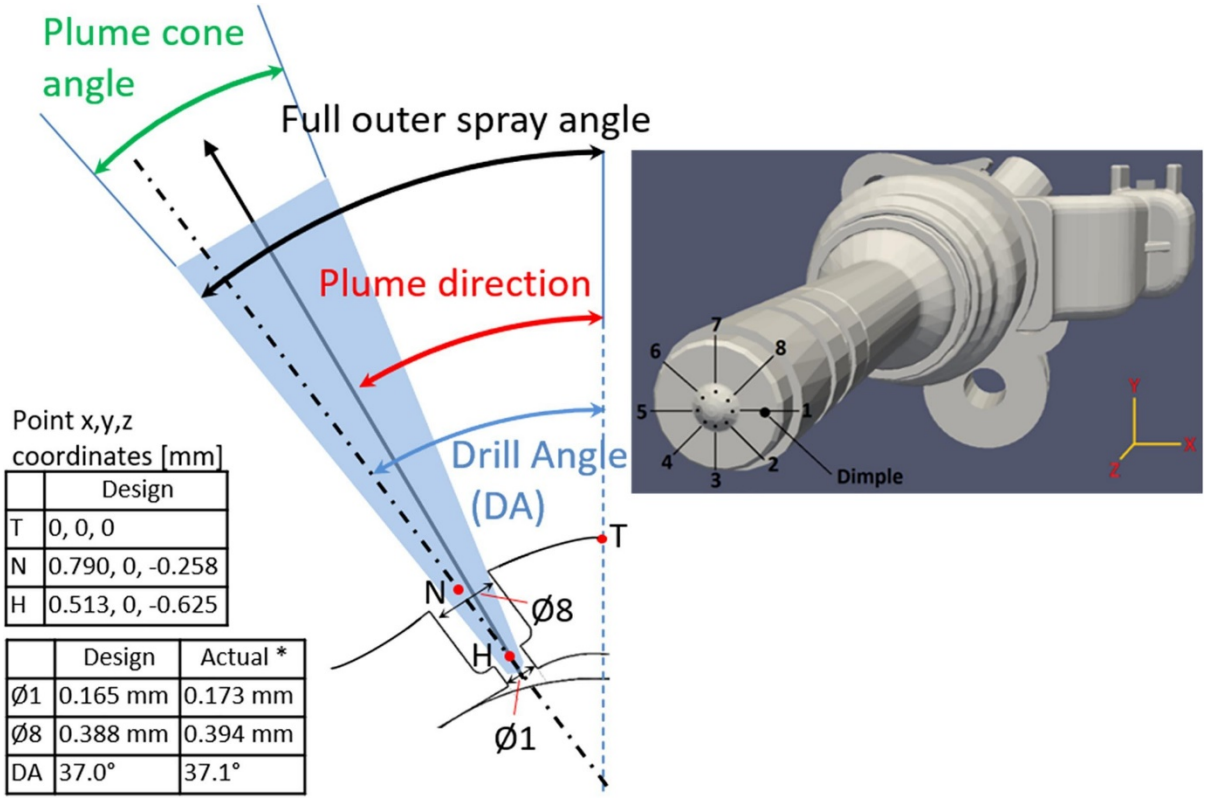

Figure 9. Cut plane image of spray G injector with dimensions (inset figure shows the 3-D rendering of the injector with primary orientation) [101].

Machine learning has been effectively employed to analyze and optimize complex engine processes, as seen in studies focusing on ignition delay times under dual-fuel engine conditions and 3D spray prediction under engine combustion network (ECN) spray G conditions. Machine learning algorithms were used to model and predict key engine behaviors that are otherwise challenging to capture with traditional methods. Utilized machine learning to predict ignition delay times in dual-fuel engines, where the interaction between two fuels and varying engine conditions can cause significant variations in combustion behavior. By training the model on experimental data, it was able to provide more accurate predictions of ignition timing, improving the understanding of dual-fuel engine performance and enhancing calibration for better fuel efficiency and emissions control. Similarly, applied learning algorithms to predict

the conditions, focusing on the dynamic and transient characteristics of the fuel spray. Here, machine learning was used to predict spray patterns, which are critical for optimizing combustion and reducing particulate emissions. In both cases, machine learning provided a powerful tool for modeling complex, nonlinear relationships, enabling more efficient and precise optimization of engine processes for improved performance and lower emissions [100-101].

In the existing literature, machine learning–based optimization studies on internal combustion engines have predominantly relied on CFD-generated datasets and surrogate modeling approaches, where spray and combustion characteristics are inferred indirectly through numerical simulations rather than direct experimental observation [102]. In such studies, injector parameters and operating conditions are optimized within data-driven frameworks, and the physical interpretation of the results is largely based on simulated in-cylinder fields and statistical trends. In contrast to these approaches, the present study integrates experimental spray visualization, engine performance measurements, and machine learning-based analysis within a unified framework, providing direct experimental evidence that links spray structure to combustion performance and emission behavior under varying injection pressures and injection timings. By visually correlating spray atomization characteristics with NOx, soot, indicated power, and ISFC trends, this work extends beyond purely simulation-based methodologies and enhances the physical interpretability of machine learning predictions. Furthermore, while previous studies have demonstrated the computational efficiency of machine learning–genetic algorithm frameworks for rapid optimization, the present results confirm that machine learning models trained on physically meaningful and experimentally validated injector parameters can accurately capture nonlinear spray–combustion interactions. As a result, this hybrid experimental–data-driven approach improves the reliability, transparency, and industrial applicability of machine learning techniques for advanced diesel engine development [102].

3. Methodology

3.1. Developed Real Engine

The engine model is designed with a 67 mm cylinder diameter and a 68 mm stroke length, providing a total engine capacity of 479 cc. It delivers a power output ranging from 9.9 kW to 13.3 HP at a maximum speed of 3600 rpm. The engine operates with an injection pressure of 137 bar, contributing to efficient fuel delivery. With a compression ratio of 23.5, it ensures optimal engine performance and fuel efficiency.

The cooling system is water-based, with a recommended water capacity of 3 liters, ensuring effective temperature management during operation. The engine's oil pressure ranges from 1 bar at idle to 4.5 bar at maximum RPM, providing the necessary lubrication at varying speeds. The lubricant oil capacity is 3.3 liters, maintaining smooth engine operation and preventing wear and tear on critical components.

This water-cooled engine is built for durability and high performance, making it suitable for demanding tasks while maintaining reliable cooling and lubrication under different operational conditions.

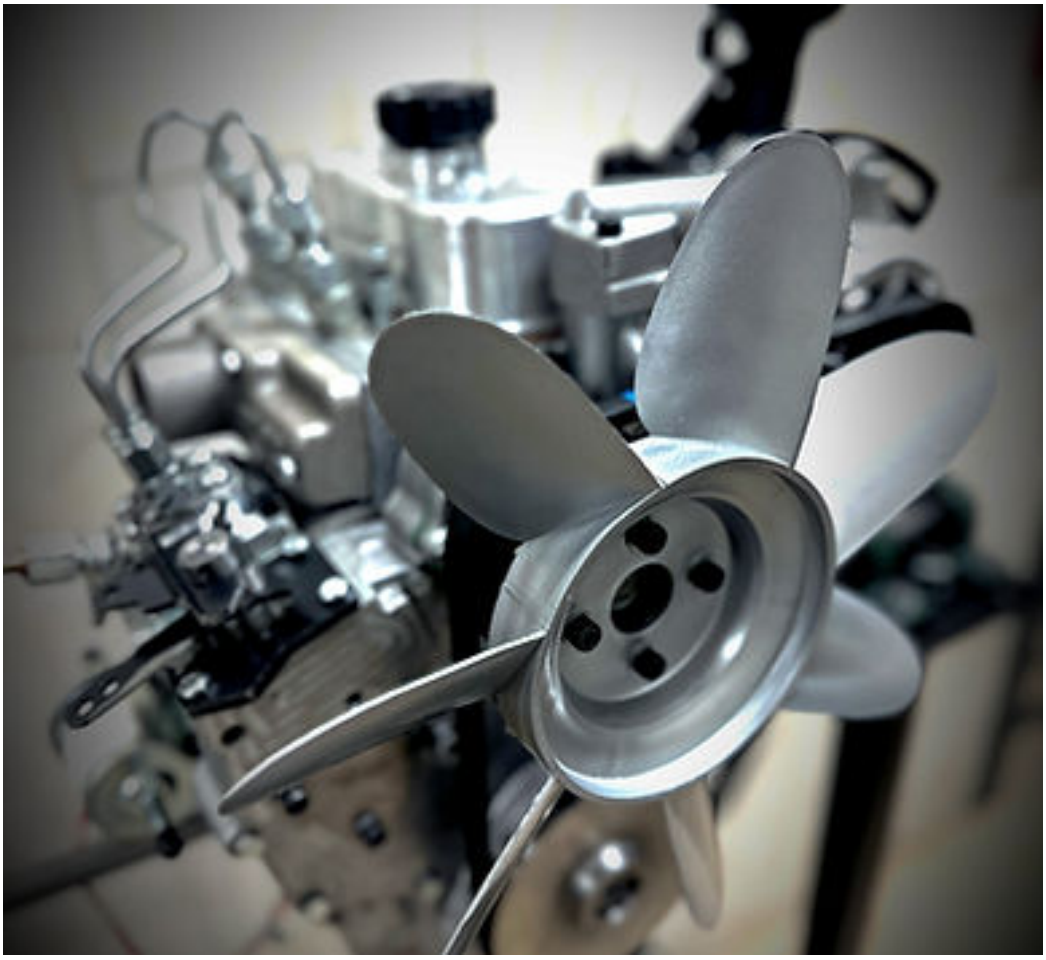

Figure 10. Illustrates the motor developed and produced by Prof. Dr. Hasan Koten via university industry collaboration and used in this thesis performance testing.

The engine has been designed through a collaborative effort between Istanbul Medeniyet University and the industry, combining academic expertise and industrial experience to create an innovative and high-performance product. Nearly 1,000 individual parts make up the engine, each crafted with precision and care to ensure optimal functionality and durability. The design and manufacturing process has been thoroughly executed using computer-aided design (CAD) software, which has allowed for detailed modeling and simulations of the engine's components and overall system.

From the choice of raw materials to the production techniques used, the entire process has been meticulously planned and executed. Casting materials have been carefully selected for their strength and suitability for high-performance engine applications. The production techniques range from advanced casting methods to precision machining, ensuring that each part meets the required standards for quality and performance.

By utilizing cutting-edge technology and CAD software, the collaboration has enabled a highly efficient and precise design process. This partnership between Istanbul Medeniyet University and the industry ensures that the engine is not only theoretically optimized but also practically viable for industrial use. This collaboration exemplifies the successful integration of academic research and industrial production, resulting in a high-quality engine designed to meet modern technological demands.

3.2. **Engine–Dynamometer Integration**

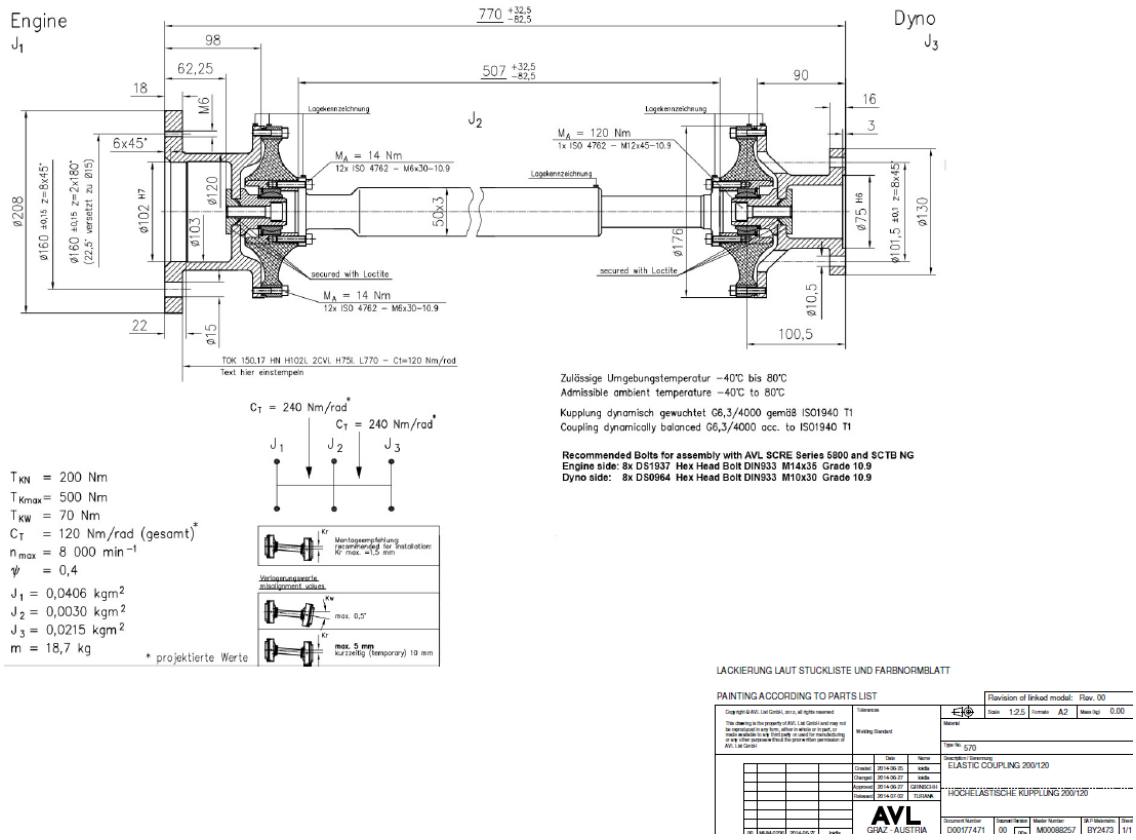

Figure 11. Technical blueprint of the engine–dynamometer coupling assembly used in this thesis

Figure 11 presents the detailed engineering drawing of the coupling mechanism used to connect the engine output shaft to the dynamometer input system. The blueprint includes precise dimensional specifications, tolerance values, torque limits, and material requirements for each segment of the coupling assembly. These measurements define the geometric compatibility between the two systems and ensure that the rotational power is transferred efficiently with minimal mechanical loss. The illustration also shows the arrangement of flanges, bolts, spline connections, and the central shaft, highlighting the fastening methods—such as the use of high-grade bolts and Loctite—to maintain structural integrity during high-speed operation. Additional parameters, including admissible temperature ranges, moment of inertia values for each rotating mass (J_1, J_2, J_3), and dynamically balanced coupling requirements, provide insight into the operational constraints and performance expectations. Overall, this schematic serves as a foundational reference for manufacturing, assembly, and verification of the power transmission interface between the engine and the motor dynamometer.

Figure 12. Custom-Designed Components for Engine–Dynamometer Interface Preparation

Figure 13. Custom-designed components for engine–dynamometer ınterface preparation during our engine dynamometer test.

Figure 12,13 presents the integration studies carried out during the preparation of the engine and dynamometer test system, offering a comprehensive view of how the entire setup is

assessed prior to experimental operation. These studies involve a systematic evaluation of the mechanical, structural, and functional interactions between the engine assembly and the dynamometer equipment. As part of this process, each connection point—such as shaft couplings, mounting brackets, alignment rails, and sensor interfaces—is inspected to verify that it is properly installed and capable of maintaining stability throughout the test cycles. The figure also reflects the careful adjustments made to minimize misalignment, reduce mechanical stress, and ensure that torque and rotational speed are transmitted accurately to the measuring device. By documenting these integration procedures, Figure 12 highlights the importance of precise setup and verification steps in achieving reliable, repeatable, and high-quality engine performance measurements.

