

Article

Evaluation of Hydrogen Peroxide Application in Compression Ignition Engine Fuels

Tomasz Osipowicz ¹, Karol Franciszek Abramek ^{1,*}, Dalibor Barta ² and Paweł Drożdżel ³

¹ Faculty of Mechanical Engineering and Mechatronics, West Pomeranian University of Technology in Szczecin, 70-310 Szczecin, Poland; tosipowicz@zut.edu.pl

² Faculty of Mechanical Engineering, University of Žilina, Univerzitná 1, 010 26 Žilina, Slovakia; dalibor.barta@fstroj.uniza.sk

³ Faculty of Mechanical Engineering, Lublin University of Technology, ul. Nadbystrzycka 36, 20-618 Lublin, Poland; p.drozdziel@pollub.pl

* Correspondence: karol.abramek@zut.edu.pl

Abstract

The article discusses the issues related to the possibility of using hydrogen peroxide in a proportion of 10% to CI engine fuel to reduce emissions in exhaust gases. The additive proposed by the authors of the paper is a 12% hydrogen peroxide solution. The paper presents the results of engine and analytical tests carried out by the authors. The paper mainly discusses the emission of toxic substances into the atmosphere for an engine running on standard and modified fuels. Laboratory tests have shown that the cetane number increased by two units for the modified fuel. The results of engine tests showed that the fuel additive reduces the concentration of nitrogen oxides and hydrocarbons, while the soot content increased slightly. The study showed that the modified fuel does not affect the operating parameters of the compression ignition engine. To assess the potential impact of hydrogen peroxide addition to fuel on the durability of fuel injection equipment, a nonlinear digital twin model was developed to enable the analysis of the relative degradation risk of the Common Rail injection system. The model was implemented in the MATLAB R2024b (September 2024) environment as an expert-based scenario model intended for comparative analysis of the influence of different fuels on potential degradation processes occurring within the fuel injection apparatus. Four fuel variants were analyzed: conventional diesel fuel (DF), diesel fuel containing 12% H₂O₂, B100 fuel (rapeseed oil methyl ester), and B100 fuel containing 12% H₂O₂. The model incorporated selected physicochemical fuel properties significantly affecting the operation of the fuel injection system, including density, kinematic viscosity, calorific value, flash point, iodine number, and oxygen content.

Keywords: diesel engine; hydrogen peroxide; fuel combustion; fumes; emission

Academic Editor: Georgios Mavropoulos

Received: 25 May 2026

Revised: 6 July 2026

Accepted: 10 July 2026

Published: 11 July 2026

Copyright: © 2026 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the [Creative Commons Attribution \(CC BY\) license](https://creativecommons.org/licenses/by/4.0/).

1. Introduction

Current trends in modern motor vehicles are focused on reducing greenhouse gas and toxic emissions into the atmosphere. Modifying fossil fuels is a method of improving the emission parameters of means of transport so that exhaust fumes meet current environmental standards. The task of modifiers used in fuels is to improve the organization of combustion processes in the cylinder working space. The combustion of a combustible mixture and the release of heat in CI engines causes physical and chemical effects that

largely determine the engine's performance. The combustion phenomena that affect the thermal efficiency of an engine primarily include the effectiveness of converting the fuel's chemical energy, the thermodynamic efficiency of its utilization, and the intensity of dynamic loading exerted on the crank–piston assembly [1]. These have been problematic throughout the entire history of diesel engine development. The chemical effects mainly relate to the composition of exhaust gases, in particular their smoke content and toxic substances. At present, due to environmental protection requirements, these are the main requirements for the design of internal combustion engines. The conditions under which combustion occurs should primarily ensure the maximum possible release of the fuel's chemical energy (complete and total combustion), optimal air–fuel mixing and utilization of the oxidizer, while maintaining minimal exhaust emissions. Thermodynamic analysis of the engine operating cycle indicates that the efficiency of heat release in each engine is strongly dependent on the phasing of the combustion process relative to the crank angle [2]. From this point of view, it would be optimal to burn the entire fuel dose at a constant combustion chamber volume when the piston is at TDC. However, in this case, the rate of heat release would become excessively high, causing impact loads on the crank mechanism and acoustic symptoms in the form of excessive noise. These adverse phenomena necessitate spreading the heat release process over a certain period of crankshaft rotation near the piston TDC. The requirements for complete heat release and its effective conversion into useful work, combined with low dynamic loading of the crank mechanism and minimized combustion noise, are inherently conflicting. Consequently, any engineering solution aimed at optimizing these parameters constitutes a compromise. This compromise is further constrained by exhaust gas composition, which must comply with currently applicable emission regulations. Experience shows that it is extremely difficult to achieve satisfactory results in each engine in terms of crankshaft loads, engine noise, exhaust gas composition, and fuel economy, and an optimal compromise solution is usually only possible with a strictly defined heat-release curve. One of the principal challenges associated with compression-ignition engines is the precise control and optimization of the combustion process so that the resulting thermo-physical and chemical phenomena satisfy the diverse and often competing requirements related to performance, fuel efficiency, durability, and emissions over the entire operating range. The combustion process in a diesel engine is very complex, as its initiation depends on meeting conditions for certain fuel self-ignition [3]. The combustion process itself also depends on many design factors and fuel properties, including the auto-ignition delay. One of the primary strategies for mitigating exhaust emissions involves the implementation of catalytic aftertreatment systems. In motor vehicles, catalytic converters are primarily integrated into the exhaust system, where they function to neutralize toxic compounds, including nitrogen oxides (NO_x), hydrocarbons (HC), carbon monoxide (CO), and particulate matter (PM). Conventional catalytic reactors do not influence the combustion process directly; their role is limited to post-combustion exhaust gas purification [3]. In contrast, liquid-phase catalysts are designed to actively support combustion, suppress the formation of toxic species during the reaction, and facilitate their in-situ neutralization. Additionally, such catalysts inhibit the proliferation of hydrocarbon-degrading microorganisms in the fuel, which contribute to fuel aging. Literature reports indicate that catalytic converters can also be deployed directly within the combustion chamber of compression-ignition (CI) engines. For instance, in [4], zinc- and vanadium-based catalysts were applied in a single-cylinder, four-stroke CI engine. Experimental results demonstrated reductions of approximately 70% in NO_x and HC, 60% in CO, and 50% in CO_2 emissions, confirming the effectiveness of in-cylinder catalytic intervention. Studies on the use of plant-based fuels have been presented in [5]. The automotive industry is currently undergoing a transition from conventional internal combustion engine technologies to a new era of electric propulsion. The

authors correctly emphasize the need to develop engineering solutions focused on electric vehicles powered by renewable energy sources or incorporating hybrid power systems. Study [6] presented the results of measurements of the characteristics of an engine running on lemon oil biofuel. Furthermore, critical engine components, including the piston crown, cylinder head, and valves, were coated with a stabilized zirconia catalyst. Experimental evaluation demonstrated that a biofuel-powered engine equipped with catalysts on these components exhibited reduced emissions of carbon monoxide (CO), hydrocarbons (HC), nitrogen oxides (NO_x), and particulate matter compared to a conventional engine operating on standard fuel. In [7], gaseous fuels such as hydrogen, methane, and natural gas were blended with liquid fuel in a 1:1 ratio for testing, with a platinum-aluminum catalyst applied within the combustion chamber. Results indicated that the catalytic system effectively decreased NO_x emissions. The addition of hydrogen to the fuel mixture led to elevated in-cylinder pressures, increased NO_x and HC emissions, and reduced smoke formation, whereas the incorporation of methane and natural gas reduced NO_x. Moreover, supplementary catalytic treatment further decreased smoke levels with these alternative fuels. In compression-ignition (CI) engines, selective catalytic reduction (SCR) systems using urea-based solutions, such as AdBlue [8], are employed to remove NO_x from exhaust gases; however, this approach is costly and requires frequent replenishment. Reference [9] investigated the use of water-in-oil (W/O) emulsions as fuel for compression-ignition (CI) engines. The experiments were conducted under controlled operating conditions, with constant engine speed and load, while measuring in-cylinder pressure, heat release rate, and exhaust gas composition. Results demonstrated that blending water into the fuel reduced nitrogen oxide (NO_x) emissions by up to 19.6% and decreased smoke opacity by up to 66.3%. The observed effects are attributed to the micro-explosion phenomenon of water droplets during combustion, which enhances fuel atomization, improves air–fuel mixing, and lowers peak flame temperatures, thereby reducing NO_x formation and particulate matter generation. According to the authors, this is because water lowers combustion temperature by absorbing heat during evaporation and through micro-explosions caused by the rapid evaporation of water droplets, which simultaneously reduces NO_x emissions and smoke. It is also possible to create an emulsion fuel using non-biodegradable plastic shopping bags (PGB) [9]. Experiments have confirmed that a water–oil emulsion made from PGB reduces nitrogen oxide emissions and smoke. The best exergy efficiency was achieved with an emulsion containing 10% diesel fuel. The study described in [10] analyzed the exergy performance of a ̸S engine powered by bio-fuel produced from cottonseed oil enriched with titanium oxide and silver nanoparticles. The results suggest that fuels with added nanoparticles exhibit reduced exergy dissipation. It should be emphasized that the incorporation of nanoparticles involves significant material costs. In [11], cerium oxide was used as a diesel fuel additive. Experiments showed that using this catalyst reduced soot and hydrocarbon emissions by 30% at partial engine load, while at full load, nitrogen oxide emissions decreased by about 5%. No significant differences in fuel consumption were observed at medium and maximum loads. Article [12] analyzed the effect of alcohol additives (methanol, ethanol, n-butanol, and their mixtures) on the combustion process. The use of such additives reduced self-ignition delay and improved combustion efficiency compared to pure diesel fuel. The best results were achieved for a mixture containing 80% diesel fuel, 10% methanol, and 10% n-butanol [13,14]. In turn, studies [15,16] described the use of a catalyst in injector nozzles in engines with direct mechanical fuel injection. The installation of a platinum catalytic reactor on the non-working part of the injector needle reduced harmful emissions. Paper [16] presents a method of partial dehydrogenation of diesel fuel to obtain high-quality hydrogen for vehicle use. The study used a platinum catalyst deposited on a zinc and aluminum carrier. According to the results of studies [17–19], platinum deposited on a tin and alu-