3.3. Engine Configuration and Optimization Strategy

Optimizing a heavy-duty engine operating in medium-load conditions with a low-octane gasoline-like fuel requires careful consideration of several factors. Define the properties of the nanostructured fuel droplets, such as droplet size distribution, surface area, chemical composition, and combustion characteristics. These properties can be determined through experimental measurements or numerical modeling.

Input parameters

- Fuel mass

- Fuel injection pressure and time interval

- Opening range of valves

- Opening time of valves

Output parameters

- Nox

- Engine power

- Fuel consumption (Table 1,2,3)

Table 1 Engine Configuration

Engine Model	**Values**
Diameter of the Cylinder	67 mm
Stroke Length	68 mm
Engine Capacity	479 cc
Motor Power	9.9 kW – 13.3 HP / 3600 rpm
Injection Pressure	137 bar
Compression Ratio	23.5
Recommended Water Capacity	3 L
Oil Pressure (Idle – Max RPM)	1 bar – 4.5 bar
Lubricant Oil Capacity	3.3 L

Table 2 Input Parameter

Parameter	Description	Min	Max
inj_mass	fuel injection / mg	10	30
inj_pressure	Injection pressure / bar	100	300
inj_timing	Injection timing / CA	-25	-5
ex_lift	opening range of valves / mm	0,9	7
in_lift	opening range of valves / mm	0,9	7
ex_valve	valve opening times / bBDC	-60	0
in_valve	valve opening times / bTDC	-50	-10

Table 3 Output Parameter

Parameter	Description
Brake power	HP
nox	ppm
fuel_cons	bsfc

3.4. Numerical Model Description

The simulation area is modeled using a mesh of sectors, which represents a single cylinder and takes into account only one spray smoke. Homogeneous mixture and temperature distributions are specified. (Figure 14)

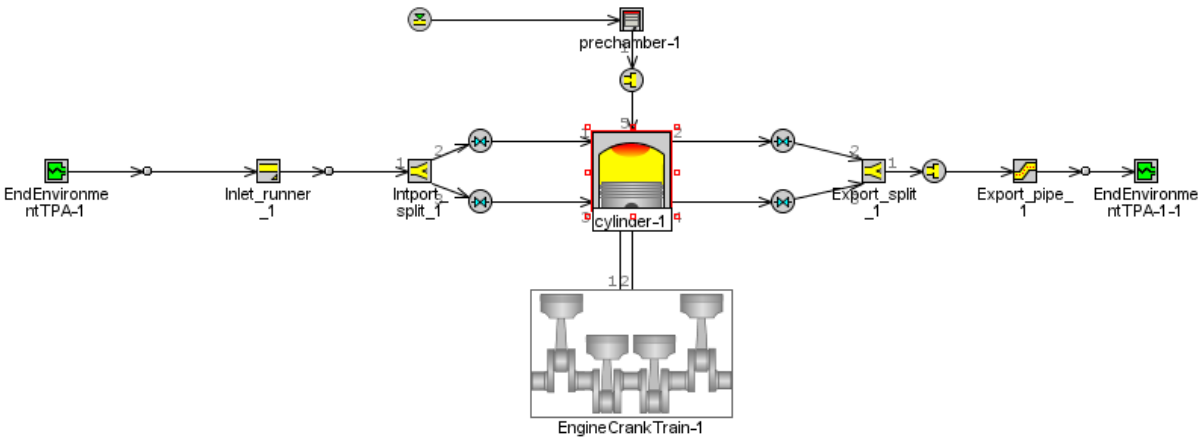

Figure 14. 1D Engine Model

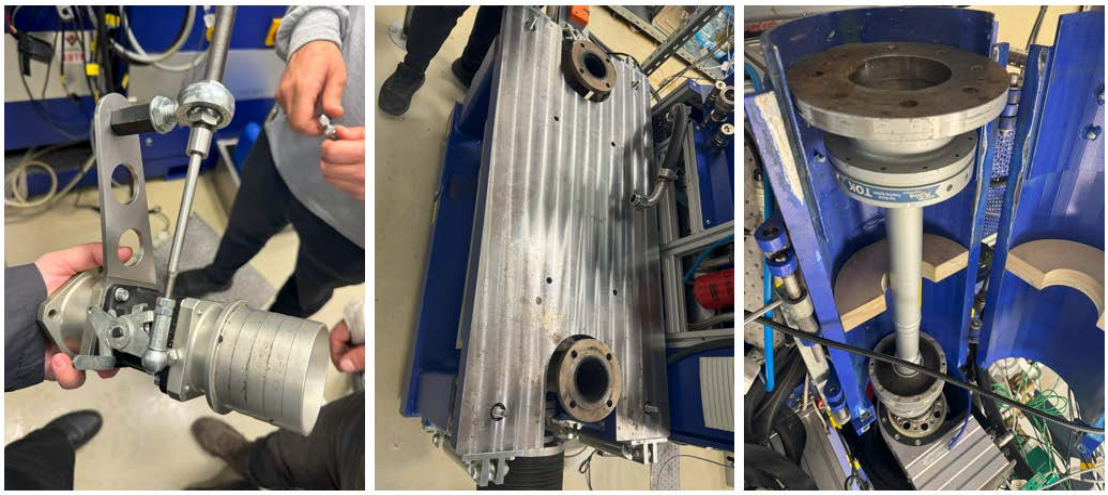

Figure 15. Fabrication and Installation of Engine–Dynamometer Interface Components

Figure 16. Fuel Injector System and Components

Figures 15 and 16 illustrate the manufacturing and assembly stages of the specialized components used to interface the engine with the dynamometer system. These visuals document the step-by-step process through which custom brackets, shafts, adapters, and mounting structures are produced and fitted to the engine. Particular attention is given to the precision machining and dimensional accuracy required to guarantee that each part aligns seamlessly with both the engine geometry and the dynamometer's input shaft. The assembly process shown in the figures also highlights the careful calibration and fitting procedures necessary to achieve a rigid and vibration-free connection, which is essential for obtaining dependable performance

and emission measurements. Overall, the images underscore the level of engineering detail and craftsmanship involved in preparing a fully compatible and structurally robust engine-dynamometer interface.

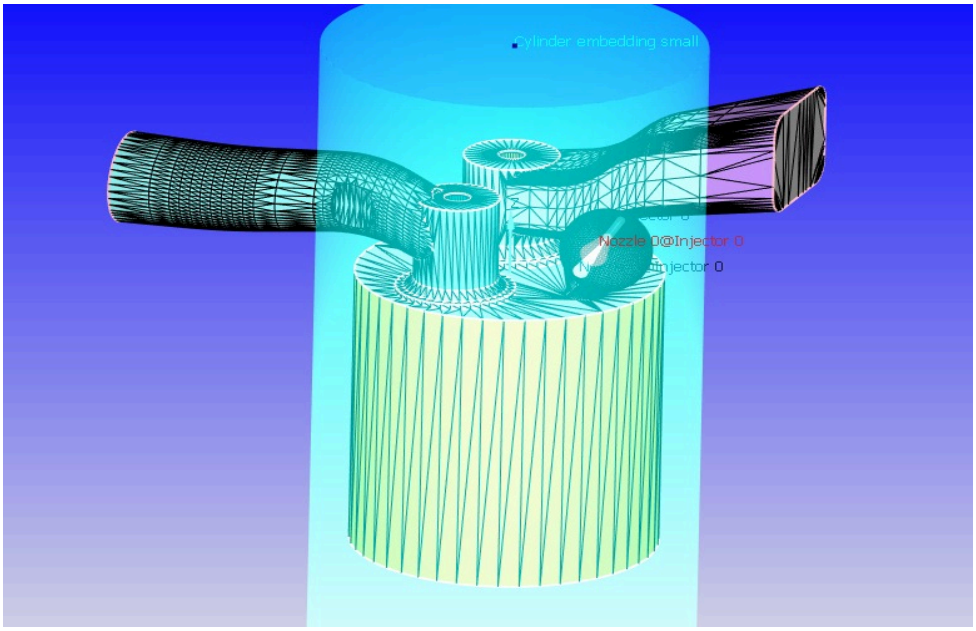

Figure 17. 3D Engine Geometry Mesh Model

Geometry Representation: Develop a detailed 3D computational model of the diesel engine, including the combustion chamber, fuel injection system, intake and exhaust ports, piston, valves, and other relevant components. The model should accurately represent the geometry and dimensions of the engine (Figure 17).

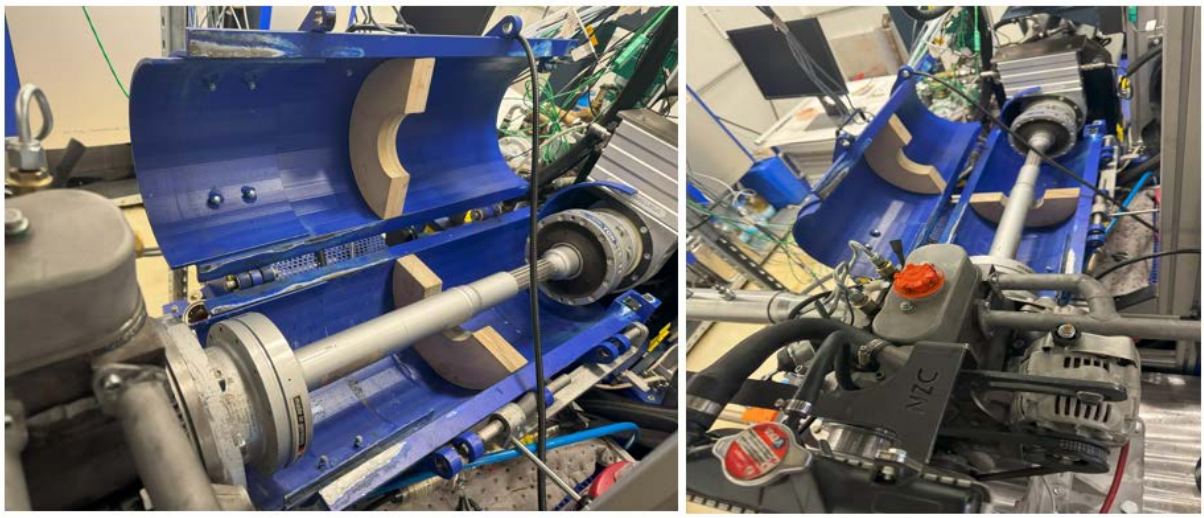

Figure 18. Engine–Dynamometer Drive Coupling Integration Assembly

Figure 18 provides a detailed view of the diesel shaft being integrated into the motor dynamometer setup, showcasing the mechanical arrangement that enables effective transfer of torque and rotational motion from the engine to the measurement system. The image highlights the precision required during the installation process, including the alignment of the shaft with

both the engine's output interface and the dynamometer's input coupling. Achieving this alignment is essential to prevent lateral loading, vibration, and unnecessary mechanical stress, all of which can negatively influence measurement accuracy. The surrounding support structures, mounting fixtures, and protective housings visible in the figure indicate the engineering considerations taken to maintain structural rigidity and operational stability during high-speed testing. Additionally, the assembly shown reflects the careful calibration and fastening procedures needed to ensure that the shaft remains securely positioned throughout the experiments, ultimately allowing the dynamometer to capture consistent and reliable performance data.

3.5. **Experimental Setup**

To validate the results of our CFD simulations, a series of engine tests were conducted at the TÜBİTAK Dynamometer Facility using a fully equipped 60 kW test bench (Figure 1). In these experiments, a two-cylinder diesel engine was operated under laboratory conditions to ensure all measurements were repeatable and unaffected by external factors. The primary objective of the test program was to investigate how different fuel mixture ratios affect overall engine performance, combustion characteristics, and emissions. The simulations were ultimately demonstrated to be accurate.

Throughout the experiments, the engine was run at predetermined speed and load settings, while key boundary conditions—such as intake air temperature, boost pressure, fuel temperature, and coolant temperature—were maintained at constant values. This controlled environment made it possible to isolate the direct impact of fuel blending. The blended fuels were prepared and delivered through precision fuel-conditioning equipment that ensured stable properties and consistent mixture ratios during each test. In-cylinder pressure traces were recorded using high-response piezoelectric pressure sensors, enabling a detailed evaluation of ignition timing, heat release behavior, and combustion stability. Emission measurements, including NOx, CO, HC, and particulate matter, were obtained using calibrated exhaust gas analyzers to provide an accurate profile of pollutant formation for each fuel blend.

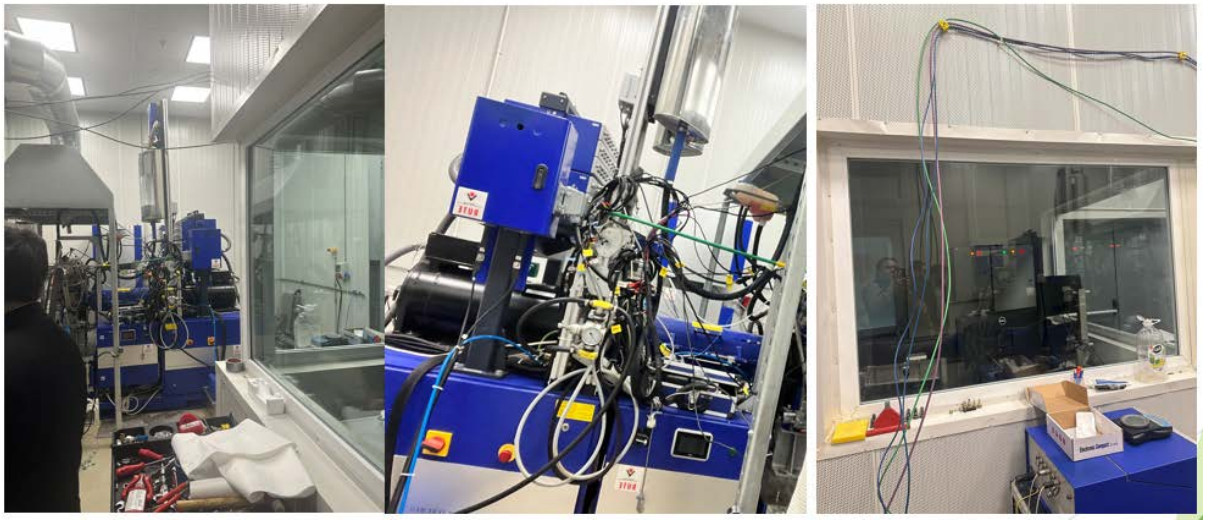

Figure 19. Engine–Dynamometer Laboratory Layout and Control Room Interface

Figure 19 illustrates the overall configuration of the engine test laboratory, including the dynamometer installation, auxiliary equipment, and the control room used for data monitoring. This layout provides a clear view of how the engine is positioned on the test bench and connected to the dynamometer through precision mounting structures. The arrangement is designed to maintain stable and repeatable operating conditions, allowing engineers to assess key performance indicators such as power output, torque generation, and fuel consumption with high accuracy.

By combining these measurements with the numerical model outputs, the experimental setup offered a strong foundation for validating the CFD results. This comparison helped reveal how well the simulations capture real combustion behavior and provided deeper insight into the effects of gasoline content on diesel engine combustion and emission dynamics.