minum substrate proved to be an effective catalyst for the dehydrogenation of hydrocarbons. Current trends in the development of internal combustion engines focus on minimizing the emission of toxic exhaust components. Studies [20] have proven that adding ethanol to fuel reduces NO_x emissions. The research described in publication [21] proposed using powdered biofuel as an additive the intake air. The analysis showed that it is possible to use this technology in internal combustion engines without compromising their durability. A solution aimed at improving the chemical properties of fuel is the use of hydrogen peroxide as an additive. There are many methods of introducing hydrogen into the engine combustion chamber. The most common technique is to install an additional system with a hydrogen cylinder, stored in gaseous or liquid form. In this case, hydrogen enters the combustion chamber together with air. However, the disadvantages of this method are high costs and the need to modify the engine design. An alternative solution is to use a chemical compound that releases hydrogen during combustion—such as hydrogen peroxide. In the presented work, the authors proposed using hydrogen peroxide with a concentration of 30%. This additive was used for 10% in the fuel mixture. Higher doses may adversely affect the operating parameters of the drive unit and contribute to faster wear of its components. The purpose of the additive proposed by the authors is to reduce toxic substances in exhaust gases and fuel consumption [22]. Due to its chemical properties, hydrogen peroxide can change the combustion process of the tested fuels and reduce the emission of toxins into the atmosphere through exhaust gases. An analysis of the literature shows that numerous studies are being conducted on the modernization and use of new fuels. In article [23], the author proposed the use of micro-emulsification in fuels based on diesel, vegetable oil, and alcohol. The research showed that due to the water content, the calorific value of all fuels improved with a reduction in nitrogen oxides and soot, aiming to reduce emissions of carbon dioxide and nitrous oxide, gases that are responsible for the greenhouse effect. Analysis of the results of studies presented by the authors of [11,24] showed that it is possible to produce oil from non-biodegradable plastic bags (PGB). The authors then proposed preparing a water–oil mixture with the addition of 10% diesel fuel from the oil produced. The tests showed that this type of fuel reduced soot and nitrogen oxide emissions in exhaust. However, the specific fuel consumption increased. In addition, the authors did not investigate how the proposed mixture affects the operation of engine components. Paper [25] published the results of research on the effect of adding t-butyl peroxide to diesel fuel and biofuel derived from Mahua oil and palm oil waste. The experiment showed that an engine operating at 100% load had lower emissions of carbon monoxide, unburned hydrocarbons, and soot by about 4% for diesel fuel with the additive, but higher emissions of nitrogen oxides by about 1% compared to biofuel with the additive. The results of the experiment on a single-cylinder, four-stroke engine powered by ON fuel with hydrogen (as the base fuel) and ON fuel with hydrogen with the addition of ditertbutyl peroxide (DTBP) are presented in [26]. The 3.50 kW engine operated at a constant speed of 1500 rpm. The paper compares the self-ignition delay period for the given mixtures. The tests showed that the ignition delay decreases with an increase in hydrogen and DTBP in diesel fuel. Research is being conducted on the use of ethanol as a fuel additive. The results of the experiments are presented in [20,21]. Ethanol lowers the combustion chamber temperature, reducing nitrogen oxide emissions. In [27], the authors described how the addition of hydrogen to diesel and biofuel affects combustion in a CI engine. The analysis showed that hydrogen as an additive not only lowers the temperature in the engine combustion chamber but also changes the physical and chemical parameters of fuels, especially those of plant origin. The authors of [28] described the effect of 10% hydrogen peroxide as an additive at concentrations of 5%, 10%, and 15% to diesel fuel and Calophyllum Inophyllum methyl ester. The tests showed that an engine powered by biodiesel with the additive produced lower emissions of carbon

monoxide and nitrogen oxides. The research presented in paper [29] concerns the use of 30% hydrogen peroxide in biofuel from *Jatropha* oil. The additive content in the emulsion was 5%, 10%, and 15%. The authors analyzed engine parameters such as cylinder pressure, ignition delay, ignition duration, heat release, and environmental parameters. The analysis showed that the engine achieved the best performance with a 15% hydrogen peroxide-to-fuel mixture ratio [30,31].

The aim of this paper was to investigate whether it is possible to reduce exhaust gas pollution from modern compression ignition engines by adding hydrogen peroxide to the fuel. Based on the analysis of the literature [32], it can be concluded that hydrogen possesses unique properties and constitutes a suitable energy source for both internal combustion engine vehicles and electric vehicles. A review of the literature has shown that research related to the topic of this paper is being conducted in many areas. However, there is little work on the use of hydrogen peroxide in fuels. The research on fuel modification should also be considered in terms of engine component operation [33,34]. According to the literature [35], most of the proposed fuel additives do not affect the operation of the fuel supply system or accelerate the wear of the CI engine. Diesel engines are central to global transportation and industry, but face persistent challenges related to emissions (NO_x, particulate matter, CO, HC) and the need for improved efficiency. Traditional emission control strategies (EGR, aftertreatment) have limitations, especially as regulatory standards tighten. The search for effective, practical fuel additives has led to renewed interest in hydrogen peroxide (H₂O₂), an oxygen-rich compound with strong oxidizing properties. H₂O₂ offers the potential to: increase the cetane number, promoting faster and more complete combustion; enhance in-cylinder oxygen availability, supporting oxidation of fuel and soot; and generate reactive radicals (OH, HO₂) that accelerate combustion chemistry and reduce emissions. These properties make H₂O₂ a promising candidate for improving diesel engine performance and emissions, especially when used in optimized concentrations and in combination with alternative fuels or advanced combustion modes.

2. Materials and Methods

The test fuel was prepared according to the following procedure. Diesel fuel was mixed with 12% hydrogen peroxide in a ratio of 10% using a 5% sodium alginate polysaccharide emulsifier [36]. The emulsifier's task is to permanently combine two liquids that do not mix. Diesel fuel is non-polar, while hydrogen peroxide is polar. These liquids form two separate layers. The emulsifier reduces surface tension, allowing droplets of one phase to disperse in the other. The first stage of the research was to analyze the cetane number of the prepared fuel and the standard diesel fuel from which the mixture was prepared. These tests were performed on a test bench for measuring the cetane number in fuel (Figure 1). The tested fuel is compared with the reference fuel using a special single-cylinder reference engine, in which the compression ratio is changed during operation until a specific self-ignition tendency is achieved, expressed as ignition delay.

The properties of the tested fuels are presented in Table 1.

Table 1. Researched fuel parameters.

Properties	RME	HME	RME + 12%H ₂ O ₂	HME + 12%H ₂ O ₂
Density [kg/m ³] (288 K)	861–888	870–900	880–905	890–915
Kinematic viscosity [mm ² /s] (313 K)	4.4–5.5	4.5–6.5	3.5–4.5	3.5–4.8
Calorific value [MJ/kg]	36–38	33–35	32–35	30–34
Ignition temperature [K]	170–190	>180	150–170	150–175
Iodine value	90–110	140–170	90–110	140–170
Oxygen content [%]	10–11	11–13	12–15	13–16



Figure 1. Test bench for measuring the cetane number of diesel.

Engine tests were carried out on a dynamometer using a 4CTI90–1BE6 engine (WSW Andoria S.A., Andrychów, Poland) with a mechanical fuel supply system. The test bench is equipped with an AVL eddy current brake (AVL List GmbH, Graz, Austria), an AVL mass fuel meter (AVL List GmbH, Graz, Austria), a Capelec exhaust gas analyzer (Capelec SAS, Montpellier, France), and a MAHA smoke meter (MAHA Maschinenbau Haldenwang GmbH & Co. KG, Haldenwang, Germany) (Figure 2). The measurement error of the test bench is 2%. Exhaust emission tests were performed in accordance with the Polish standard PN–EN ISO 8178–1: 2020 [37]. The research conditions are presented in Table 2.

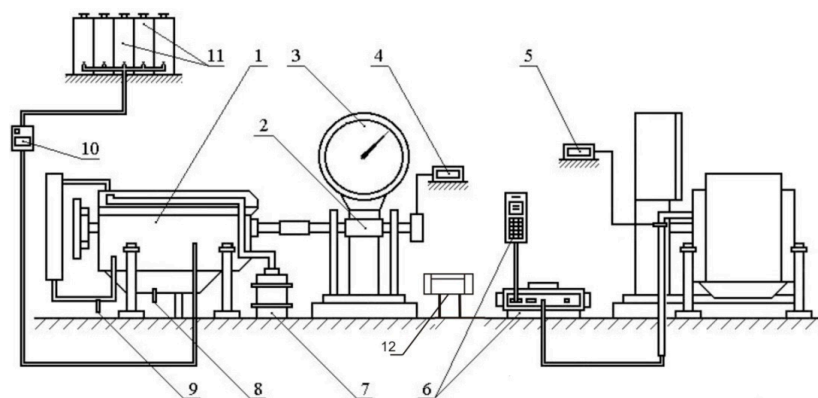


Figure 2. Engine dynamometer with a 4CTI90–1BE6 engine and an AVL brake 1—engine, 2—eddy current brake, 3—dynamometer, 4—controller, 5—exhaust temperature sensor, 6—MDO smoke meter, 7—air filter, 8—oil temperature sensor, 9—engine coolant outlet temperature sensor, 10—electronic gravimetric fuel consumption meter, 11—fuel tank, 12—Capelec exhaust gas analyzer.

Table 2. Research conditions.

Measurement Equipment	Measurement Error	Operating Conditions
4CTI90–1BE6 engine	Not applicable	Temperature: 295,15 K
AVL eddy current brake	2%	Atmospheric pressure: 99 kPa
AVL fuel mass meter	2%	Relative humidity: 31%
Capelec exhaust gas analyser	5%	

MAHA smoke meter	5%	Fuels: Diesel, Diesel and 10% mixture of sodium ascorbate with a 12% hydrogen peroxide solution
Matlab software R2024b	Not applicable	

The specific fuel consumption was calculated based on the external characteristics of the engine using the following equation [1]:

$$g_e = \frac{3600 \cdot G_e}{N} \quad (1)$$

The following fuels were used for the tests: standard diesel fuel with 12% hydrogen peroxide added to the fuel in a proportion of 10%. The cetane number of the tested fuels was measured on an IDT-69 engine test bench in accordance with PN-EN ISO 5165 2021-02 [38]. Based on the cetane number, the activation energy of the fuels and the self-ignition delay period were calculated. Formula (2) shows the relationship for calculating the activation energy [2]:

$$E_a = \frac{618.840}{LC + 25} \quad (2)$$

LC—cetane number of the fuel.

The self-ignition delay period of the tested fuels was calculated using Equation (3) [2,3]:

$$\tau_s = (0.36 + 0.22 \cdot c_m) \cdot \exp\left[E_a \left(\frac{1}{RT} - \frac{1}{17.19}\right) \cdot \left(\frac{21.2}{P-12.4}\right)^{0.63}\right] \quad (3)$$

c_m —piston speed,

E_a —activation energy value,

R —individual gas constant of the combustible mixture,

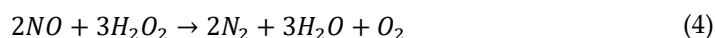
T —temperature in the combustion chamber,

P —pressure in the combustion chamber.