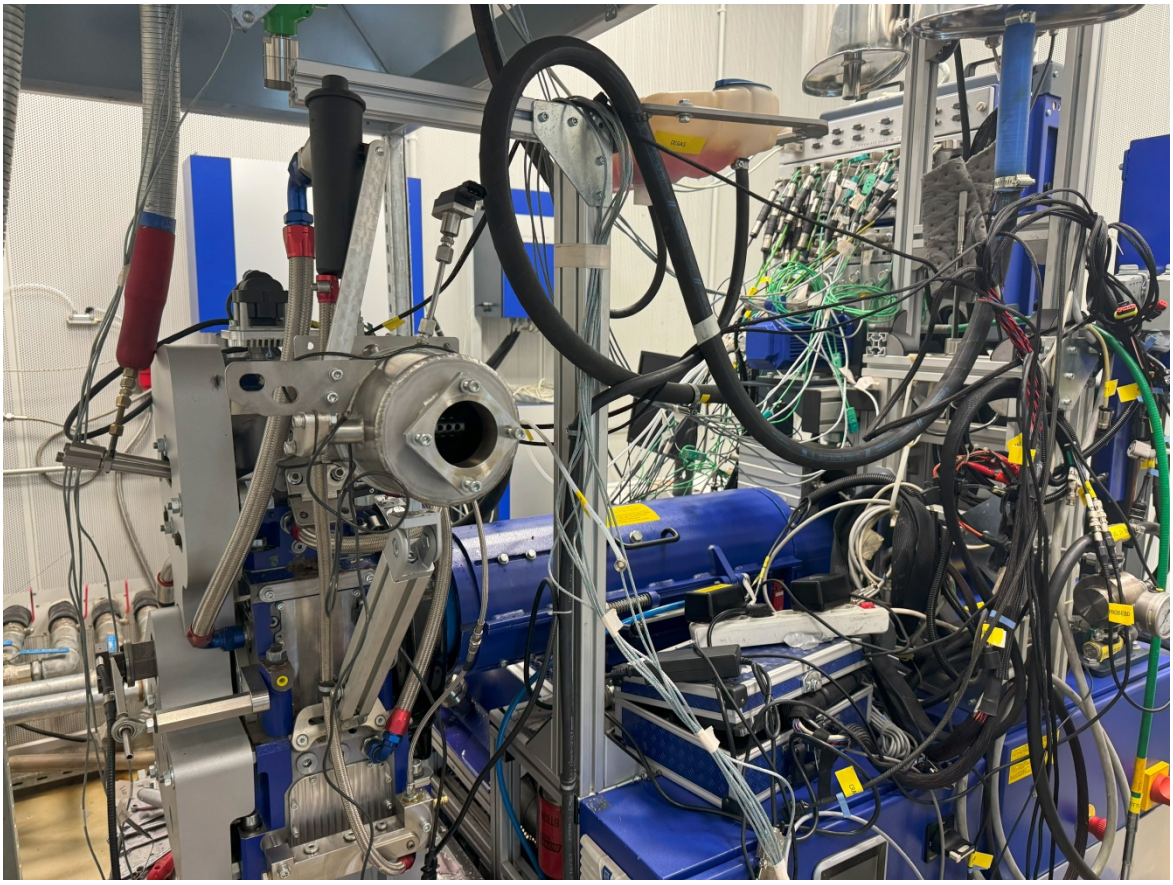

Figure 20. Fully Instrumented Engine–Dynamometer Test Configuration

This figüre 20 provides a detailed view of the engine mounted on the dynamometer test bench, showcasing the extensive instrumentation required for high-precision data acquisition. The image highlights the complex arrangement of sensors, wiring harnesses, pressure transducers, and control units used to monitor critical parameters such as combustion pressure, exhaust temperature, fuel flow, and rotational speed. The turbocharger assembly and associated plumbing are clearly visible, indicating that the engine is configured to replicate real-world operating conditions. Various measurement lines—such as thermocouple cables, in-cylinder pressure sensor leads, and ECU communication lines—are systematically routed to avoid interference and ensure accurate signal transmission. Overall, this setup demonstrates the high

level of technical integration necessary to carry out controlled and repeatable engine performance and emissions measurements.

The image also highlights the separation between the test cell and the operator area, where the control room—visible through the large observation window—houses the data acquisition systems and supervisory instruments. Electrical harnesses and sensor cables run neatly across the wall and window frame, linking the engine to real-time monitoring equipment. This controlled laboratory configuration minimizes external disturbances and ensures that performance measurements reflect the true behavior of the engine under test.

In addition to the mechanical setup, the figure emphasizes the importance of a well-organized test environment for reliable performance evaluation. The structured placement of ventilation ducts, exhaust handling systems, and safety barriers contributes to a stable and secure testing atmosphere. Overall, the figure provides a comprehensive representation of a professional dynamometer facility designed to support detailed investigations of engine behavior under standardized and repeatable conditions.

3.6. Test Parameters and Measurement Techniques

- **Performance Evaluation:** Engine performance was assessed through the measurement of key indicators such as brake thermal efficiency (BTE), brake-specific fuel consumption (BSFC), and torque output. These parameters were recorded under steady-state operating conditions to ensure repeatability and accuracy. BTE was calculated using fuel flow rate and measured power output to determine the conversion efficiency of the fuel's chemical energy into useful mechanical work. BSFC measurements provided insight into the overall fuel economy of the engine, enabling a direct comparison of how different gasoline–diesel blend ratios influenced combustion efficiency. Torque measurements were obtained directly from the dynamometer, allowing for a detailed evaluation of the engine's mechanical performance across various load and speed points.

- **Emissions Analysis:** Emission characteristics were examined using high-precision exhaust gas analyzers capable of accurately detecting a wide range of pollutant species. Concentrations of carbon monoxide (CO), nitrogen oxides (NOx), unburned hydrocarbons (HC), and particulate matter (PM) were continuously monitored during each test cycle. These measurements allowed for a comprehensive evaluation of how fuel blending influenced combustion completeness, pollutant formation mechanisms, and overall environmental impact. Special emphasis was placed on NOx and PM levels due to their strong dependence on combustion temperature, mixture quality, and ignition characteristics, all of which can vary significantly with changes in gasoline content.
- **Fuel Properties Assessment**: Physical properties of the gasoline–diesel blends—including density, viscosity, and volatility—were analyzed prior to engine testing to verify consistency with the inputs used in the CFD simulations. These properties play a critical role in spray formation, atomization, ignition delay, and overall combustion behavior. Density and viscosity measurements ensured accurate fuel metering during injection, while volatility analysis provided insights into evaporation dynamics and

mixture formation quality. By confirming that the experimental fuel characteristics matched the numerical parameters used in the computational model, the reliability and validity of the CFD-to-experiment comparison were strengthened.

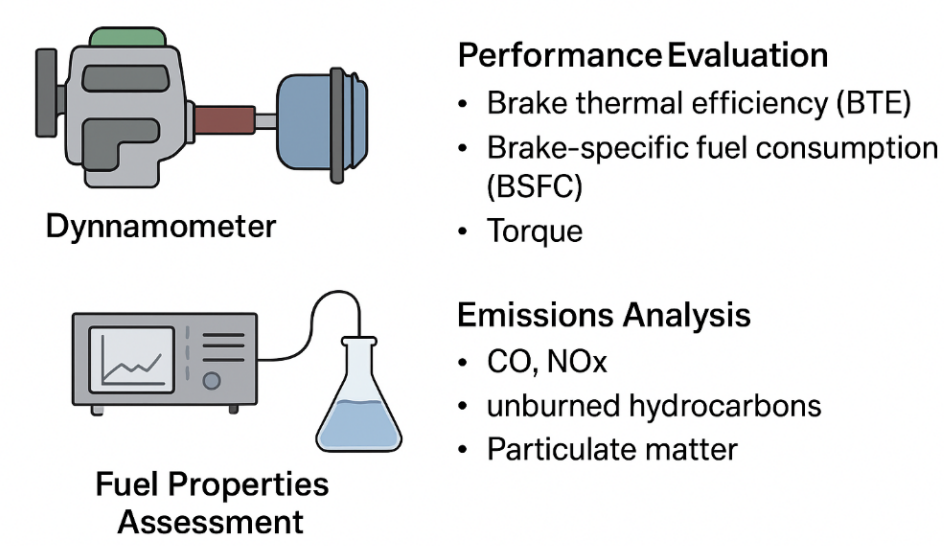

Figure 21. Test Parameters and Measurement Techniques

3.7. Data Analysis and Validation

The experimental results were systematically analyzed and compared with the CFD simulation outputs to assess the reliability and predictive capability of the computational model. This comparison included evaluating trends in combustion behavior, fuel consumption, ignition delay, in-cylinder pressure development, and emission characteristics across different gasoline–diesel blend ratios. To quantify the level of agreement between the numerical predictions and the measured data, statistical evaluation methods were employed, including regression analysis, error metrics, and correlation coefficients. These methods enabled a detailed assessment of how accurately the simulation captured real engine behavior under varying operating conditions.

Based on the discrepancies identified during the comparison phase, several calibration adjustments were performed on the numerical model. Key parameters such as fuel injection pressure, timing, and recirculation rates have been improved to increase the accuracy of combustion and emissions predictions. These adjustments not only enhanced the fidelity of the CFD model but also provided valuable insights into optimal operational settings for engines running with gasoline–diesel blends.

The validation process ensured that the computational framework can reliably predict combustion performance, enabling its use as a supportive tool for further optimization studies. Overall, the combined experimental and numerical analyses strengthened the robustness of the study by demonstrating strong agreement between predicted outcomes and real-world engine behavior.

Table 4. Dynamometer specifications.

Category	Details
Motor Type	Liquid-cooled, three-phase asynchronous electric motor
Continuous Power Output	60 kW rated power capacity
Nominal Torque	180 Nm under standard operating conditions
Maximum Operating Speed	Up to 7950 revolutions per minute
Speed Measurement Resolution	Incremental encoder with 500-line resolution (1000-line option depending on model)
Cooling Configuration	Closed-loop cooling using a water–glycol mixture (up to 50% glycol)
Maximum Coolant Temperature	45 °C allowable coolant outlet temperature
Required Coolant Flow	Motor dynamometer: 5 L/min; inverter cabinet: 5 L/min
Overload Capability	Designed to withstand high overload conditions
Bearing Design	Robust heavy-duty bearings requiring minimal maintenance
Control Method	High-performance speed regulation with servo-like response characteristics
Electrical Supply Requirements	3-phase 400 VAC power input with protective earth (PE)
Total Power Consumption	Approximately 110 kVA including AVL 577 systems

The boosting simulation unit is designed to artificially reproduce various boost conditions, allowing the engine to be evaluated under controlled intake and exhaust pressure environments. To achieve this, the system incorporates an electrically actuated exhaust backpressure valve that provides precise and rapid adjustment of exhaust-side pressure levels throughout testing. The unit is capable of generating boost pressures up to the maximum exhaust gas pressure permitted by the engine's test configuration, ensuring that a wide range of operating scenarios can be replicated. An adjustable backpressure chamber further enhances the system by enabling detailed simulation of different exhaust flow and pressure states, allowing researchers to study how the engine responds to changing boundary conditions. The boosting simulation equipment is fully compatible with AVL single-cylinder research engines and integrates seamlessly with laboratory instrumentation. This setup supports investigations of both turbocharged and naturally aspirated operating modes, enabling accurate replication of real-world boosting effects for performance, combustion, and emissions analysis.

3.8. Machine Learning Methodology

Machine learning algorithms and rapid optimization are used in engine design and optimization of parameters. This process includes these steps:

Data collection: Collecting data on the effects of engine components and parameters is important for training machine learning models. This can be accomplished through experimental testing and simulations.

Machine learning model training: Using collected data, machine learning models are trained to predict engine parameters and performance. These models can be implemented using supervised learning techniques (eg, regression, classification).

Applying rapid optimization technique: Using the machine learning model, it is possible to quickly search and find the most suitable parameter combinations to optimize the performance of the engine. This can be done using methods such as genetic algorithms, particle swarm optimization or gradient descent.

The optimum parameter combinations found should be verified by testing on real engines and/or in more detailed simulations. This step allows to evaluate how effective the optimized design is in real-world conditions.

Refinement and re-optimization: According to the validation results, the optimized engine design can be further developed and the process started again. In this way, further performance increase and emission reduction can be achieved.

In summary, examining the effects of nanostructured fuel droplets on engine performance with machine learning models and fast optimization techniques can yield better results in the field of engine design. This process contributes to optimizing engine components and parameters, thereby increasing the overall performance of the engine and reducing emissions. These methods can be used to speed up engine design and development processes and create more sustainable, energy efficient engines.

3.9. Machine Learning Approach

Investigating the effects of nanostructured fuel droplets in diesel engines using a machine learning approach and rapid optimization techniques involves a multidisciplinary approach combining expertise in combustion, fluid dynamics, nanotechnology, and machine learning. In this approach, a machine learning model was obtained using the data obtained from the CFD simulation. Below are the steps to generate data for machine learning model training.

In Machine Learning Model Training, 80 percent of the data obtained from the simulation was used for training and 20 percent for testing. In this study, comparison was made using linear model, random forest, ridge regression, k-nearest neighbor algorithms.

Boosted Decision Tree Regression (BDT) is a machine learning algorithm. It combines the techniques of decision trees to create a robust prediction model for regression.

Decision Trees: Decision trees are models used for both classification and regression. They separate the input space by its values and predict the output variable for each region.

Boosting: A learning technique in which multiple weak learners are combined to create a strong algorithm. Boosting algorithms operate sequentially, with each model focusing on the problems and challenges of the previous model.

Boosted Decision Tree Regression works by adding data sequentially. The purpose of the trees is to correct for errors in the previous data, allowing subsequent trees to examine difficult-to-predict data. Weighted Voting: When making predictions, each decision tree in the ensemble contributes to the final prediction, but their contributions are weighted according to their performance on the training data. Trees that perform well have a higher weight, meaning their predictions have a greater impact on the final output.

Training Process: The training process of Boosted Decision Tree Regression involves iteratively adding decision trees to the ensemble. At each iteration, a new tree is trained to predict the residuals (differences between the actual and predicted values) from previous trees. The predictions from all trees are then combined to obtain the final prediction.

Regularization: Various regularization techniques can be applied during the training process to prevent overfitting. These may include limiting the depth of each decision tree, adding a penalty term to the loss function, or early stopping.

Overall, Boosted Decision Tree Regression is a powerful algorithm that can capture complex nonlinear relationships in data while reducing overfitting through ensemble learning and regularization techniques. It is widely used in various regression tasks where accurate predictions are required, such as finance, healthcare, and marketing.

Decision Forest Regression, is a regression method where multiple decision trees are used. It can produce better predictions than a single decision tree.

Decision Trees: It is a learning algorithm used for classification and regression. It divides the dataset into smaller units based on the properties of the input parameters. It makes predictions about the variable.

Ensemble Learning: Decision Forest Regression uses ensemble learning to combine multiple models to create a more robust model. Instead of just one decision tree, multiple decision trees are used.

Randomization: Decision Forest Regression creates a generalizable regression model by randomly generating each tree in the training process. This helps reduce overfitting and improve generalization performance.

Bagging (Bootstrap Aggregating): Many decision trees are trained using randomly selected data from the training data. This random sampling allows for a more general model to be obtained.

Voting: During prediction, each decision tree in the forest makes a prediction, and the final output is determined by aggregating the predictions of all trees. For regression tasks, the predictions of individual trees are typically averaged to obtain the final prediction.