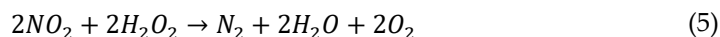
During engine tests, the following engine parameters were measured: power, torque, specific fuel consumption, emissions of nitrogen oxides, hydrocarbons, particulate matter, and carbon dioxide in the exhaust gases.

The purpose of adding hydrogen to fuel is to reduce toxic substances in exhaust gases such as nitrogen oxides, hydrocarbons, and soot. Simplified relationships (4–7) illustrate the mechanism by which the above toxic substances are reduced.

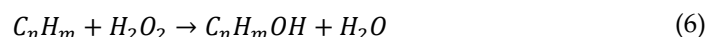
Equation (4) shows the mechanism of nitrogen oxide reduction [2]:



Equation (5) shows the mechanism of nitrogen dioxide reduction:



Equation (6) shows the general mechanism of hydrocarbon oxidation:



Equation (7) shows the general mechanism of solid particle oxidation:



The results of laboratory tests and calculations are presented in Figures 3 and 4.

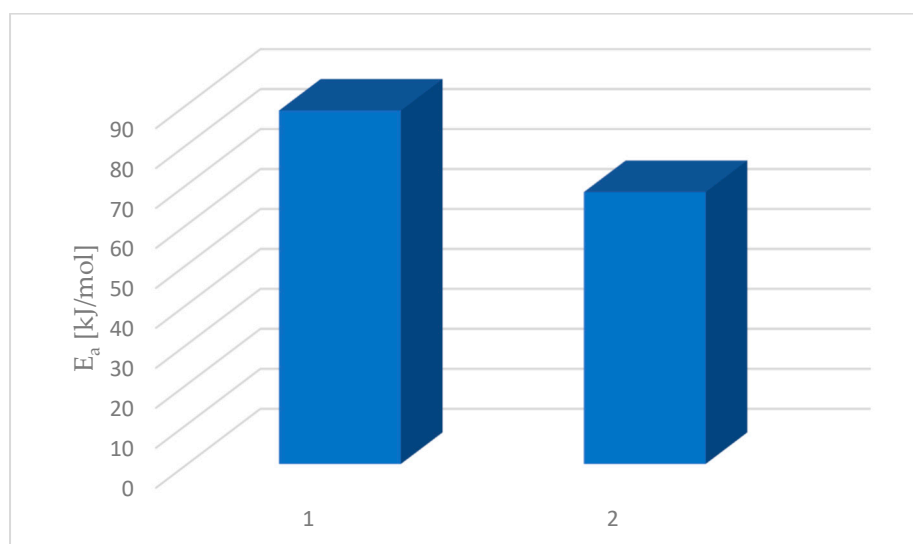


Figure 3. Calculated energy activation value 1. standard fuel, 2 modified fuel.

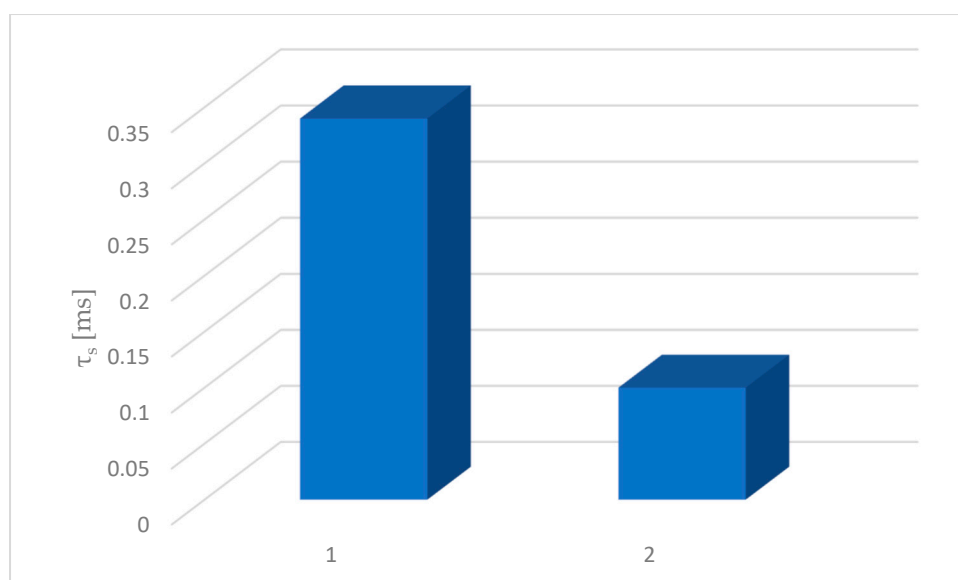


Figure 4. Calculated ignition delays for researched fuels 1. modified fuel, 2 standard fuel.

The initiator of a chemical reaction is activation energy (E_a). It is an energy barrier that reacting molecules must overcome for substrates to be converted into products. The activation energy value determines the rate of the chemical reaction. The higher the activation energy, the slower the reactions occur due to the high energy barrier to carry out a given reaction. Factors that accelerate chemical reactions are temperature and catalyst. The activation energy value was calculated from Equation (2).

The self-ignition delay period is the time from the injection of fuel into the combustion chamber to the appearance of the first self-ignition points of the mixture. During this phase, the fuel evaporates and mixes with the air. The shorter this moment, the faster and more efficient the combustion process is, with lower emissions. The self-ignition delay is calculated using Formula (3) [2].

Fuel properties were adopted based on literature data concerning diesel fuel, fatty acid methyl esters, and fuel blends containing hydrogen peroxide.

The digital twin model was based on the assumption that degradation of the fuel injection apparatus is a multifactorial process resulting from the simultaneous interaction

of oxidation and corrosion processes, reduced lubricity, changes in fuel viscosity, cavitation phenomena, pressure-induced loads, thermal degradation, and deposit formation.

To reproduce the nonlinear character of degradation phenomena, exponential temperature-acceleration functions and saturation functions describing damage accumulation during engine operation were applied. The model considered the effect of fuel temperature at three levels, namely, 30 °C, 50 °C, and 70 °C, adopted as representative operating scenarios corresponding to low, moderate, and elevated fuel temperatures within the Common Rail system.

An original Wear Risk Index (WRI), ranging from 0 to 1, was introduced to evaluate the relative degradation tendency. WRI does not represent a direct measure of the actual wear of fuel injection components, but rather an expert-based comparative parameter enabling assessment of the potential impact of the analyzed fuels on the degradation risk of the injection system.

Simulations were conducted for engine operating times ranging from 0 to 100 h under constant injection pressure conditions characteristic of modern Common Rail systems. The modeling results were presented in the form of WRI variation curves as a function of engine operating time for different fuel variants and fuel temperatures.

3. Results

The results of laboratory tests and calculations are presented in Figures 5–10.

The specific fuel consumption was calculated using Equation (1). To determine this value, engine power and instantaneous fuel consumption are required.

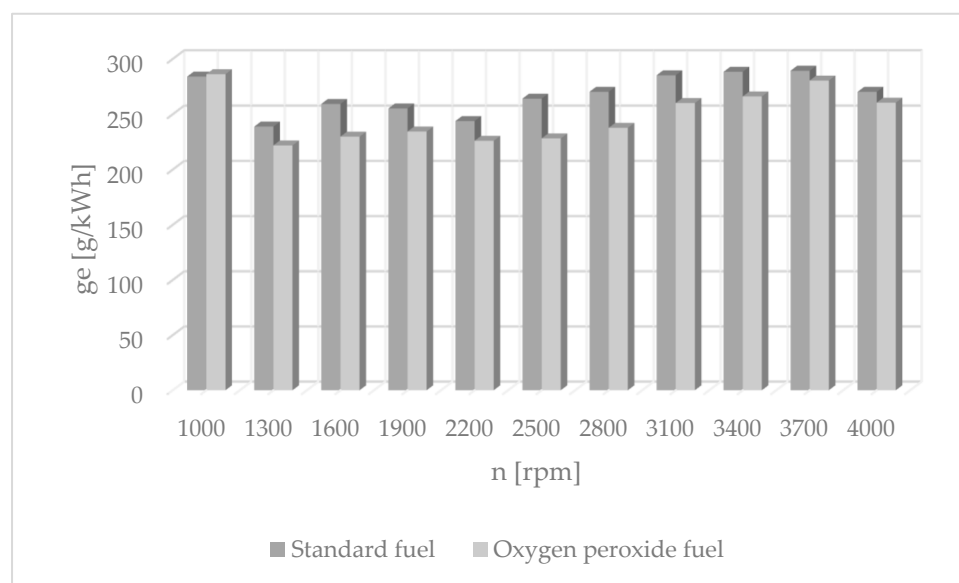


Figure 5. Engine-specific fuel consumption.

Nitrogen oxides (NOx) are inorganic chemical compounds consisting of nitrogen and oxygen atoms. They are formed during combustion at high temperatures and in the presence of excess air. These compounds are harmful to health—they are toxic, weakening the immune system in the lungs, which increases susceptibility to respiratory infections. Long-term exposure to NOx is associated with an increased risk of respiratory diseases. Nitrogen oxide emissions can be reduced by decreasing the excess air ratio, reducing the amount of heat emitted, lowering the temperature in the combustion chamber, and using appropriate fuel additives. In addition, catalytic converters are often used in exhaust systems to effectively reduce the NOx content in exhaust gases.

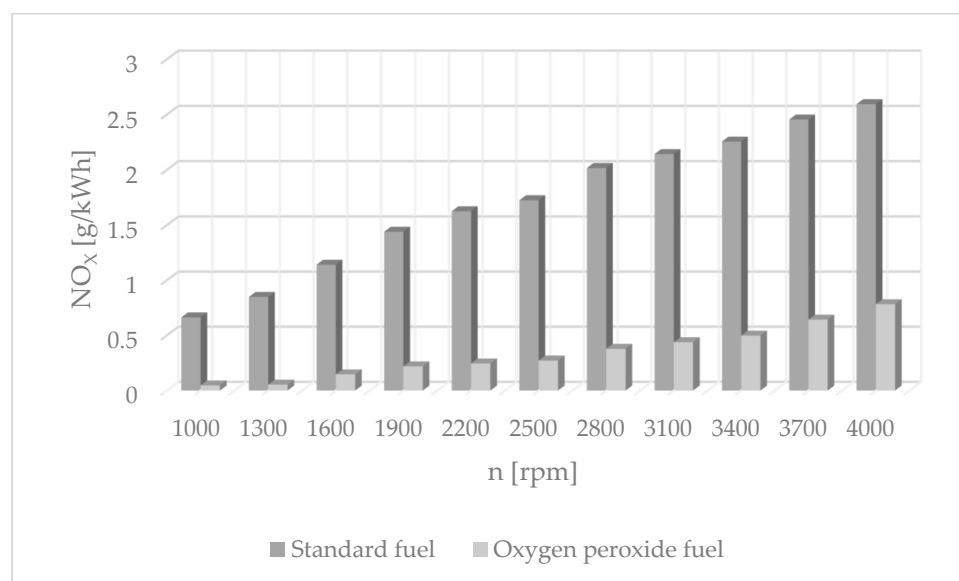


Figure 6. Nitrogen oxides emission into fumes.