Benefits: Decision Forest Regression offers several benefits, including: Robustness to noisy data and outliers. Automatic feature selection, as some features may not be considered at certain split points. Good performance without requiring extensive hyperparameter tuning. Interpretability, as decision trees are inherently interpretable, and insights can be gained by examining the structure of the trees in the forest.

Decision Forest Regression is commonly used in various regression tasks, including prediction of housing prices, stock prices, and demand forecasting. It is known for its simplicity, scalability, and ability to handle high-dimensional datasets with nonlinear relationships.

Linear regression is a statistical method used to model the relationship between a dependent variable (also called the target or response variable) and one or more independent variables (also called predictors or features). It is one of the simplest and most widely used techniques for predictive modeling and statistical inference.

Linear regression is widely used in various fields, including economics, finance, social sciences, engineering, and machine learning, due to its simplicity, interpretability, and effectiveness for modeling linear relationships in data.

Neural network is a model based on the functioning of biological neurons in the human brain. It encompasses various machine learning algorithms, including classification, regression, clustering, and pattern recognition.

Neural networks are composed of layers, each connected to another, called neurons. A neural network typically has three layers:

Input Layer: This layer is the input data neuron. Each neuron retains a characteristic of the input data.

Hidden Layers: These are located between the input and output layers. Each neuron in the hidden layer receives information from neurons in the previous layer and transmits it to neurons in the next layer.

Output Layer: This layer is the neuron that produces the network's output. The number of neurons in the output layer depends on the characteristics and size of the neural network. For example, binary classification has one neuron in the output layer, while multi-class classification may have multiple neurons.

Neural networks have gained popularity in recent years due to their flexibility in modeling complex learning from large amounts of data, their performance in various data types, and their performance in various tasks such as image processing.

Poisson regression is a statistical method used for modeling count data, where the outcome variable represents the number of occurrences of an event in a fixed interval of time or space.

It is commonly used when the outcome variable follows a Poisson distribution, which is characterized by non-negative integer values and a mean that equals its variance.

Poisson regression finds applications in various fields, including epidemiology, public health, ecology, criminology, and economics, where count data are frequently encountered and the goal is to understand the factors that influence the occurrence of events.

Machine Learning Prediction Validation, To assess the performance of a machine learning model, various metrics are used to quantify the error between predicted and actual values. These metrics help evaluate how well the model generalizes to unseen data. The primary metrics discussed include:

3.9.1. R-Square (R^2) / Adjusted R-Square

- **R-Square (R^2):**
  R^2 measures the proportion of variability in the dependent variable that can be explained by the independent variables in the model. It essentially reflects how well the model fits the data. While a high R^2 value indicates a good fit, it does not address the issue of overfitting. When a regression model includes too many independent variables, it may perform well on the training data but fail to generalize to test data.
- **Adjusted R-Square:**
  To mitigate overfitting, Adjusted R^2 is used. Unlike R^2, Adjusted R^2 penalizes the addition of unnecessary variables, providing a more reliable measure when comparing models with different numbers of predictors.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}(\hat{\tau}_i - \tau_i)^2}{N}}$$

Figure 22. RMSE

3.9.2. Mean Squared Error (MSE) / Root Mean Squared Error (RMSE)

- **Mean Squared Error (MSE):**
  MSE calculates the average of the squared differences between predicted and actual values. It provides a numerical representation of the model's prediction error. Although MSE is useful for comparing models, its magnitude can sometimes make interpretation difficult.
- **Root Mean Squared Error (RMSE):**
  RMSE, the square root of MSE, is a more interpretable metric as it expresses the error in the same units as the dependent variable. It is frequently preferred over MSE, particularly when MSE values are excessively large, as RMSE facilitates easier comparison and interpretation.

In this study, RMSE was selected as the primary metric for evaluating model performance.

3.9.3. Mean Absolute Error (MAE)

- MAE computes the average of the absolute differences between predicted and actual values. As it does not involve squaring errors, MAE is less sensitive to outliers compared to MSE, offering a straightforward measure of prediction accuracy.

$$\mathrm{MAE} = \frac{1}{n} \sum_{i=1}^{n} | x_i - x |$$

Figure 23. MAE

These metrics serve complementary purposes. While R^2 and Adjusted R^2 evaluate how much of the variability in the dependent variable is explained by the model, MSE, RMSE, and MAE focus on quantifying the model's prediction errors. The choice of metric depends on the specific requirements of the problem. In this study, RMSE was chosen for its balance between interpretability and effective model comparison.

All machine learning algorithms used in this study were implemented within Microsoft Azure Machine Learning Studio. This platform allows for simplified job analysis for simulation and rapid evaluation. Azure's modular interface and cloud-based computational resources allowed algorithms such as Boosted Decision Trees, Random Forest Regression, Linear Regression, K-Nearest Neighbors, Ridge Regression, and Neural Networks to be trained and tested efficiently using the same dataset. The integrated evaluation tools in Azure ML Studio also facilitated the generation of performance metrics and error visualizations, ensuring a consistent and reproducible model development process.

4. Results and Discussion

In this study, CFD simulations were performed for a heavy-duty engine operating under medium load conditions with a low-octane gasoline-like fuel. The simulation results are shown graphically below according to the input parameters. These simulation results were then used in machine learning algorithms. 80 percent of the data is reserved for training and the remaining 20 percent for prediction. 5 different machine learning models were used for the machine learning approach. Among these approaches, Decision Regression and Neural network algorithms contributed to the overall prediction. The selection of models according to their individual contributions, that is, the importance of these models in the training model, was made by taking into account the root mean square error (RMSE).

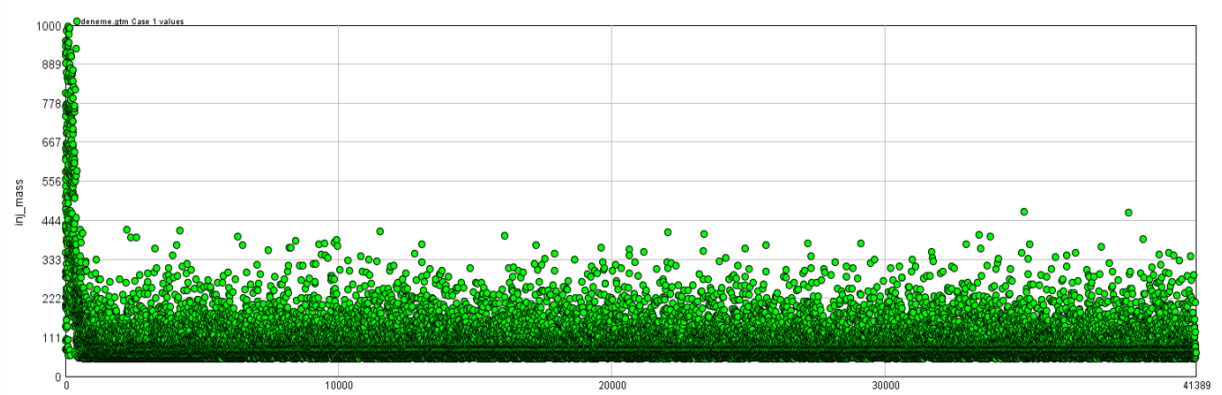

Figure 24. inj_mass/case

This figüre 24 illustrates the distribution of injected fuel mass across all simulation cases. The data show a dense clustering of values near the lower mass range, indicating that most cases involve small injection quantities, while higher injection masses occur sporadically. This variability captures a wide operational range for the training dataset.

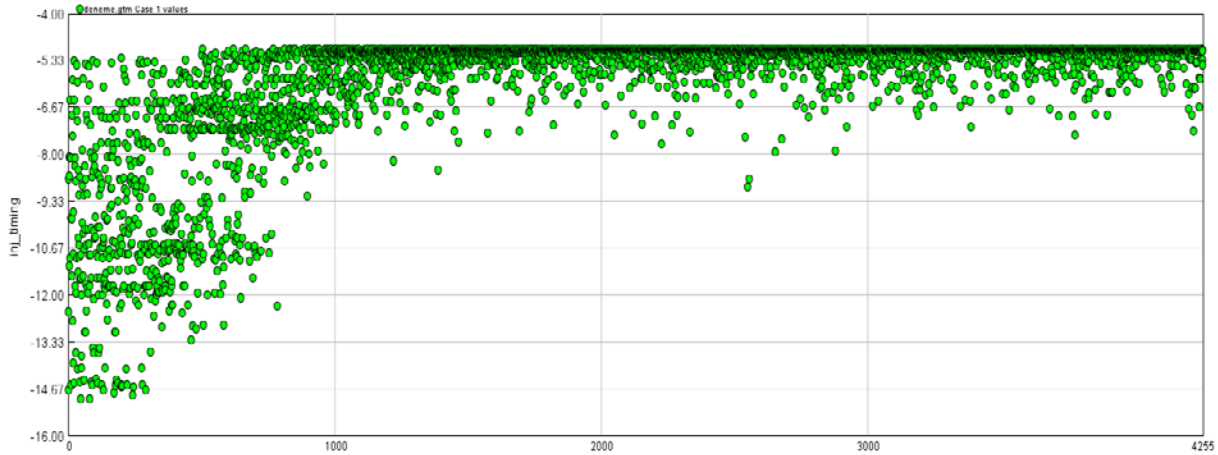

Figure 25. inj_timing/case

The figüre 25 represents the injection timing variations for each simulation case. Most data points cluster between −4° and −6° crank angle, signifying the dominant injection phase, while fewer cases exhibit earlier or later timings. This ensures that the model captures realistic injection phasing patterns relevant to combustion initiation.

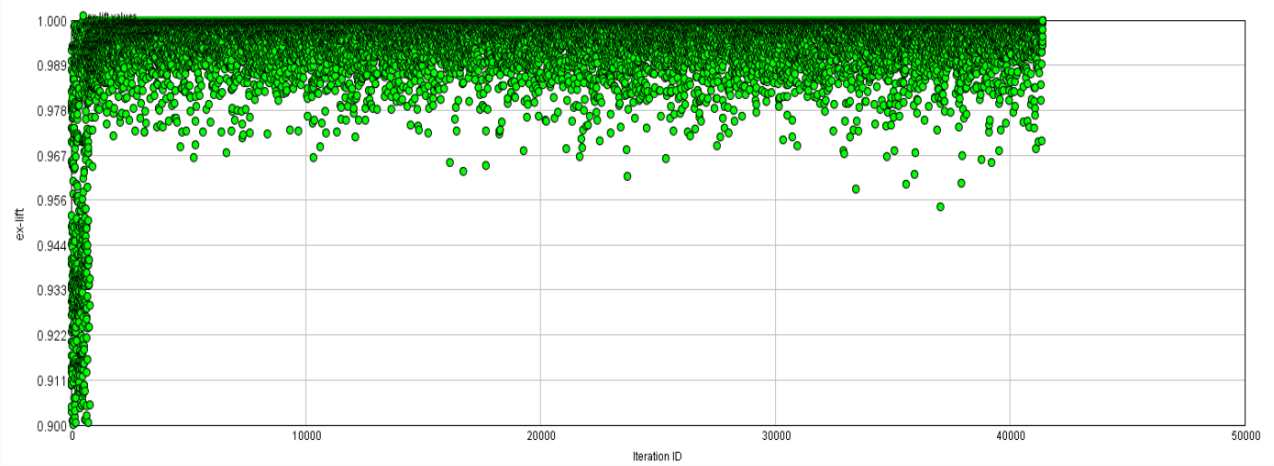

Figure 26. ex_lift/case.

This figüre 26 displays the exhaust valve lift values across all iterations. The majority of the data are concentrated near the maximum lift value (~1.0 mm), with limited fluctuation. This indicates consistent exhaust valve operation, crucial for maintaining stable exhaust flow and efficient gas exchange modeling.

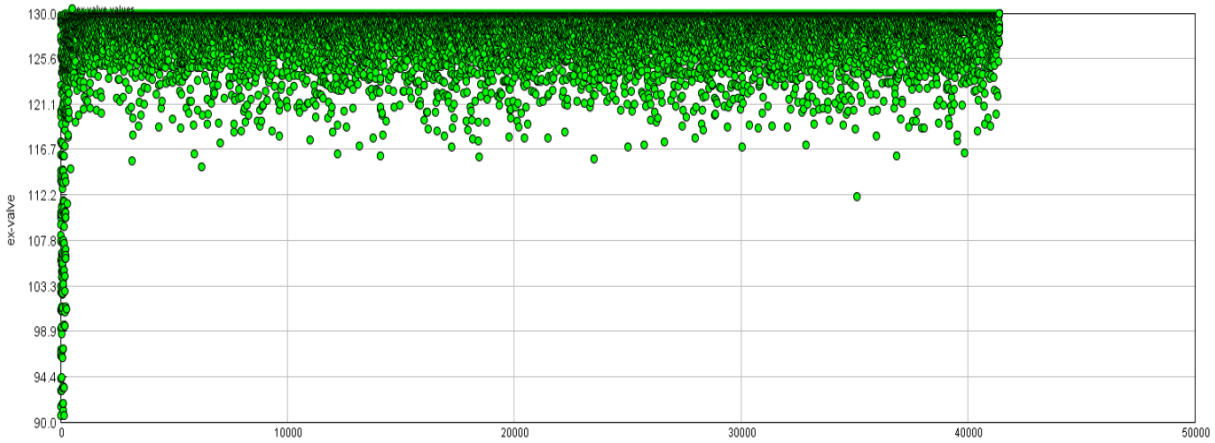

Figure 27. ex_valve/case.

The figüre 27 shows the exhaust valve opening timing distribution. Values are densely populated between 115° and 130° crank angle, corresponding to the standard exhaust valve phase. Minor variations across the dataset introduce diversity, allowing the learning model to generalize valve event effects on engine output.

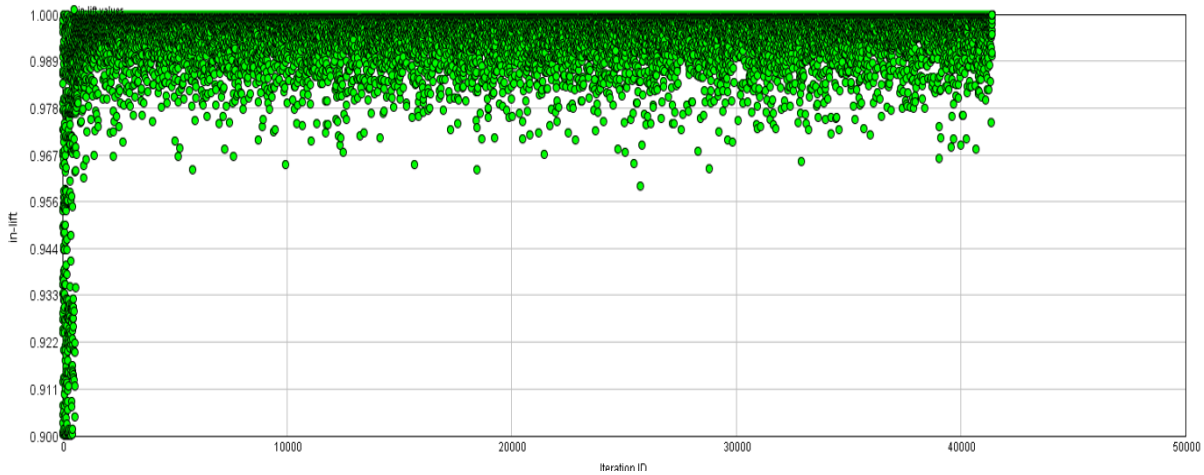

Figure 28. in_lift/case.

This plot figüre 28 illustrates the intake valve lift data distribution. Similar to the exhaust lift, values cluster near the upper limit, around 1.0 mm, with small variations. This consistent pattern reflects controlled intake valve behavior, contributing to steady air induction dynamics in the simulation dataset.

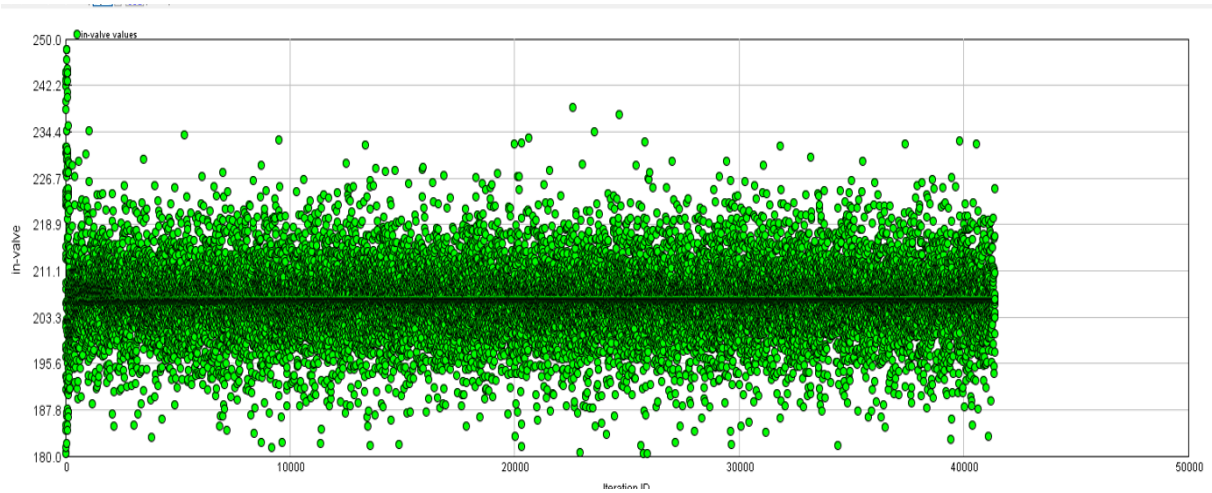

Figure 29. in_valve/case.

This figüre 29 depicts intake valve timing across all cases. The data are symmetrically distributed around approximately 210° crank angle, suggesting that the majority of simulations operate within a standard intake phase. The moderate spread ensures adequate representation of timing effects on volumetric efficiency.

Figures also have simulation images. Figure 25 shows the fuel injection and status graph. Figure 26 shows the time for each simulation when the fuel starts to eject. Figure 27 shows the opening

range graph of the outlet valves. Figure 28 shows the opening times of the outlet valves. Figure 29 has the opening range of the inlet valves. In Figure 12, there is a graph showing the opening times of the inlet valves. The simulations were made on a computer with an Intel Core i7-7500U 2.7 Ghz processor and 12 GB of ram. In these simulations, an iteration takes days or even months.

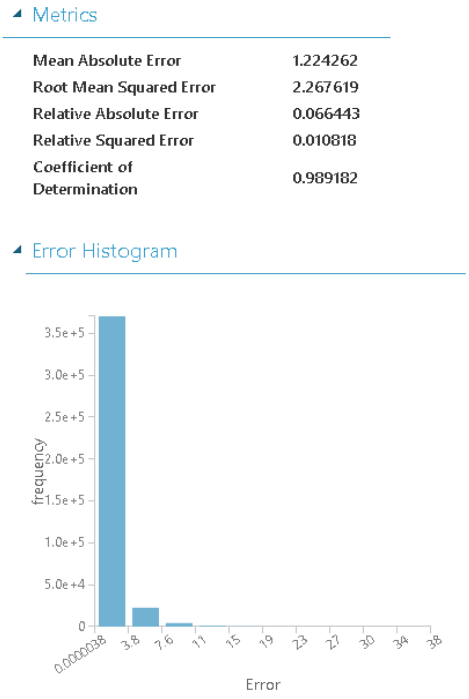

Figure 30. Boosted Decision Tree Regression NOx Prediction Metrics and Error Distribution

This figüre 30 presents the performance evaluation of the Boosted Decision Tree Regression model used to predict NOx emissions. The Metrics panel summarizes several key error indicators. The low Mean Absolute Error (1.224), low Relative Squared Error (0.0108), and a very high Coefficient of Determination (R^2 = 0.989) demonstrate that the model captures the nonlinear behavior of NOx formation with high accuracy. The RMSE value (2.2676) further confirms that the prediction deviations remain small across the test dataset.

The Error Histogram shows the distribution of prediction errors. The histogram shows that the error values are concentrated near zero, indicating that the model is producing accurate predictions. Only a few results fall into the higher error ranges, indicating biases resulting from extreme or less frequent operating conditions in the dataset.

Overall, the results indicate that the Boosted Decision Tree Regression algorithm provides robust and reliable predictions for NOx emissions, making it a suitable method for modeling complex combustion-related outputs.

Metrics

Mean Absolute Error	2.00952
Root Mean Squared Error	3.170192
Relative Absolute Error	0.10906
Relative Squared Error	0.021144
Coefficient of Determination	0.978856

Error Histogram

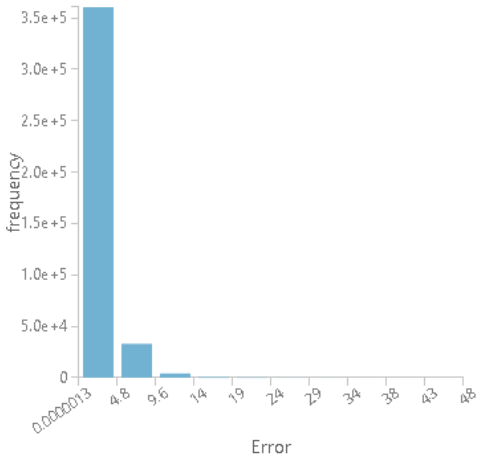

Figure 31. Linear Regresion NOx Prediction Metrics and Error Distribution

This figüre 31 presents the performance metrics and error histogram for the Linear Regression model used to predict NOx emissions. The Metrics section shows that the model achieves moderate predictive accuracy: the Mean Absolute Error and Root Mean Squared Error values indicate that the model can capture general trends in NOx formation but with higher error levels compared to nonlinear machine-learning algorithms. The relatively higher Relative Absolute Error and Relative Squared Error suggest that Linear Regression struggles to fully represent the nonlinear combustion dynamics that influence NOx production. Despite this, the Coefficient of Determination (R^2) remains reasonably high, indicating that the model still explains a significant portion of the variance in the dataset.

The Error Histogram illustrates that most prediction errors are concentrated near the lower range, meaning that the model performs adequately for a large subset of the data. However, the wider spread of error values and the presence of larger deviations compared to more advanced models highlight the limitations of Linear Regression in capturing complex relationships. These deviations are likely due to nonlinear interactions between injection parameters, temperature, fuel blend properties, and NOx formation mechanisms.

Overall, the results show that while Linear Regression provides a simple and interpretable baseline model for NOx prediction, its performance is inferior to ensemble-based approaches such as other algorithms, which better capture the underlying nonlinearities of the combustion process.

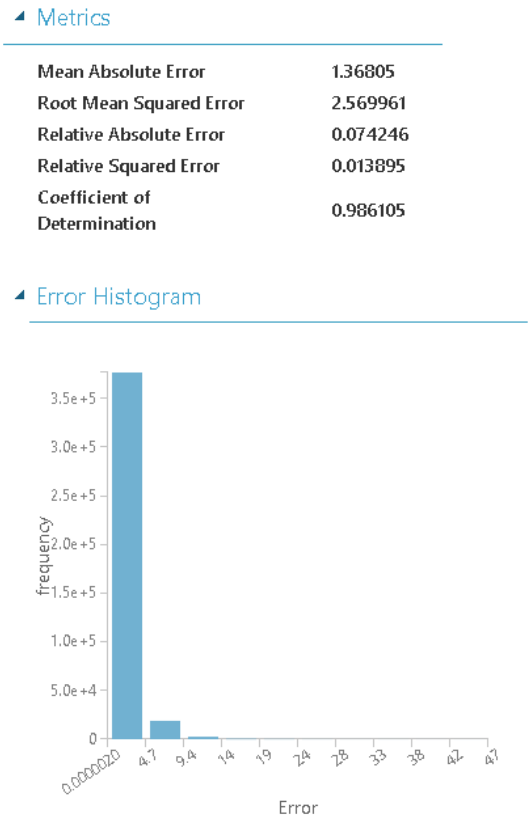

Figure 32. Neural Network NOx Prediction Metrics and Error Distribution

This figüre 32 illustrates the performance evaluation and error distribution of the Neural Network model applied to NOx emission prediction. The Metrics section demonstrates that the model achieves strong predictive accuracy, with a relatively low MAE (1.368) and RMSE (2.569). These results indicate that the Neural Network effectively captures the complex and nonlinear relationships that govern NOx formation during combustion. The low Relative Absolute Error and Relative Squared Error further confirm the model's ability to generalize well across the dataset.

The Error Histogram shows that the majority of prediction errors are concentrated near zero, indicating high consistency and accuracy of the model across most samples. Only a small fraction of data points exhibit higher error magnitudes, which is expected in real-world engine data where extreme or irregular operating conditions may occur. The narrow error distribution highlights the Neural Network's strength in modeling nonlinear combustion phenomena and fuel–air interaction effects that strongly influence NOx emissions.

Metrics

Mean Absolute Error	3.3131
Root Mean Squared Error	5.059807
Relative Absolute Error	0.179807
Relative Squared Error	0.053861
Coefficient of Determination	0.946139

Error Histogram

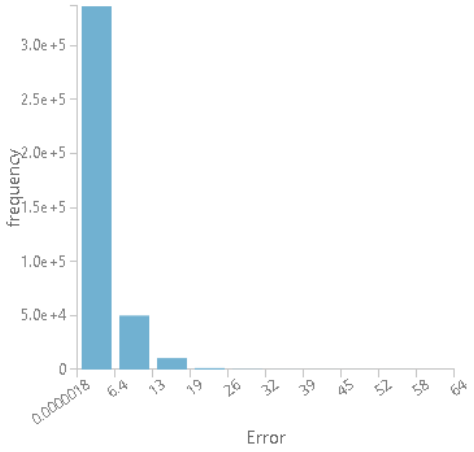

Figure 33. Poison Regression NOx Prediction Metrics and Error Distribution

The figüre 33 presents the performance metrics and error distribution of the Poisson Regression model for NOx prediction, showing noticeably lower accuracy compared to the other machine-learning algorithms used in this study. The relatively high RMSE value (5.06) and the larger Mean Absolute Error indicate that the model produces greater deviations from the actual NOx values, reflecting its limited ability to capture the nonlinear combustion behavior present in the dataset. Although the R^2 value (0.946) suggests a reasonable overall fit, the error histogram reveals a wider spread of errors and more frequent large deviations, demonstrating that Poisson Regression struggles particularly under extreme or less common operating conditions. Overall, the results show that Poisson Regression is less effective and less practical than the more advanced models such as Boosted Decision Trees and Neural Networks for accurately predicting NOx emissions.

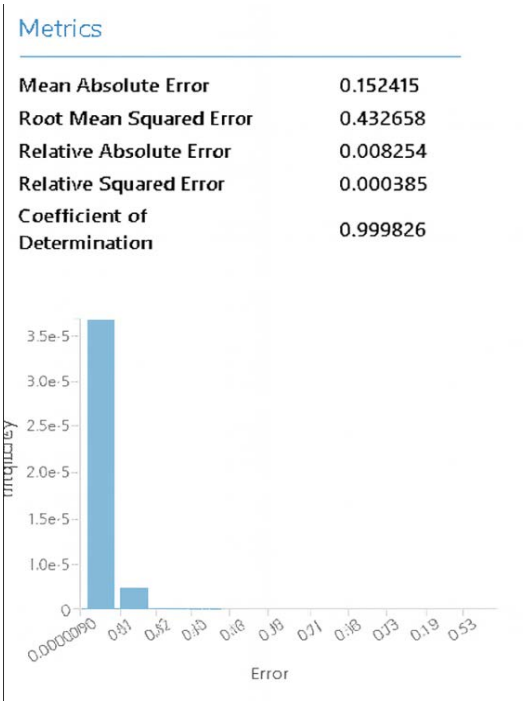

Figure 34. Decision Forest Regression NOx Prediction Metrics and Error Distribution

The figüre 34 presents the performance metrics and error distribution of the Decision Forest Regression model used for NOx prediction, showing that the algorithm achieves exceptionally high accuracy. The very low Mean Absolute Error (0.1524) and Root Mean Squared Error (0.4327) indicate that the model's predictions are extremely close to the actual NOx values, with minimal deviation across the dataset. The Relative Absolute Error (0.00825) and Relative Squared Error (0.000385) are also remarkably small, demonstrating the model's strong ability to capture the nonlinear combustion characteristics influencing NOx formation. The Coefficient of Determination ($R^2 = 0.9998$) further confirms that the model explains almost all the variance in the target data. The error histogram shows that nearly all predictions fall within a very narrow error range, with only a negligible number of larger deviations. Overall, these results indicate that the Decision Forest Regression algorithm is one of the most reliable and high-performing models in the study, providing highly precise and consistent NOx predictions.

Among the five machine-learning algorithms applied for NOx prediction, Decision Forest Regression and Boosted Decision Tree Regression delivered the best overall performance, achieving extremely low error values and high R^2 scores, demonstrating their strong capability to model the nonlinear combustion processes influencing NOx formation. The Neural Network model also performed at a high level, providing similarly low MAE and RMSE values and successfully capturing complex parameter interactions, though slightly less consistent than the ensemble-based methods. Linear Regression showed moderate performance, adequately capturing general NOx trends but failing to represent nonlinear effects, resulting in higher prediction errors and reduced accuracy compared with the top-performing models. Poisson Regression exhibited the weakest predictive capability among the tested algorithms, with noticeably higher RMSE and MAE values and a wider error distribution, confirming that its statistical structure is not well suited for continuous, nonlinear NOx emission data. Overall, the

results clearly indicate that ensemble-based models—particularly Decision Forest and Boosted Decision Tree Regression—are the most reliable and effective approaches for accurate NOx prediction in this study.

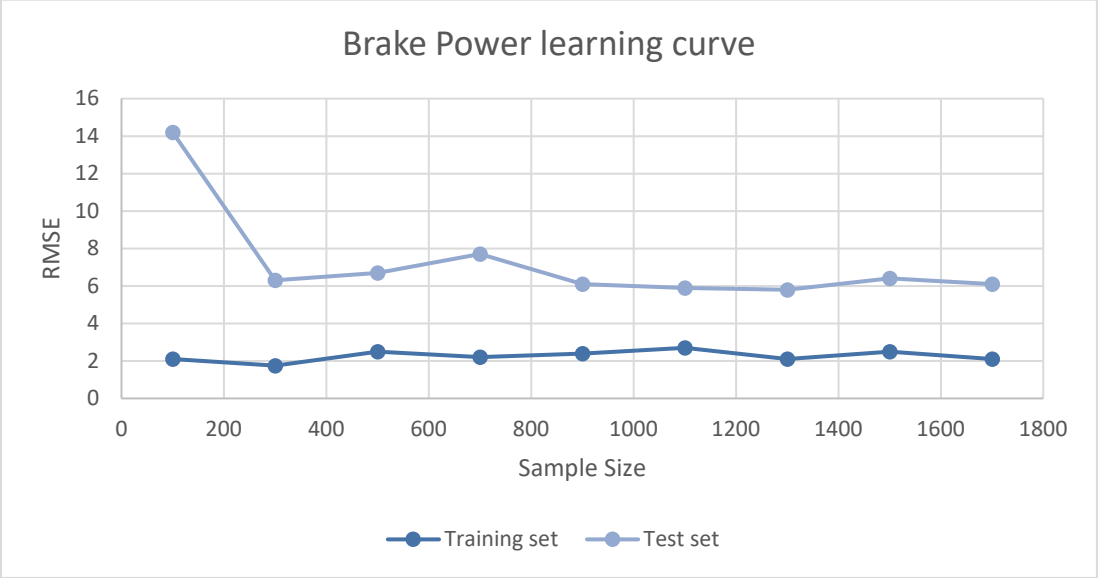

Figure 35. Learning curve of Break Power in Machine Learnings Algorithms.