Hydrocarbons (HCs) are chemical compounds consisting of carbon and hydrogen atoms. They are mainly produced because of incomplete or partial fuel combustion, as well as the decomposition of hydrocarbon compounds in chain reactions occurring during the combustion of fuel fractions. Their emission occurs particularly near the walls of the combustion chamber, where too low a temperature limits the formation of soot. Prolonged exposure to hydrocarbons can lead to serious health problems such as cancer, a weakened immune system, kidney and liver damage, and the development of cataracts.

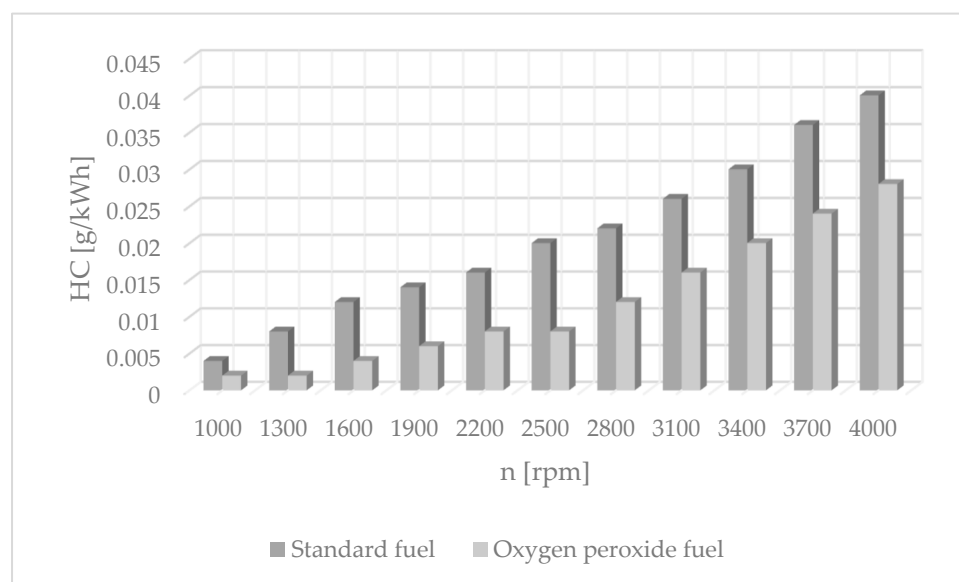


Figure 7. Hydrocarbon emission concentration in fumes.

Carbon dioxide is a gas that is not toxic to living organisms. However, excessive atmospheric concentrations trap heat radiation, contributing to the greenhouse effect. For this reason, it is important to take measures to reduce emissions of this compound into the environment.

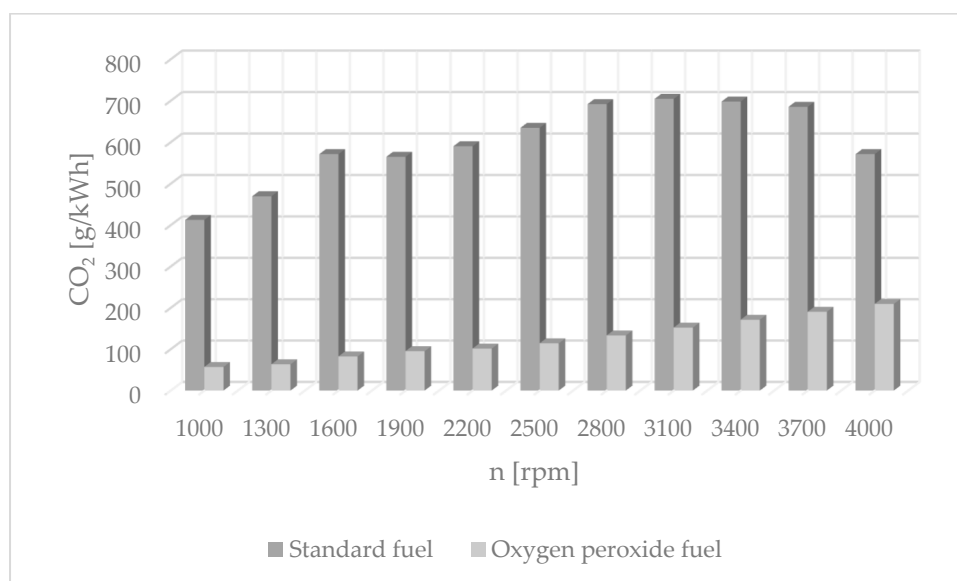


Figure 8. Carbon dioxide emission into fumes.

Soot, or particulate matter (PM), is a harmful airborne particle produced by incomplete fuel combustion. The level of exhaust smoke is most often assessed in compression-ignition (CI) engines. The main cause of particulate matter emissions is improper fuel atomization, which negatively affects its evaporation. Soot formation occurs mainly in areas of the combustion chamber where oxygen access is limited. Soot particles can enter the alveoli and then the bloodstream, causing respiratory and circulatory diseases. In addition, soot contains aromatic hydrocarbons, which increase the risk of cancer.

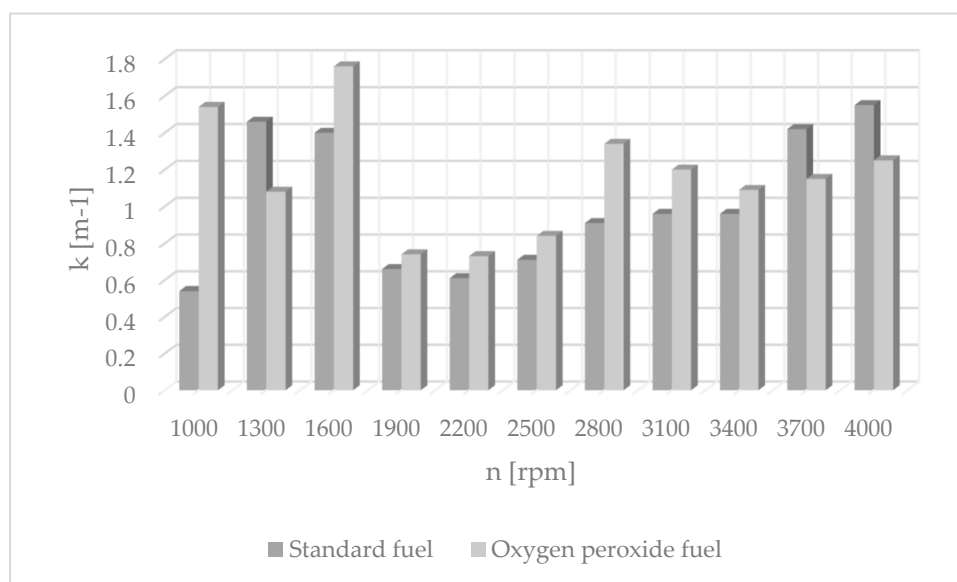


Figure 9. Solid particles concentration in fumes.

An important parameter for analyzing the processes occurring in the cylinder is the heat of combustion (Figure 10). It determines how fuel additives or the chemical properties of the fuel affect the pressure and temperature in the combustion chamber.

Modeling of the combustion process of diesel fuel and a mixture of diesel fuel with hydrogen peroxide was carried out in the Matlab environment. The simulation results are shown in Figures 11 and 12.

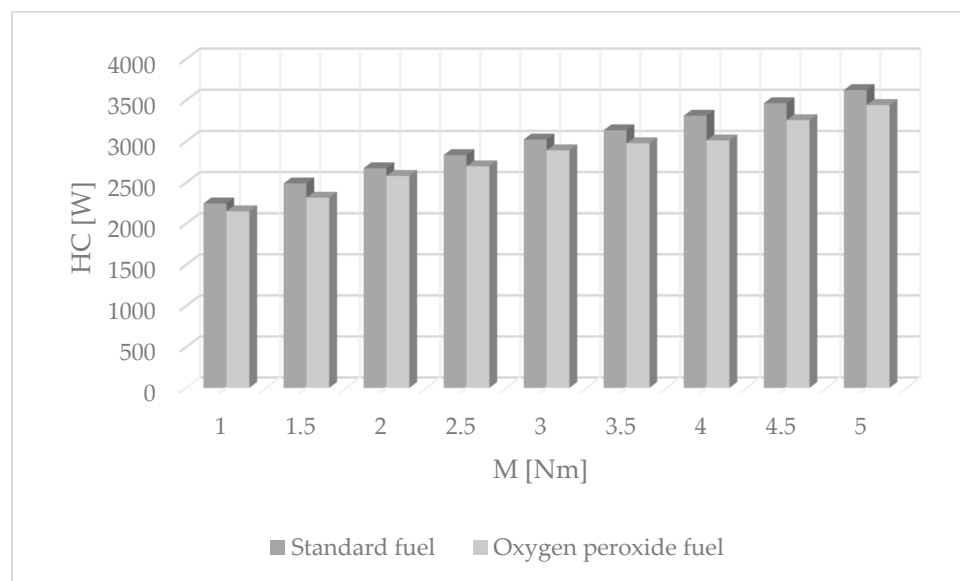


Figure 10. Heat release characteristics as a function of torque.