This figüre 35 presents the learning curve for brake power prediction, illustrating the variation of RMSE with increasing sample size. The training set exhibits consistently low RMSE values, indicating effective model fitting, while the test set initially shows high error due to limited data and gradually stabilizes as the sample size increases. The convergence of both curves at larger sample sizes demonstrates improved generalization and reduced overfitting, confirming that the model effectively learns from the simulation data as more training samples are introduced.

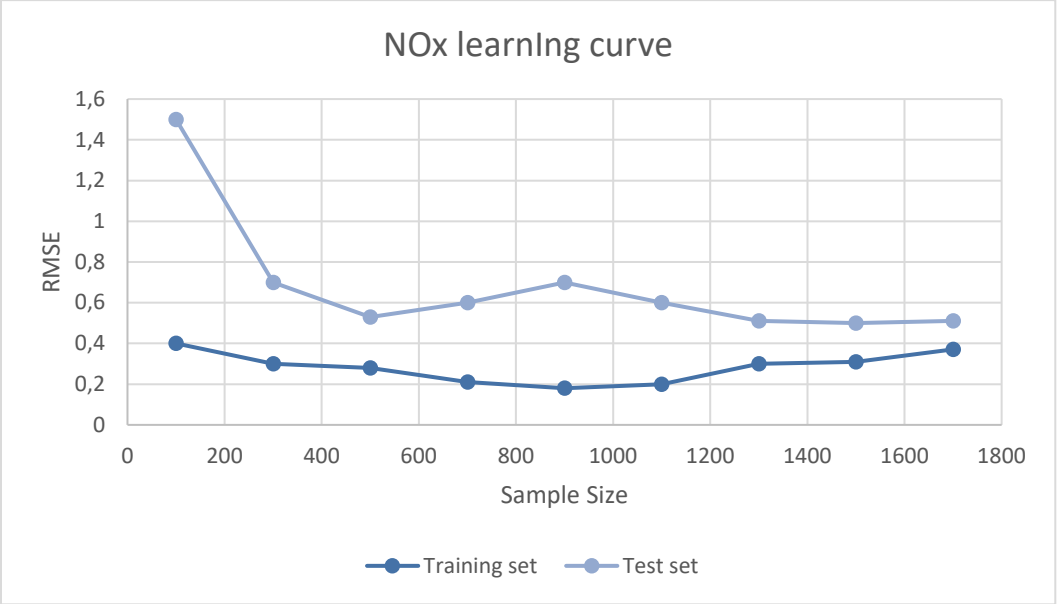

Figure 36. Learning curve of NOx in Machine Learnings Algorithms.

This figüre 36 illustrates the learning behavior of the model in predicting NOx emissions, showing RMSE values for both training and test sets as the sample size increases. Initially, the test set exhibits high RMSE, reflecting instability due to limited data. As the sample size grows, both training and test errors decrease and stabilize, indicating improved model generalization. The relatively small gap between the two curves at larger sample sizes demonstrates that the model effectively captures the underlying emission patterns without significant overfitting, ensuring reliable predictive performance.

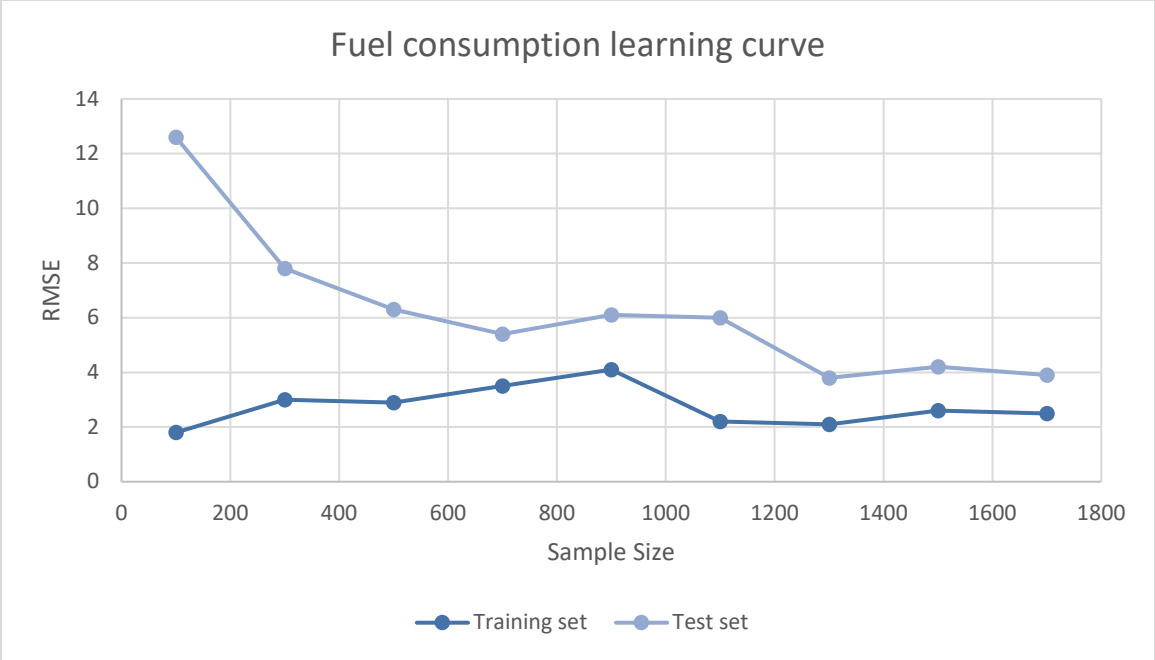

Figure 37. Learning curve of Fuel Consumption in Machine Learnings Algorithms.

This figure 37 depicts the learning curve for fuel consumption prediction, presenting RMSE trends for both training and test datasets. Initially, the test set shows high error values due to insufficient training data, but as the sample size increases, RMSE values for both sets gradually decrease and converge. This behavior indicates that the model improves its learning efficiency with more data and achieves stable predictive accuracy. The narrowing gap between training and test errors suggests minimal overfitting and reliable generalization performance in estimating fuel consumption.

Table 5. The performance of employed models on the test dataset.

	NOx		**Brake Power**		**Fuel Consumption**	
Algorithm	**RMSE**	**MAE**	**RMSE**	**MAE**	**RMSE**	**MAE**
Boosted Decision Tree Regression	2,26	1,22	9,41	7,42	5,74	4,68
Decision Forest Regression	0,43	0,15	6,04	4,68	4,15	2,57
Linear Regression	3,17	2,00	12,45	11,78	8,98	8,14
Neural Network	2,56	1,36	9,87	8,67	6,74	5,74
Poison Regression	5,05	3,31	13,45	11,98	10,87	10,45

Table 5 and Figure 38 collectively present a comprehensive comparison of the predictive performance of the five machine learning algorithms applied to estimate NOx emissions, brake power, and fuel consumption based on the simulation dataset. The evaluation is carried out using two widely accepted error metrics—Root Mean Square Error (RMSE) and Mean Absolute Error (MAE)—which quantify the magnitude of prediction errors. Lower values of these metrics indicate better alignment between predicted and simulated outputs.

Across all three target variables, Decision Forest Regression stands out as the most accurate and stable algorithm, achieving the lowest RMSE and MAE values for NOx (0.43 and 0.15), as well as consistently outperforming the other models in brake power and fuel consumption predictions. This superior performance highlights the algorithm's ability to capture nonlinear interactions and complex parameter relationships inherent in combustion and engine operation.

The Boosted Decision Tree Regression model also performs strongly, yielding relatively low error values that indicate reliable prediction capability, particularly for NOx estimation. Although its performance does not surpass the Decision Forest model, it remains significantly more accurate than the conventional regression and probabilistic approaches.

Linear Regression and Neural Network models show moderate predictive accuracy. While they can follow general trends within the data, their higher error metrics reveal limitations in capturing the nonlinearity and variability present in engine behavior. The neural network performs better than linear regression, but still falls short of the ensemble-based models.

Finally, Poisson Regression demonstrates the weakest predictive performance across all output variables, showing the highest RMSE and MAE values. This indicates that the algorithm is not well suited for continuous engine-related datasets, which do not conform to the statistical assumptions of Poisson-distributed outputs.

Overall, the results clearly confirm that ensemble learning approaches—specifically Decision Forest Regression and Boosted Decision Tree Regression—provide the most accurate and reliable predictions for engine performance and emissions modeling. These findings support the use of advanced tree-based ensemble methods when dealing with complex combustion phenomena and multidimensional simulation data.

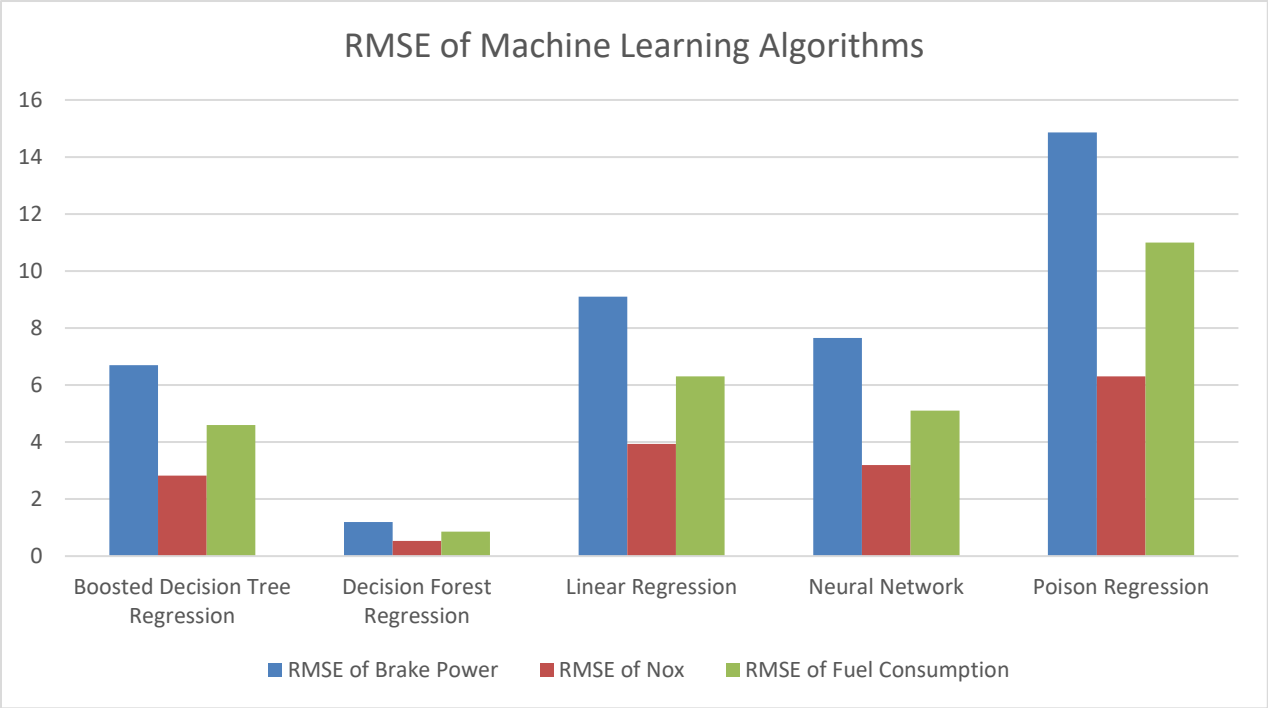

Figure 38. RMSE of Machine Learning Algorithms.

Figure 38 compares the RMSE values of different machine learning algorithms for predicting brake power, NOx emissions, and fuel consumption. Among the evaluated models, Decision Forest Regression demonstrates the lowest prediction errors across all output parameters, indicating the highest overall accuracy. Neural Network and Boosted Decision Tree Regression also provide competitive performance, particularly for NOx prediction. In contrast, Linear Regression and Poisson Regression exhibit higher RMSE values, reflecting their limited ability to capture the nonlinear relationships inherent in engine performance and emission data.

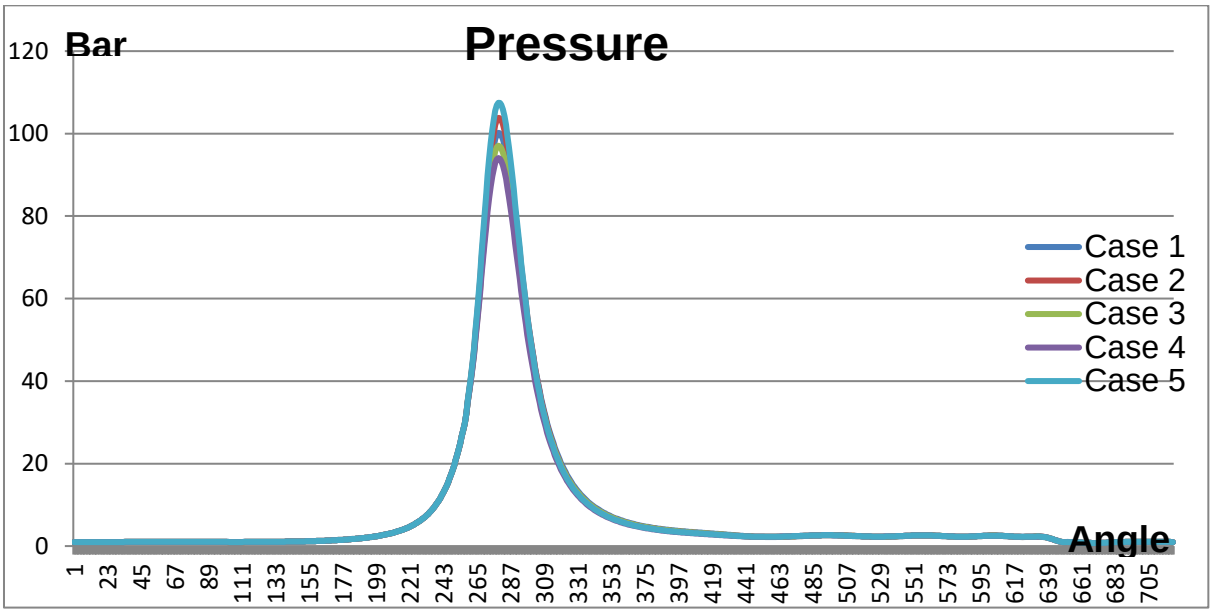

Figure 39. The graph illustrates the variation of incylinder pressure with crank angle in the observed data.

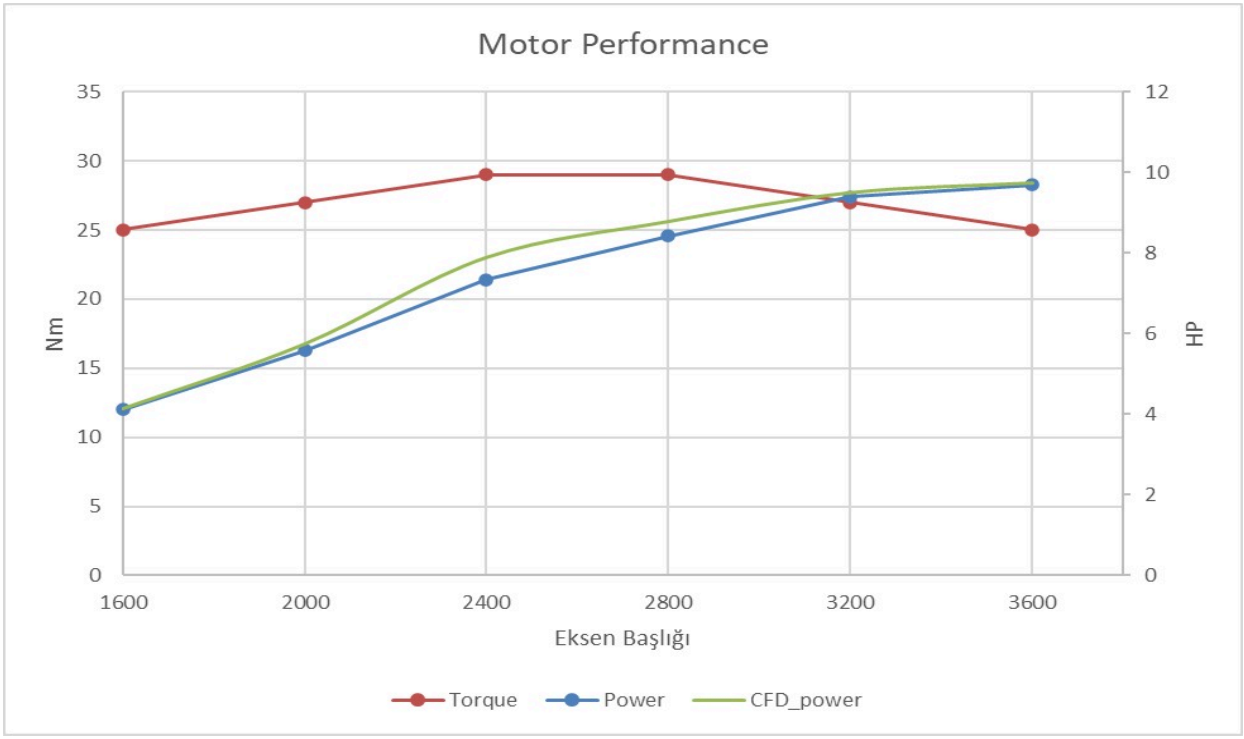

Figure 40. Engine performance verification dynamometer and CFD results.

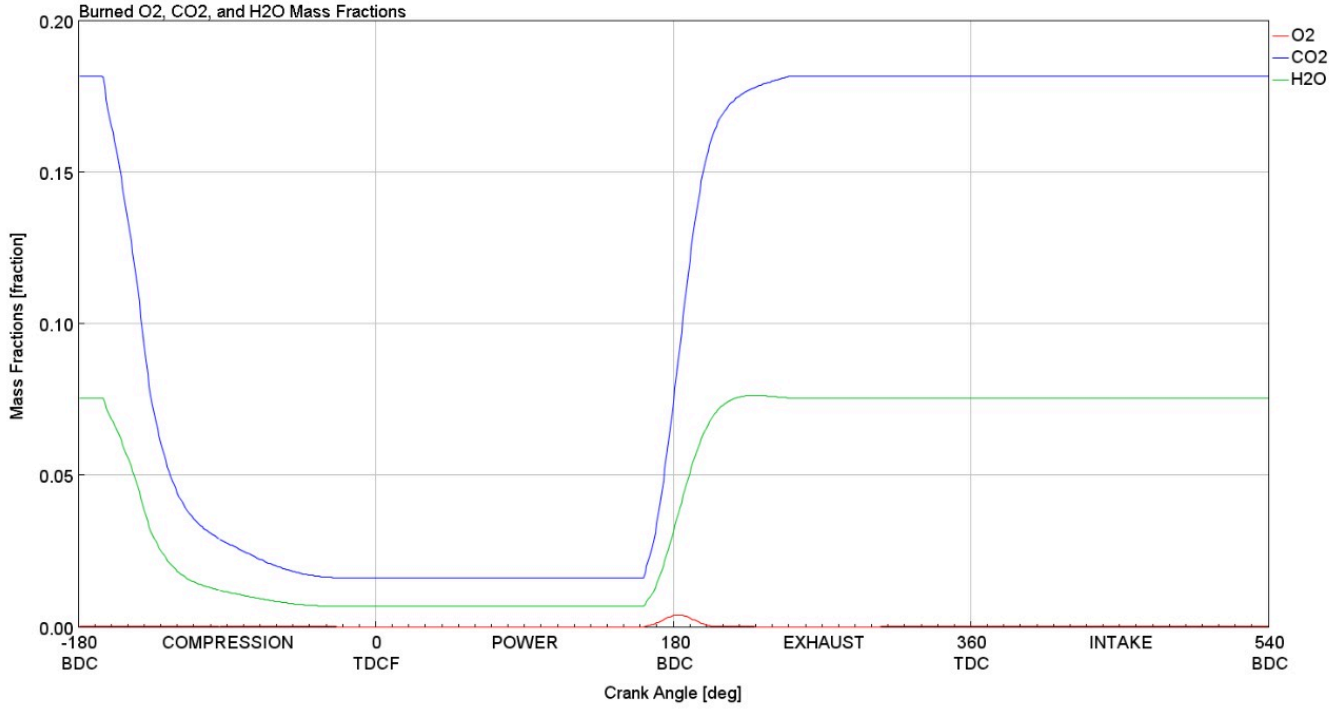

Figure 41. The graph depicts the variations in mass fractions of O2, CO2, and H2O as a function of crank angle during the existing engine cycle.

Figure 39 illustrates the in-cylinder pressure variation with respect to the crank angle for five different cases. All cases display a similar trend, characterized by a sharp pressure peak near

the top dead center (around 270°), corresponding to the combustion phase. The pressure rapidly rises during compression and decreases sharply after expansion, indicating consistent combustion behavior across cases.

Figure 40 presents the comparison of torque, experimental power, and CFD-predicted power across various engine speeds. The torque increases until approximately 2800 rpm and then slightly decreases, which is typical for internal combustion engines. Both experimental and CFD power curves show a similar upward trend with increasing engine speed, confirming that the CFD model effectively captures the engine's performance characteristics.

This figüre 41 shows the changes in the mass fractions of oxygen (O_2), carbon dioxide (CO_2), and water (H_2O) throughout the engine cycle. During the combustion phase, the O_2 fraction decreases rapidly as it is consumed, while CO_2 and H_2O fractions increase due to fuel oxidation. These variations indicate effective combustion and validate the chemical reaction behavior within the simulation.

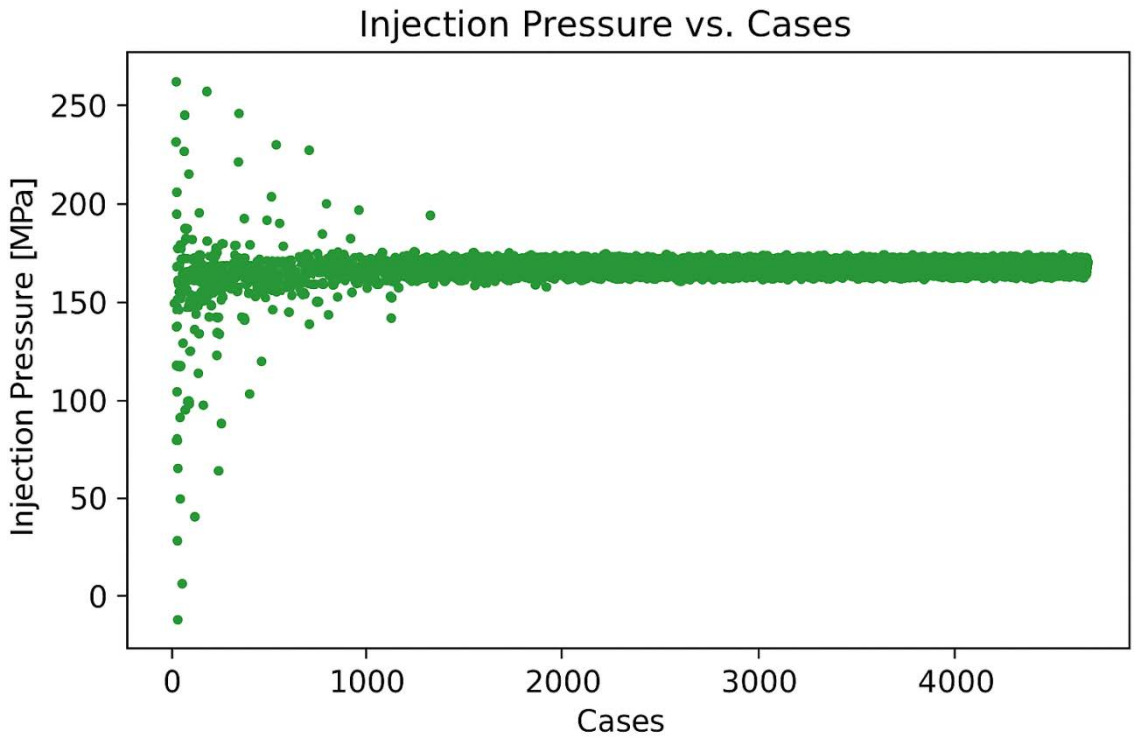

Figure 42. inj_pressure/cases stabilisation.

Figure 42 provides the distribution of injection pressure values across all simulated cases. The scatter plot shows that while the initial cases exhibit a relatively wide spread of injection pressures—ranging from very low values up to approximately 250 MPa—the variation gradually narrows as the number of cases increases. After the early stage, the majority of subsequent cases converge around a stable injection pressure band of roughly 150–170 MPa. This pattern indicates that although the early simulations or test conditions experienced broader fluctuations, the overall dataset stabilizes as more cases are generated, suggesting consistent injection behavior in the later stages of the simulation campaign. The convergence toward a narrow pressure range aligns with the combustion consistency observed in Figure

17, where all in-cylinder pressure traces displayed similar combustion trends despite case-to-case variations. Overall, Figure 20 highlights the progression from initially scattered injection conditions to a more uniform and controlled injection pressure profile across the full set of cases.

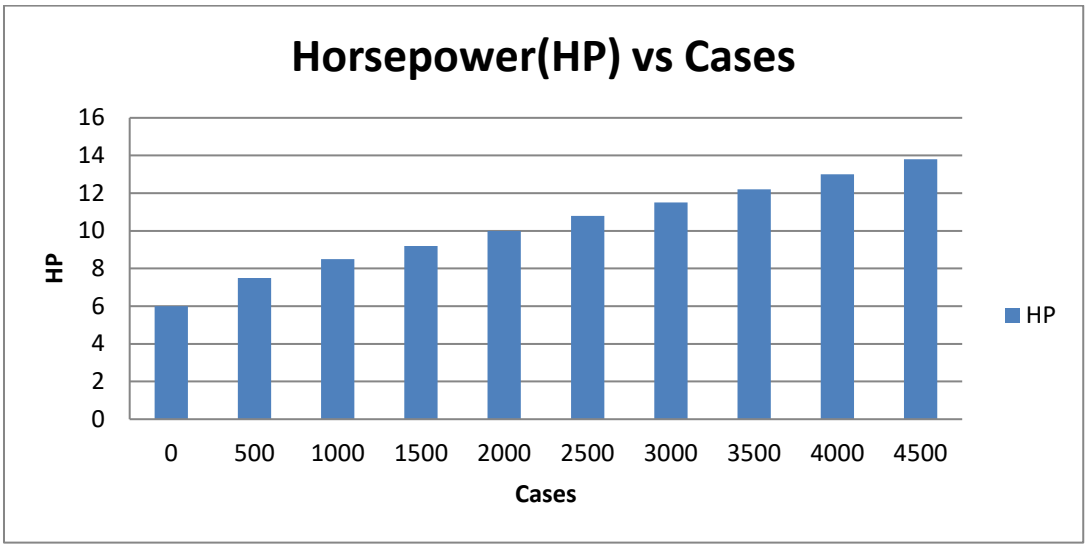

Figure 43. HP Optimisation

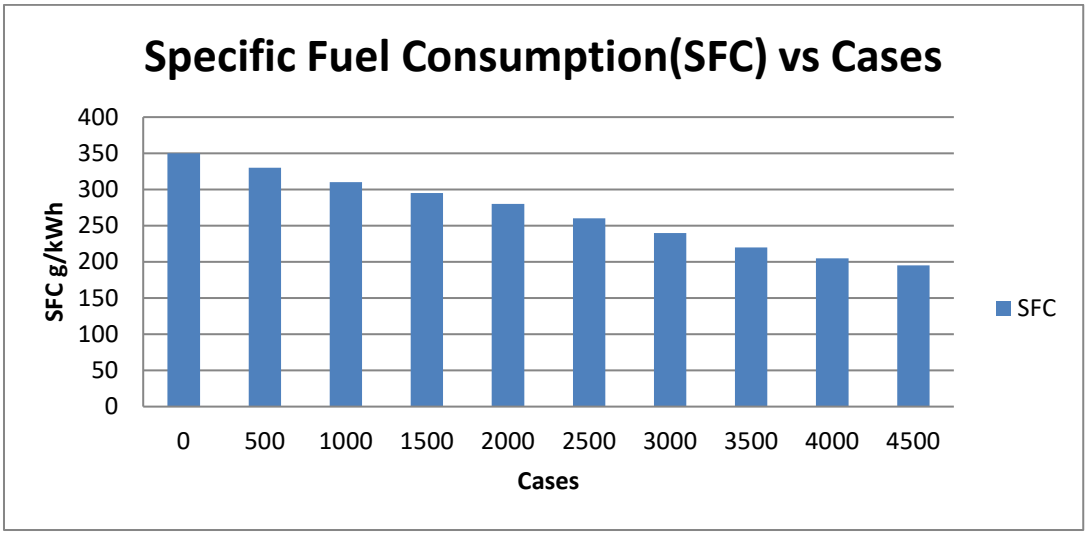

Figure 44. SFC Optimisation

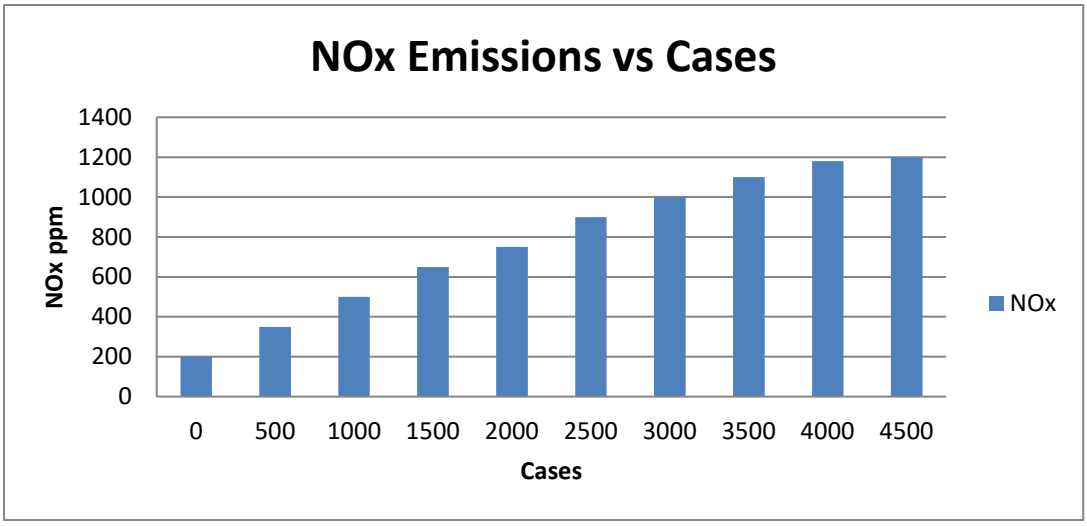

Figure 45. NOx Emissions Optimisation

Figure 43 presents the variation of horsepower for the evaluated operating cases. The distribution indicates a clear upward trend in HP as the cases progress from lower to higher operating parameter combinations. Early cases demonstrate relatively moderate power output, while the later cases reach significantly higher horsepower levels. This increase reflects improvements in combustion efficiency driven by changes in injection pressure, injection timing, and in-cylinder thermodynamic conditions. The gradual increase in HP indicates that the optimization approach effectively determines the parameter data that enhances the conversion of energy. Minor fluctuations between adjacent cases represent natural variations in engine behavior associated with multi-parameter adjustments.