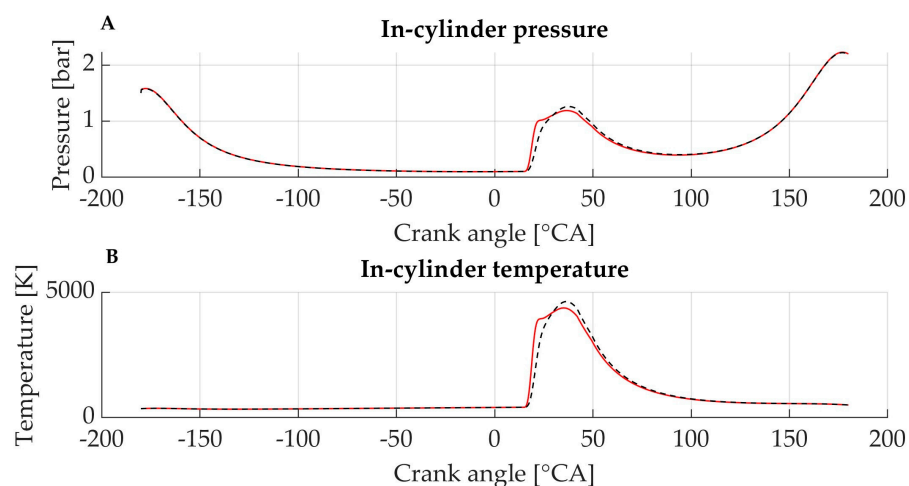


Figure 11. (A) Predicted global pressure in the cylinder. (B) Predicted global temperature in the cylinder. Black line—standard fuel, red line—oxygen peroxide fuel.

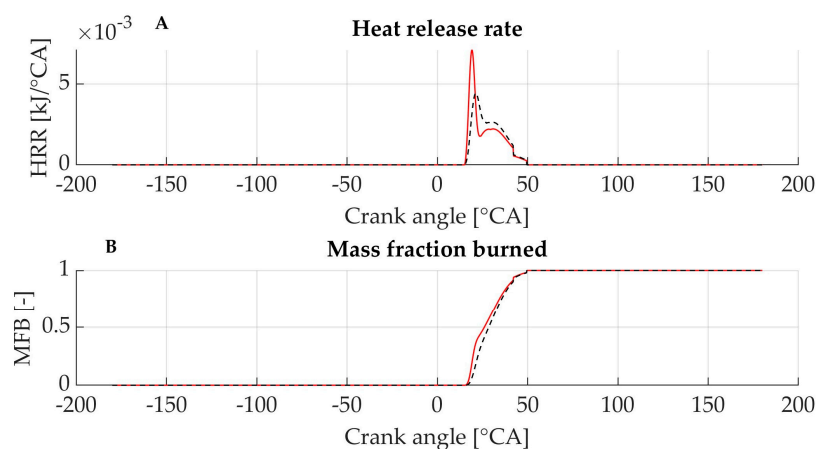


Figure 12. (A) Predicted global heat release rate. (B) Predicted global mass fraction burned. Black line—standard fuel, red line—oxygen peroxide fuel.

Due to the lack of long-term experimental data concerning the durability of the Common Rail injection system supplied with a diesel fuel–hydrogen peroxide blend, a nonlinear digital twin model was developed (Figures 13–15).

The purpose of the developed model was not to directly determine the actual geometrical or mass wear of injection system components, but rather to evaluate the relative degradation tendency of the system operating under chemically aggressive fuel conditions.

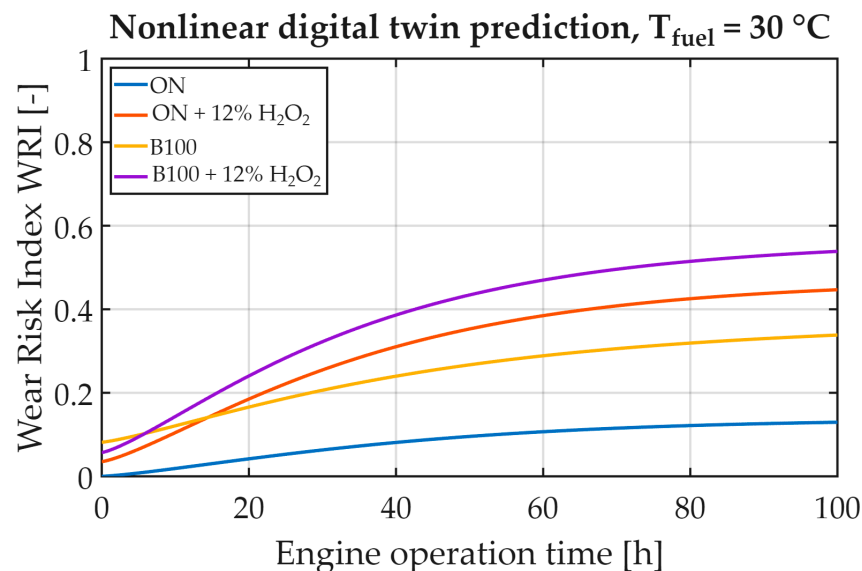


Figure 13. Nonlinear digital twin prediction model of injection system wear for selected fuels at a fuel temperature of 30 °C.

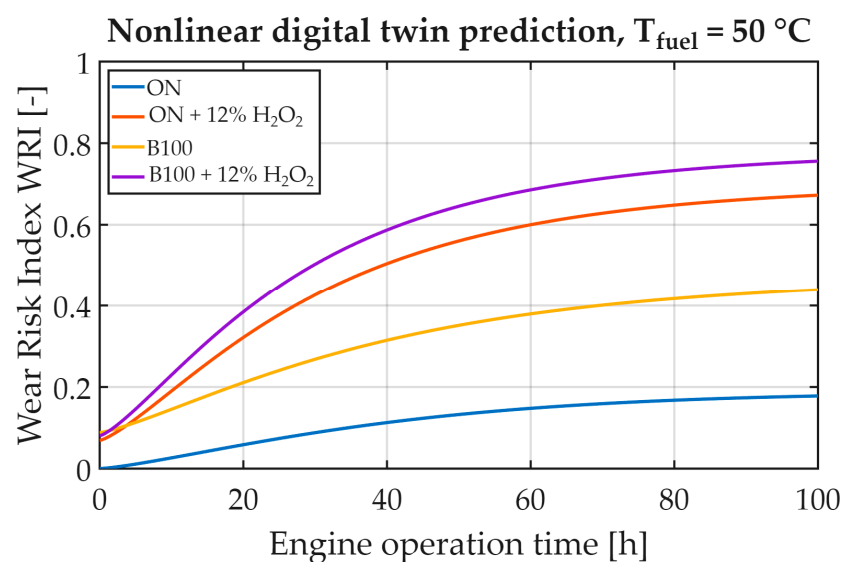


Figure 14. Nonlinear digital twin prediction model of injection system wear for selected fuels at a fuel temperature of 50 °C.

The model was developed for three fuel-temperature operating scenarios within the fuel supply system:

- 30 °C—low/moderate fuel-temperature conditions, corresponding, for example, to engine start-up or mild operating conditions;
- 50 °C—a typical fuel temperature during stabilized engine operation;
- 70 °C—elevated fuel temperature conditions, which may occur during prolonged engine operation, fuel recirculation, and heating of the Common Rail system.

These temperatures were not selected arbitrarily but were chosen based on fuel-flow modelling in the injector nozzle reported in the literature [1].

The current model does not represent the actual physical wear of the injector but rather a relative degradation risk index (WRI). WRI may be interpreted as follows:

- $WRI < 0.30$ —low degradation risk,
- $0.30 \leq WRI < 0.60$ —moderate degradation risk,
- $WRI > 0.60$ —high potential degradation risk.

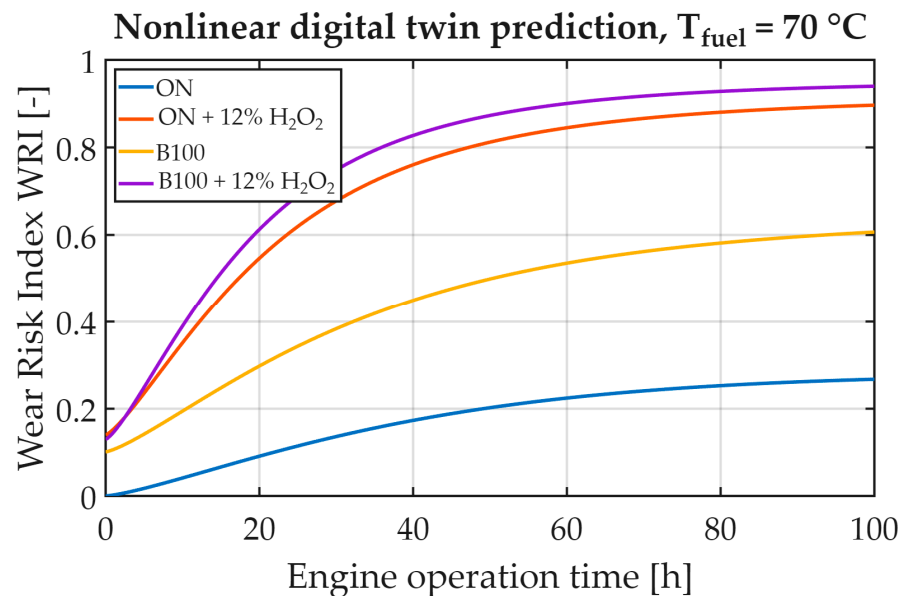


Figure 15. Nonlinear digital twin prediction model of injection system wear for selected fuels at a fuel temperature of $70\text{ }^{\circ}\text{C}$.

4. Discussion

Diesel engines remain pivotal in transportation, power generation, and industrial applications due to their high thermal efficiency and durability. However, their operation is closely linked to the formation of regulated pollutants, such as nitrogen oxides (NO_x) and particulate matter (soot), which are governed by the underlying combustion kinetics. Understanding and modeling the kinetic processes of diesel combustion is thus essential for improving engine efficiency, meeting stringent emission standards, and enabling the adoption of alternative fuels and advanced combustion strategies [39,40]. Diesel combustion involves a complex network of chemical reactions, spanning from low-temperature oxidation to high-temperature pyrolysis and soot formation. During the combustion process of a fuel–air mixture, numerous physicochemical phenomena occur [41]:

- ignition delay and two-stage ignition phenomena,
- high- and low-temperature reactivity,
- soot precursor (PAH, acetylene) formation,
- NO_x and other pollutant pathways.

For the theoretical analysis of the combustion process, a single-zone zero-dimensional thermodynamic model of a CI engine was employed to analyze the combustion of two fuels: conventional diesel fuel and diesel fuel with the addition of 10% of a 12% hydrogen peroxide solution. The model accounts for the effect of additional oxygen introduced through the decomposition of H₂O₂, using a three-stage Wiebe function and a modified Arrhenius correlation for autoignition delay. Both the three-stage Wiebe function and the modified Arrhenius correlation serve as essential tools for modeling autoignition delay in combustion. The Wiebe function excels at detailing combustion progress (i.e., the

evolution of mass fraction burned and heat release rate) across distinct combustion phases, while the modified Arrhenius correlation provides a robust framework to capture temperature-dependent kinetic behaviors, especially under variable operating pressures and in regimes exhibiting negative temperature coefficient behavior. Although they address different aspects, one being more empirical and the other more kinetic-based, their integration in unified frameworks offers complementary strengths for enhanced predictive accuracy under a wide range of operating conditions [42].