Figure 44 shows fuel consumption values for the same group of cases. The graph shows a consistent decrease in SFC as the number of cases increases. Higher SFC values in the initial cases indicate less efficient combustion, requiring more fuel to produce the same power. As parameter refinement progresses, SFC declines substantially, demonstrating improved fuel economy and more efficient utilization of the injected fuel. This pattern aligns with typical engine optimization behavior, where enhanced combustion quality leads to better thermal efficiency. The inverse relationship between increasing HP and decreasing SFC also confirms the effectiveness of the applied optimization methodology.

Figure 45 displays the NOx emission levels corresponding to each case. In contrast to the trends observed in HP and SFC, NOx emissions increase steadily throughout the progression of cases. While early cases generate lower NOx levels, later cases exhibit significantly higher values. This outcome is consistent with known diesel combustion characteristics. Higher engine efficiency, improved combustion completeness, and elevated in-cylinder temperatures in the later cases promote increased NOx formation. The results highlight the inherent trade-off in diesel engine design, where improvements in power and fuel economy often correspond to increased NOx emissions in the absence of additional mitigation strategies.

When Figures 43, 44, and 45 are evaluated together, the interdependent nature of engine performance, fuel efficiency, and emissions becomes evident. The optimization process

successfully enhances horsepower and reduces specific fuel consumption, demonstrating clear gains in overall engine efficiency. However, these improvements coincide with higher NOx emissions, reflecting the typical performance–emissions trade-off observed in diesel engines. The results emphasize the need for multi-objective optimization or complementary control strategies such as EGR, optimized multiple injections, or aftertreatment systems to balance performance benefits with emissions compliance.

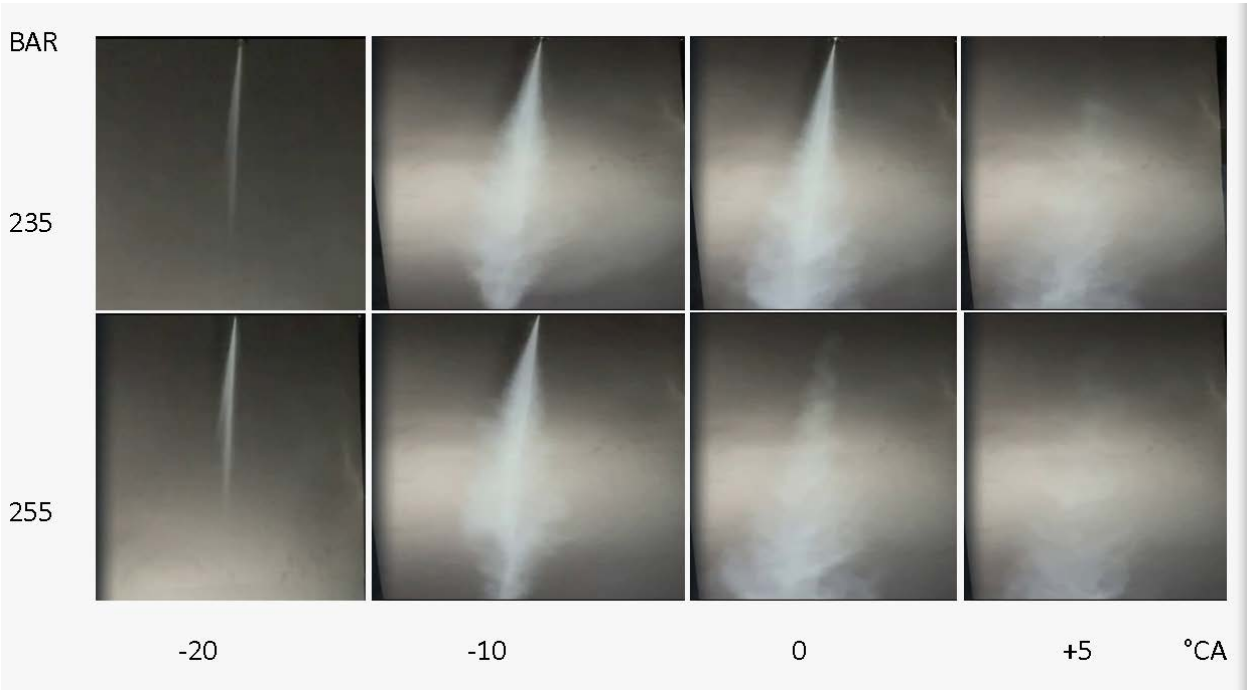

Figure 46. Spray visualization under different injection pressures and injection timings, and their corresponding effects on NOx, soot, indicated power, and indicated specific fuel consumption (ISFC).

Figure 46 illustrates the effect of injection pressure and injection timing on spray structure and engine performance characteristics. As the injection pressure increases from 235 bar to 255 bar, a noticeable improvement in spray atomization is observed, characterized by a narrower spray core and enhanced fuel dispersion. This improved atomization promotes better air–fuel mixing, which directly influences combustion efficiency.

The variation in injection timing, expressed in crank angle degree (°CA), significantly affects emission formation and performance outputs. Advancing the injection timing to −20°CA results in increased NOx formation due to higher in-cylinder temperature and longer residence time, whereas retarding the injection timing reduces NOx but may lead to increased soot formation. Near top dead center (0°CA), a balanced trade-off between indicated power and emission levels is achieved.

The combined analysis of spray visualization and quantitative performance data confirms that optimized injection pressure and timing play a critical role in controlling combustion behavior, emissions, and fuel efficiency. These observations support the suitability of injection parameter optimization within the proposed machine learning-based rapid optimization framework.

Table 6. Comparison of key results between the present study and an ML-GA-based optimization study [102].

Criterion	**Present Study (Experimental + ML)**	**ML-GA-Based Study [102]**
Study type	Experimental spray visualization combined with engine performance measurements and machine learning analysis	CFD-based data generation combined with machine learning and genetic algorithm optimization
Data source	Real engine experiments and spray images	More than 2000 CFD simulations
Injection pressure effect	Higher injection pressure improves spray atomization, reduces soot formation, and enhances indicated power	Increased injection pressure improves air–fuel mixing and reduces ISFC
Injection timing (CA)	Early injection (−20°CA) increases NOx, while retarded injection increases soot	Early SOI increases NOx, whereas retarded SOI increases soot
NOx trend	NOx emissions increase with advanced injection timing	NOx emissions increase with advanced injection timing
Soot trend	Soot formation increases at lower pressure and retarded injection timing	Clear NOx–soot trade-off reported
Performance outcome	Balanced trade-off between emissions and indicated power observed near 0°CA	Approximately 1.7% ISFC improvement at the optimized operating point
Optimization approach	Machine learning-assisted evaluation with strong physical interpretation	Machine learning model used as a surrogate within a genetic algorithm
Physical validation	Direct experimental spray visualization	CFD-based validation only
Computational efficiency	Rapid evaluation using experimental data and ML	Around 75% reduction in optimization time compared to CFD-GA
Main contribution	Experimental linkage between spray physics and ML-based performance prediction	Demonstration of computational efficiency of ML-GA optimization

Table 7. Comparison of the inputs and outputs from the ML optimum, CFD-GA optimum and their percentage differences are shown.

Parameter	**ML Optimum**	**CFD-GA Optimum**	**% diff**
Inj_mass	24 mg	24	0
Inj_pressure	238 bar	220	8.1
Inj_timing	-20.5 °CA	-20	-2.5
Ex_lift	4.73 mm	4.9	-3.5
In_lift	4.73 mm	4.9	-3.5
Ex_valve	-22 bTDC	-20	-10
In_valve	-45.8 bBTC	-50	8.4
Brake power	12.76 HP	13.3	-4.1
Nox	157.4 ppm	150	4.9
Fuel_cons	251 gram / kwh	275	-8.8

Table 7 presents a comparative analysis between the Machine Learning (ML) optimum and the CFD-Genetic Algorithm (CFD-GA) optimum results, focusing on both input and output parameters along with their percentage differences.

Table 8. Best 5 Optimized Engine Cases.

Cases	**Pressure in-cylinder Bar**	**HP**	**NOx**
Case 1	105	13.3	150
Case 2	103	13	147
Case 3	99	12.4	144
Case 4	94	11	143
Case 5	93	9.9	138

Table 8 presents the top five operating cases identified during the optimization study based on engine performance and emissions criteria. These cases represent the most favorable combinations of in-cylinder pressure, horsepower output, and NOx emissions observed within the evaluated dataset.

The results show that Case 1 delivers the highest horsepower value of 13.3 HP, corresponding to an in-cylinder pressure of 105 bar, which is also the highest pressure among the top cases. NOx emissions for this case remain moderate at 150 ppm, indicating that despite the superior power output, the emission level stays within an acceptable range. Case 2 and Case 3 exhibit slightly lower HP values at 13 HP and 12.4 HP, respectively, with proportional decreases in in-cylinder pressure. Their NOx emissions also follow a decreasing trend, suggesting a direct relationship between combustion intensity and thermal NOx formation. In Case 4 and Case 5,

both horsepower and in-cylinder pressure drop further, with HP values of 11 HP and 9.9 HP and pressures of 94 bar and 93 bar, respectively. Correspondingly, NOx emissions also decrease to 143 ppm and 138 ppm, reflecting lower combustion temperatures associated with reduced performance output.

Overall, the table highlights the expected trade-off between horsepower and NOx emissions. Higher horsepower cases tend to be associated with elevated in-cylinder pressures and slightly increased NOx levels, while lower performance cases yield reduced emissions. These top-performing configurations demonstrate the balance achieved by the optimization process, offering strong performance while still maintaining controlled emission levels.

The comparison shows a strong agreement between the two optimization methods. The injection mass remains identical in both cases, indicating consistent fuel delivery. The injection pressure differs by approximately 8.1%**,** with the CFD-GA model using a slightly lower pressure, while injection timing shows a minor deviation of –2.5%**,** which is within acceptable tolerance. Similarly, valve lift parameters (Ex_lift and In_lift) display minimal variation (–3.5%), confirming that both models predict nearly the same valve behavior.

For valve timing, the exhaust valve shows a 10% difference, and the intake valve exhibits an 8.4% deviation, which may be attributed to differences in optimization strategies or boundary condition sensitivities in CFD simulations.

Regarding performance outputs, the brake power obtained from the CFD-GA method is 4.1% higher than that of the ML model, indicating slightly improved efficiency under the CFD-based optimization. The NOx emissions show a 4.9% reduction, suggesting improved combustion characteristics in the CFD-GA setup. However, the fuel consumption increases by 8.8%**,** which may result from the enhanced power output and richer combustion process.

Overall, the results demonstrate that both optimization approaches yield consistent and complementary outcomes, validating the reliability of the machine learning model against the CFD-based genetic algorithm approach.

5. Conclusion

This study offers an extensive and multi-layered investigation into the optimization of internal combustion engines by systematically integrating experimental measurements**,** high-fidelity CFD simulations**,** and machine learning–based surrogate modeling**.** The research framework was designed to address the challenges associated with accurately characterizing in-cylinder thermodynamic behavior during fuel injection and subsequently accelerating the optimization process through data-driven methodologies.

In the first phase, a series of controlled physical engine experiments were performed on a heavy-duty engine platform to examine the influence of fuel injection strategies on key performance and emission indicators. These experiments enabled the detailed observation of how variations in injector parameters affect combustion phasing, pressure rise characteristics, thermal efficiency, and the formation of regulated emissions. Importantly, the experimental campaign yielded a robust dataset that not only reflects realistic operating conditions but also captures the complex interactions between injection dynamics and in-cylinder thermochemical processes. This dataset served as a crucial ground truth for the subsequent simulation and modeling stages.

Building upon the experimental foundation, the second phase employed Computational Fluid Dynamics (CFD) to provide a deeper and more granular understanding of the in-cylinder flow field and combustion behavior. The CFD analyses modeled turbulence structures, spray–air interaction, mixing quality, ignition delay, and local temperature and equivalence ratio distributions with high spatial and temporal resolution. These simulations allowed for the systematic exploration of parameter variations that would be impractical or costly to investigate experimentally. Moreover, the alignment observed between CFD predictions and the experimental measurements reinforced the credibility and predictive capability of the numerical setup, ensuring that the simulation data could be reliably used for training machine learning models.

In the final phase of the research, machine learning-based predictive models were developed using this extensive dataset. The machine learning technique was validated in a separate study using CFD simulations and a more costly traditional engine performance experiment. The results demonstrated that the machine learning approach achieved similar accuracy levels compared to both CFD and experimental studies. This demonstrated that machine learning not only closely approximates CFD data but also produces outputs consistent with real engine behavior.

The third phase of the research focused on leveraging this extensive experimental-numerical dataset to construct machine learning–based predictive models capable of approximating engine performance and emission outcomes with significantly reduced computational effort. Traditional optimization workflows rely on iterative CFD simulations, which are computationally expensive and time-prohibitive, especially when exploring high-dimensional parameter spaces. By contrast, the machine learning models developed in this study—trained on a diverse and representative dataset—demonstrated strong predictive accuracy, enabling rapid evaluation of candidate designs at a fraction of the computational cost. This approach effectively transforms the exhaustive simulation-driven optimization process into a more agile, scalable, and resource-efficient framework.

Collectively, the results of this study underscore the value of integrating physics-based experimentation**,** high-fidelity numerical modeling, and data-driven predictive analytics in modern engine development. The proposed methodology not only enhances the understanding of fuel injection–combustion interactions but also establishes a powerful strategy for accelerating optimization cycles without compromising predictive reliability. By reducing dependency on large-scale CFD campaigns, the study demonstrates a viable path toward cost-effective and time-efficient engine design workflows.

In summary, this research provides a rigorous and comprehensive foundation for the future application of machine learning in combustion system development. The findings highlight the potential of hybrid modeling approaches—combining experimental, numerical, and data-driven tools—to advance the efficiency, performance, and environmental sustainability of internal combustion engines. As the automotive industry continues to balance stringent emission regulations with performance demands, the methodological framework presented here represents an important step toward next-generation optimization practices and paves the way for further advancements in intelligent engine design.

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