Hydrogen peroxide is a compound that indirectly governs the course of autoignition and the transition between low-temperature and high-temperature oxidation regimes during the combustion process in a CI engine. Its significance primarily arises from its involvement in chain-branching and chain-propagation reactions, leading to the formation of highly reactive $\text{OH}\cdot$ and $\text{HO}_2\cdot$ radicals.

Hydrogen peroxide influences the diesel engine combustion process by enhancing combustion efficiency, reducing ignition delay, and promoting radical formation, which assists in fuel oxidation and soot reduction. When optimally dosed (typically between 5% and 15% by volume), H_2O_2 improves brake thermal efficiency and reduces emissions (CO , HC , particulate matter, and NO_x), but excessive concentrations may cause higher combustion temperatures and increased NO_x emissions. Its effectiveness is rooted in both chemical and physical mechanisms, including enhanced atomization and micro-explosions in emulsified fuels.

The combustion characteristics of hydrogen peroxide in diesel engines affects ignition delay and flame in the following ways [28,32,43]:

- H_2O_2 addition consistently shortens ignition delay in diesel combustion, primarily by increasing the cetane number and promoting early radical formation (notably OH). This effect is most pronounced at low to moderate concentrations (5–10% by volume), with diminishing returns or even adverse effects (e.g., slowed heat release) at higher concentrations.
- Enhanced laminar flame speed and more complete combustion are observed with H_2O_2 , attributed to increased radical pool and improved fuel–air mixing. However, excessive H_2O_2 can destabilize the flame or lead to abnormal combustion.
- The ignition-promoting effect of H_2O_2 is robust, but optimal dosing is critical to avoid negative impacts on combustion stability.

The ignition delay was calculated based on the Arrhenius equation extended by the oxygen availability factor OA . This factor determines the extent to which oxygen limits the rate of the chemical reaction (8) [44]:

$$\tau_{\text{ID}} = A_s \exp\left(\frac{E_a}{RT_{\text{ref}}}\right) \left(\frac{p_{\text{ref}}}{p_0}\right)^{-n_p} OA^{-k_{OA}} \quad (8)$$

where:

- A_s — constant,
- E_a — activation energy,
- $T_{\text{ref}}, p_{\text{ref}}$ — kinetic values at TDC,
- n_p — pressure exponent,
- k_{OA} — additional oxygen influence exponent,
- OA — oxygen availability index.

The oxygen availability (OA) index was introduced to quantitatively determine the relative availability of the oxidizer in the combustion chamber in relation to the stoichiometric oxygen requirement resulting from the fuel dose. This parameter describes the extent to which the fuel–air mixture is oxygen-lean or oxygen-rich, and allows for the influence of oxygen additives such as hydrogen peroxide (H_2O_2) (9) [44]:

$$OA = \frac{m_{O_2, \text{powietrze}} + m_{O_2, H_2O_2}}{m_{O_2, \text{stoich}}} \quad (9)$$

where:

- $m_{O_2, \text{powietrze}}$ — the mass of oxygen contained in the intake air (a mass fraction of 21% oxygen is usually assumed),
- m_{O_2, H_2O_2} — additional mass of oxygen released because of the exothermic decomposition of hydrogen peroxide according to the reaction



- $m_{O_2, \text{stoich}}$ — the theoretical (stoichiometric) amount of oxygen required for the complete combustion of the mass of injected fuel with a known stoichiometric AFR_{st}.

Values of ' $OA > 1$ ' indicate increased oxygen availability relative to stoichiometric conditions, which promotes a reduction in ignition delay, more intense premixed combustion, and a faster progression of the high heat release phase. Conversely, values of ' $OA < 1$ ' indicate an oxygen deficiency, which promotes a longer ignition delay, a weaker premix phase, a prolonged diffusion combustion phase, and increased soot emissions.

The use of the OA index allows the influence of hydrogen peroxide to be considered both through increased oxygen availability and the thermal effect resulting from its exothermic decomposition. This parameter is particularly useful in simplified zero-dimensional models, where it allows the changes in mixture reactivity following the introduction of oxygen additives to be modeled without the need for complex kinetic models.

Combustion in the model was modeled using the sum of three Wiebe functions, describing respectively:

- the premixed burn phase,
- the mixing-controlled phase (mixing-controlled/diffusion burn),
- the late burn phase.

Each of the three stages is described by a classical Wiebe function.

The total mass fraction burned (MFB) is expressed as the weighted sum of the three Wiebe functions (11) [45]:

$$MFB(\theta) = E_1 M_1(\theta) + E_2 M_2(\theta) + E_3 M_3(\theta) \quad (11)$$

where E_1 , E_2 , E_3 denote the energy contributions corresponding to the premix phase, the mixing-controlled phase and the late burn phase, respectively.

The Wiebe function for the stage i takes the form (12) [46]:

$$M_i(\theta) = 1 - \exp \left[- \left(\frac{\theta - SOC_i}{\Delta \theta_i} \right)^{m_i+1} \right] \quad (12)$$

where:

- a_i — shape factor,
- m_i — the Wiebe exponent,
- $\Delta \theta_i$ — duration of the combustion stage,
- SOC_i — start of the combustion stage.

The derivative of the Wiebe function describes the combustion rate, and when multiplied by the total reaction energy, it determines the heat release rate (HRR) (13) and (14) [45]:

$$\frac{dM_i}{d\theta} = \frac{a_i(m_i+1)}{\Delta \theta_i} \left(\frac{\theta - SOC_i}{\Delta \theta_i} \right)^{m_i} \exp \left[-a_i \left(\frac{\theta - SOC_i}{\Delta \theta_i} \right)^{m_i+1} \right] \quad (13)$$

$$HRR(\theta) = Q_{\text{total}} \left(E_1 \frac{dM_1}{d\theta} + E_2 \frac{dM_2}{d\theta} + E_3 \frac{dM_3}{d\theta} \right) \quad (14)$$

where Q_{total} considers the combustion energy of diesel fuel and the energy released during the exothermic decomposition of H_2O_2 .

The start of combustion (SOC) was defined as the sum of the start of fuel injection (SOI) and the ignition delay (ID). The characteristic combustion angles were determined in accordance with the standard MFB definition:

$$\text{MFB}(\text{CA}10) = 0.1,$$

$$\text{MFB}(\text{CA}50) = 0.5,$$

$$\text{MFB}(\text{CA}90) = 0.9.$$

The CA50 parameter serves as the main measure of combustion phasing, whilst CA10 and CA90 indicate the start and end of the main combustion phase, respectively.

The decomposition of H_2O_2 generates additional heat of approximately 95–100 kJ/mol, which increases the reaction rate in the initial combustion phase and enhances the Wiebe derivative ($\frac{dM}{d\theta}$) in the premixed region [47].

This has been considered in the model by:

- increasing the proportion of energy in the premix phase,
- shortening its duration,
- increasing the shape factor a_1 , which corresponds to a more rapid, intense phase of volumetric combustion.

Wiebe's three-stage model, supported by the OA relationship that modifies the ignition delay, provides a compromise between computational complexity and the accuracy of representing combustion trends in compression-ignition engines. This model captures the key characteristics of the combustion process and enables the analysis of the effect of H_2O_2 addition on combustion dynamics without the need for advanced chemical kinetics.

An analysis of the test results shows that nitrogen oxide emissions were lower for the modified fuel across the entire speed range, whilst the modeled heat release rate was higher. The difference stems from the fact that H_2O_2 increases the amount of water, whilst the simplified model does not account for the increased water content in the engine combustion chamber. During the combustion process, the medium within the engine's working space is not homogeneous. There are areas with higher and lower temperatures. The overall higher HRR does not imply a higher global temperature in the engine chamber; consequently, the NO_x content has decreased, which is typical for fuels mixed with water vapor. At minimum engine loads, the combustion temperature is low. Under such engine operating conditions, unfavorable conditions prevail in the cylinder working space:

- fuel atomization is poorer,
- fuel evaporation is slower,
- formation of the combustible mixture is poorer,
- H_2O molecules increase the cooling of the fuel stream,
- fuel-rich zones are formed.

Such an environment promotes the formation of soot during combustion. Therefore, when analyzing the characteristics of soot emissions during tests at minimum engine speeds, they are higher for the modified fuel. Only when the engine begins to operate at medium and maximum loads does the soot content decrease compared to standard fuel. This is because:

- the combustion temperature rises,
- mixing is more intense,
- soot oxidation is more effective,

- the decomposition products of hydrogen peroxide oxidize soot more rapidly.

Soot undergoes oxidation at higher temperatures and with a higher oxygen content. At low engine loads, there is a shortage of oxygen and a lower temperature. The observed effects of the research are the result of the simultaneous interaction of chemical mechanisms (oxygen release, radical generation) and physical mechanisms characteristic of emulsion fuels (microexplosions, charge cooling). The reduction in emissions cannot be attributed solely to the chemical effects of hydrogen peroxide. The presence of about 8.8% water in the fuel mixture introduces a significant thermal effect, consisting in lowering the combustion temperature due to the high heat of water evaporation.

Hydrogen peroxide has strong oxidizing properties, which can affect the durability of fuel supply system components, especially in common rail systems. Possible hazards include corrosion, cavitation and deterioration of the lubricating properties of the fuel. No negative effects were observed in these studies in the short service life; however, the long-term effects require further durability studies.

The model calculates the relative wear-risk index of the fuel injection system, denoted as (15) [48–50]:

$$WRI \in [0,1] \quad (15)$$

where $WRI = 0$ indicates a very low degradation risk, while $WRI = 1$ represents a very high degradation risk. The index does not represent the percentage wear of the injector but rather the relative degradation risk resulting from fuel properties, fuel temperature and operating time. The model consists of several nonlinear degradation sub-models (16):

$$WRI = f(R_{ox}, R_{lub}, R_{vis}, R_{cav}, R_p, R_T, R_{dep}, R_{fuel}) \quad (16)$$

where:

- R_{ox} represents oxidation and corrosion risk,
- R_{lub} represents lubricity deterioration risk,
- R_{vis} represents viscosity-related degradation risk,
- R_{cav} represents cavitation risk,
- R_p represents high-pressure-related degradation risk,
- R_T represents thermal degradation risk,
- R_{dep} represents deposit formation risk,
- R_{fuel} represents the degradation associated with the overall change in fuel properties.

For each fuel, relative property values were calculated with respect to conventional diesel fuel [50]:

$$F_\rho = \frac{\rho}{\rho_{ON}} \quad (17)$$

$$F_v = \frac{v}{v_{ON}} \quad (18)$$

$$F_Q = \frac{Q}{Q_{ON}} \quad (19)$$

$$F_{Tz} = \frac{T_z}{T_{z,ON}} \quad (20)$$

$$F_O = \frac{O}{O_{ref}} \quad (21)$$

$$F_I = \frac{I}{I_{ref}} \quad (22)$$

where:

- ρ —fuel density,
- ν —kinematic viscosity,
- Q —calorific value,
- T_z —ignition temperature,
- O —oxygen content,
- I —iodine value,
- the subscript ON denotes the reference value for diesel fuel.

The influence of fuel temperature was described using an exponential function:

$$A_T = \exp\left(\frac{T_f - T_{ref}}{T_s}\right) \quad (23)$$

where:

- T_f —fuel temperature,
- $T_{ref} = 40\text{ }^\circ\text{C}$ —reference temperature,
- $T_s = 25\text{ }^\circ\text{C}$ —temperature sensitivity is coefficient.

This means that an increase in fuel temperature does not increase degradation risk linearly but exponentially. Therefore, at $70\text{ }^\circ\text{C}$, the model predicts a significantly higher degradation risk than at $30\text{ }^\circ\text{C}$.

The effect of operating time was described using a saturation function (24):

$$A_t = 1 - \exp\left[-3\left(\frac{t}{t_{ref}}\right)^{1,35}\right] \quad (24)$$

where:

- t —engine operating time,
- $t_{ref} = 100\text{ h}$ —reference operating time.

This function indicates that degradation risk increases rapidly during the initial period and then gradually approaches saturation.

The oxidation and corrosion risk was expressed by the following Equation (25):

$$R_{ox} = F_{ox}(1 + 0.08H^{1,25})A_TA_t \quad (25)$$

where:

- F_{ox} —fuel oxidation susceptibility,
- H — H_2O_2 concentration in the fuel [%],
- A_T —temperature influence,
- A_t —time influence.

The oxidation susceptibility coefficient F_{ox} was calculated as follows (26):

$$F_{ox} = 0.15 + 0.35F_O^{1,2} + 0.35\left(\frac{H}{12}\right)^{1,4} + 0.20F_I^{1,1} \quad (26)$$

This means that the oxidation risk increases with oxygen content, H_2O_2 concentration, iodine value, fuel temperature, and operating time.

The lubricity deterioration risk was calculated using Equation (27):

$$R_{lub} = \left(\frac{1}{F_{lub}} - 1\right)^{1,4} A_T(1 + 0.015t^{0,85}) \quad (27)$$

The relative lubricity coefficient was calculated from Equation (28):

$$F_{lub} = 1.00 + 0.12(F_v - 1) - 0.25\left(\frac{H}{12}\right) \quad (28)$$

If F_{lub} decreases, the risk of lubricity deterioration increases. The addition of H_2O_2 reduces relative lubricity, while the higher viscosity of B100 partially improves it.

The viscosity-related degradation risk was calculated from Equation (29):

$$R_{vis} = |F_v - 1|^{1.25} (1 + 0.006t) [1 + 0.01 \max(T_f - T_{ref}, 0)] \quad (29)$$

The model assumes that both excessively low and excessively high viscosity relative to diesel fuel may deteriorate injector operating conditions.

The cavitation risk was calculated using Equation (30):

$$R_{cav} = F_{cav} \left(\frac{p_{inj}}{p_{ref}} \right)^{1.7} (1 + 0.035H) [1 + 0.012 \max(T_f - T_{ref}, 0)] A_t \quad (30)$$

The cavitation susceptibility coefficient F_{cav} was calculated using Equation (31):

$$F_{cav} = 0.30 + 0.25 |F_v - 1|^{1.2} + 0.30 \left(\frac{H}{12} \right)^{1.3} + 0.15 F_p \quad (31)$$

The cavitation risk increases with injection pressure, H₂O₂ concentration, viscosity deviation from diesel fuel, fuel density, and fuel temperature.

The pressure fatigue risk was calculated using Equation (32):

$$R_p = \left(\frac{p_{inj}}{p_{ref}} \right)^2 A_t \quad (32)$$

where:

- p_{inj} —injection pressure,
- $p_{ref} = 160$ MPa—reference pressure.

The higher the injection pressure, the greater the mechanical loading risk of injector components.

Equation (33) describes thermal degradation risk:

$$R_T = \left(\frac{T_f}{80} \right)^{2.2} A_t \quad (33)$$

The thermal degradation risk increases nonlinearly with increasing fuel temperature [51].

The deposit formation risk was described by Equation (34):

$$R_{dep} = F_{dep} \left[1 - \exp\left(-2.2 \left(\frac{t}{t_{ref}} \right)^{1.15} \right) \right] [1 + 0.01 \max(T_f - T_{ref}, 0)] \quad (34)$$

The deposit formation coefficient F_{dep} was calculated using Equation (35):

$$F_{dep} = 0.25 + 0.35 F_I^{1.25} + 0.20 F_O + 0.10 |F_v - 1| \quad (35)$$

The deposit formation risk increases with iodine value, oxygen content, viscosity deviation from the reference fuel, fuel temperature, and operating time.

The degradation risk resulting from the overall change in fuel properties was described by Equation (36):

$$R_{fuel} = F_{fuel} A_T A_t \quad (36)$$

The coefficient describing fuel-property-related degradation risk was calculated using Equation (37):

$$F_{fuel} = 0.30 |F_p - 1|^{1.2} + 0.30 |F_v - 1|^{1.2} + 0.20 |1 - F_Q|^{1.2} + 0.20 |1 - F_{Tz}|^{1.2} \quad (37)$$

This term describes the overall deviation of a given fuel from the physicochemical properties of conventional diesel fuel.

The total raw degradation-risk index was calculated as a weighted sum of all degradation mechanisms (38):

$$R_{raw} = w_{ox} R_{ox} + w_{lub} R_{lub} + w_{vis} R_{vis} + w_{cav} R_{cav} + w_p R_p + w_T R_T + w_{dep} R_{dep} + w_{fuel} R_{fuel} \quad (38)$$

The following weighting coefficients were assumed:

- $w_{ox} = 0.25$,

- $w_{lub} = 0.18$,
- $w_{vis} = 0.12$,
- $w_{cav} = 0.14$,
- $w_p = 0.08$,
- $w_T = 0.08$,
- $w_{dep} = 0.10$,
- $w_{fuel} = 0.05$.

The sum of all weighting coefficients equals: $\sum w_i = 1$

The final degradation-risk index was calculated using the saturation function (39):

$$WRI = 1 - \exp(-R_{raw}) \quad (39)$$

Therefore:

$$0 \leq WRI \leq 1$$

The WRI values were interpreted as follows:

- $WRI < 0.30$ —low degradation risk,
- $0.30 \leq WRI < 0.60$ —moderate degradation risk,
- $WRI \geq 0.60$ —high degradation risk.

The cavitation susceptibility coefficient [52] was introduced as an expert-defined nonlinear parameter describing the relative tendency of the fuel to intensify cavitation-related degradation processes inside the injector nozzle. The equation considers viscosity deviation, hydrogen peroxide concentration, and fuel density relative to conventional diesel fuel. The model does not directly calculate cavitation number or multiphase flow parameters but instead provides a simplified comparative approximation of cavitation-related degradation tendency.

5. Conclusions

An analysis of the test results shows that using hydrogen peroxide as a fuel additive in a compression ignition engine mainly affects the emission of nitrogen oxides, hydrocarbons, and carbon dioxide. When analyzing the environmental characteristics of engine operation, hydrogen peroxide slightly increases the soot content in the exhaust gases. Soot is crystallized carbon that forms at low temperatures. Analysis of the measurement results indicates that adding hydrogen peroxide increases particulate emissions in the minimum and medium range of engine operations. This means that the oxidizing effect of hydrogen peroxide does not compensate for the deterioration of the fuel atomization process and local oxygen shortages under these conditions. Only at higher loads, where the combustion temperature and mixing intensity are higher, is an improvement in the soot oxidation process observed. Laboratory tests have shown that the use of a 10% additive of a 12% hydrogen peroxide solution increased the cetane number of the fuel from approximately 50.0 to 52.0. The increase in the cetane number reduced the activation energy of the combustion reaction and shortened the self-ignition delay period, which contributed to a more stable combustion process in a compression ignition engine. The tests carried out on an engine dynamometer showed a significant impact of the hydrogen peroxide additive on the ecological parameters of engine operation. A reduction in nitrogen oxide (NOx) and unburned hydrocarbon (HC) emissions was observed across a wide range of engine crankshaft speeds. This effect can be explained by the presence of additional oxygen and hydrogen in the fuel, which intensifies oxidation reactions and lowers local combustion temperatures, promoting NOx reduction. At the same time, the test results showed a slight increase in particulate matter (soot) emissions, which may be due to changes in the diffusion combustion and afterburning phases, as well as modifications to the fuel atomi-

zation conditions in the combustion chamber. Carbon dioxide emissions did not change significantly, indicating that the addition of hydrogen peroxide does not worsen the CO₂ emissions balance or the energy efficiency of the engine. It should be emphasized that the proposed solution does not require any interference with the engine design or the use of costly external hydrogen supply systems, which is a significant advantage for practical application. Further research should focus on long-term engine operation and the impact of the additive on the durability of fuel system components and the combustion chamber. The next stage of research into the possibility of reducing the content of solid particles in exhaust gases will involve the use of modified fuel injectors for an engine running on the presented fuel additive. It should be emphasized that in this paper no studies of the long-term storage stability of the prepared fuel emulsion have been carried out, which is a limitation of the work. Hydrogen peroxide is a thermodynamically unstable compound and can decompose slowly according to the reaction: $\text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + 1/2\text{O}_2$. This process can be catalyzed by the presence of metal ions and organic compounds, which can lead to an increase in pressure in the fuel system and fuel degradation. Additionally, the presence of sodium alginate as an emulsifier may affect the stability of the system. Therefore, future research should include analysis of fuel stability, including changes in chemical composition, phase separation and changes in storage pressure.

The performed modeling using a nonlinear digital twin demonstrated a significant influence of fuel type, hydrogen peroxide addition, and fuel temperature on the predicted degradation tendency of the Common Rail injection system. The lowest values of the Wear Risk Index (WRI) were obtained for conventional diesel fuel, confirming its highest operational stability among the analyzed fuels. The addition of 12% H₂O₂ to diesel fuel increased the predicted degradation risk of the injection system, mainly due to the increased oxidation activity of the fuel, deterioration of lubricating properties, and increased susceptibility to cavitation phenomena.

The B100 fuel exhibited a higher predicted degradation tendency than conventional diesel fuel, which may result from the higher oxygen content, higher viscosity, and higher iodine value of fatty acid methyl esters. The highest WRI values were obtained for the B100 + 12% H₂O₂ blend. The model indicates that the simultaneous presence of methyl esters and hydrogen peroxide may lead to a synergistic increase in degradation-related processes such as oxidation, deposit formation, lubricity deterioration, cavitation intensification, and thermal degradation of injection system components.

Increasing fuel temperature from 30 °C to 70 °C significantly increased the predicted degradation risk for all analyzed fuels. The modeling results indicate that fuel temperature may be one of the key parameters affecting the durability of modern Common Rail systems. The applied nonlinear model enabled the inclusion of the progressive character of injector degradation. The model demonstrated that the increase in degradation risk is not linear but accelerates with increasing fuel temperature, operating time, and H₂O₂ concentration.

The developed digital twin does not represent a direct model of the actual physical wear of injection system components. The WRI should be interpreted as a relative degradation tendency indicator enabling a comparative assessment of the potential influence of different fuels on injection system durability. The obtained results indicate that the application of fuels containing H₂O₂ may require additional investigations concerning fuel chemical stability, material compatibility, seal durability, corrosion resistance of injection system components, and long-term operation of injectors and high-pressure pumps.

The developed model may serve as a preliminary engineering tool for assessing the relative degradation risk of injection systems operating with alternative and oxygenated fuels; however, its full validation requires long-term experimental investigations and calibration of the model based on real measurements of Common Rail component wear.

Author Contributions: Supervision, writing—review, T.O., K.F.A., D.B. and P.D.; Conceptualization, data acquisition and interpretation, investigation and writing—original draft preparation and editing, T.O.; software, investigation, writing—review and editing, K.F.A. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: The original contributions presented in this study are included in the article. Further inquiries can be directed to the corresponding author.

Conflicts of Interest: The authors declare no conflicts of interest.

References

1. Eliaz, J.; Osipowicz, T.; Abramek, K.F.; Mozga, Ł. Model Issues Regarding Modification of Fuel Injector Components to Improve the Injection Parameters of a Modern Compression Ignition Engine Powered by Biofuel. *Appl. Sci.* **2019**, *9*, 5479.
2. Ambrozik, A. *Selected Issues of Thermal Processes in Piston Internal Combustion Engines*; Kielce University of Technology: Kielce, Poland, 2003.
3. Heywood, J.B. Correlations for ignition delay in engines. In *Internal Combustion Engines Fundamentals*; McCraw–Hill Book Co.: New York, NY, USA, 1988; Volume 1, pp. 553–554.
4. Vembathu Rajesh, A.; Mathalai Sundaram, C.; Sivaganesan, V.; Nagarajan, B.; Harikishore, S. Emission reduction techniques in CI engine with catalytic converter. *Mater. Today Proc.* **2020**, *21*, 98–103.
5. Milojević, S.; Stopka, O.; Kontrec, N.; Orynycz, O.; Hlatka, M.; Radojković, M.; Stojanović, B. Analytical Characterization of Thermal Efficiency and Emissions from a Diesel Engine Using Diesel and Biodiesel and Its Significance for Logistics Management. *Processes* **2025**, *13*, 2124.
6. Udhayakumar, N.; Mani, M.; Ramesh Babu, S.; Karthikkeyan, G.; Peace John Samuel, K.; Karna, V. An experimental investigation on emission characteristics in CI engine with zinc and vanadium coated catalytic converter. *Mater. Today Proc.* **2022**, *62*, 2250–2255.
7. Karthikkeyan, V.; Thiyagarajan, S.; Edwin Geo, V.; Ashok, B.; Nanthagopal, K.; Ong Hwai Chyuan Vignesh, R. Simultaneous reduction of NO_x and smoke emissions with low viscous biofuel in low heat rejection engine using selective catalytic reduction technique. *Fuel* **2019**, *255*, 115854.
8. Abu-Jrai, A.M.; Al-Muhtaseb, A.H.; Hasan, A.O. Combustion, performance, and selective catalytic reduction of NO_x for a diesel engine operated with combined tri fuel (H₂, CH₄, and conventional diesel). *Energy* **2017**, *115*, 901–910.
9. Guziłkowska Tic, J.; Tic, W.J. Modifiers used in the combustion process of fuel oils and solid fuels. *Chemik* **2012**, *66*, 1203–1210.
10. Park, J.; Oh, J. Study on the characteristics of performance, combustion, and emissions for a diesel water emulsion fuel on a combustion visualization engine and a commercial diesel engine. *Fuel* **2022**, *311*, 122520.
11. Saha, D.; Roy, B. Effects of plastic-grocery-bag derived oil-water-diesel emulsions on combustion, performance and emission characteristics, and exergoeconomic aspects of compression ignition engine. *Sustain. Energy Technol. Assess.* **2022**, *54*, 102877.
12. Dogan, B.; Celik, M.; Bayindirli, C.; Erol, D. Exergy, exergoeconomic, and sustainability analyses of a diesel engine using bio-diesel fuel blends containing nanoparticles. *Energy* **2023**, *274*, 127278.
13. Leach, F.C.P.; Davy, M.; Terry, B. Combustion and emissions from cerium oxide nanoparticle dosed diesel fuel in a high speed diesel research engine under low temperature combustion (LTC) conditions. *Fuel* **2021**, *288*, 119636.
14. Zhang, S.; Tian, J.; Li, J.; Lv, J.; Wang, S.; Zhang, Y.; Dong, R.; Gao, S.; Cao, C.; Tan, D. Investigation on combustion, performance and emission characteristics of a diesel engine fueled with diesel/alcohol/n-butanol blended fuels. *Fuel* **2022**, *320*, 123975.
15. Klyus, O. The use of turbulization in preliminary fuel treatment in self-ignition engines. *Combust. Engines* **2009**, *138*, 49–53.
16. Sa, B.; Klyus, O.; Markov, V.; Kamaltdinov, V. A numerical study of the effect of spiral counter grooves on a needle on flow turbulence in a diesel injector. *Fuel* **2021**, *290*, 120013.
17. Gianotti, E.; Taillades-Jacquín, M.; Carmona, A.R.; Taillades, G.; Rozière, J.; Jones, D.J. Hydrogen generation via catalytic partial dehydrogenation of gasoline and diesel fuels. *Appl. Catal. B Environ.* **2016**, *185*, 233–241.
18. Wang, N.; Qiu, J.; Wu, J.; Yuan, X.; You, K.; Luo, H. Microwave assisted synthesis of Sn-modified MgAlO as support for platinum catalyst in cyclohexane dehydrogenation to cyclohexene. *Appl. Catal. A Gen.* **2016**, *516*, 9–16.
19. Echeverri, A.; Gomez, T.; Hadad, C. Ammonia borane dehydrogenation tendencies using Pt₄, Au₄, and Pt₂Au₂ clusters as catalysts. *Mol. Catal.* **2019**, *471*, 9–20.

20. Lodi, F.; ☉are, A.; Arora, P.; Stevanovic, S.; Ristovski, ☉.; Brown, R.J.; Bodisco, T. Combustion characteristics of microalgae-based diethyl phthalate biofuel during ambient, preheated, and hot engine operation. *Fuel* **2023**, *331*, 125890.
21. Mendiburu, A.☉.; Lauermann, C.H.; Hayashi, T.C.; Marinos, D.J.; Rodrigues da Costa, R.B.; Coronado, C.J.R.; Roberst, J.J.; De Carvahlo, J.A., Jr. Ethanol as a renewable biofuel: Combustion characteristics and application in engines. *Energy* **2022**, *257*, 124288.
22. Elfasakhany, A. Investigation of biomass powder as a direct solid biofuel in combustion engines: Modelling assessment and comparisons. *Ain Shams Eng. J.* **2021**, *12*, 2991–2998.
23. Abrar, I.; Bhaskarwar, A.N. Microemulsion fuels for compression ignition engines: A review on engine performance and emission characteristics. *Fuel* **2019**, *257*, 115944.
24. Saha, D.; Roy, B.; Pattanyak, S.; Mishra, L.; Kundu, P.P. Performance, emission, combustion, exergy, exergoeconomic and sustainability analyses of EGR incorporated CI engine fuelled with areca nut husk nano-additive dosed plastic oil–water-diesel emulsion blend. *Therm. Sci. Eng.* **2024**, *47*, 102317.
25. Nayak, S.K.; Nizatic, S.; Pham, V.V.; Huang, ☉.; Ölcer, A.I.; Bui, V.G.; Wattanavichien, K. Influence of injection timing on performance and combustion characteristics of compression ignition engine working on quaternary blends of diesel fuel, mixed biodiesel, and t-butyl peroxide. *J. Clean. Prod.* **2022**, *333*, 130160.
26. Kumar, C.B.; Lata, D.B.; Mahto, D. Analysis of ignition delay by taking Ditertiary-butyl peroxide as an additive in a dual fuel diesel engine using hydrogen as a secondary fuel. *Int. J. Hydrogen Energy* **2020**, *45*, 14806–14820.
27. Nguyen, V.N.; Ganesan, N.; Ashok, B.; Balasubramanian, D.; Anabayan, K.; Lawrence, K.R.; Tamilvanan, A.; Le, D.T.N.; Truong, T.H.; Tran, V.D.; et al. Eco-Friendly perspective of hydrogen fuel addition to diesel engine: An inclusive review of low-temperature combustion concepts. *Int. J. Hydrogen Energy* **2025**, *104*, 344–366.
28. Chebattina, K.R.R.; Vadapalli, S.; Pathem, U.C.; Sirasapalli, A.; Lodagala, C.C.; Billakurthi, S.M.S.R.; Annamdevara, N.C.S.; Mohammad, A.R. H₂ O₂ as fuel additive in bio-diesel for emission reduction and performance enhancement of variable compression ratio (VCR) diesel engine. *Mater. Today Proc.* **2021**, *47*, 5697–5700.
29. Nguyen, K.B.; Dan, T.; Asano, I. Combustion, performance and emission characteristics of direct injection diesel engine fueled by Jatropa hydrogen peroxide emulsion. *Energy* **2014**, *74*, 301–308.
30. Famfulik, J.; Richtar, M.; Smirau, J.; Muckova, P.; Sarkan, B.; Dresler, P. Internal combustion engine diagnostics using statistically processed Wiebe function. *Eksplot. Niezawodn. — Maint. Reliab.* **2021**, *23*, 505–511.
31. Moujдин, I.A.; Khan, M.S.; Abulkhair, H.A.; Shaiban, A.A.; Organji, H.A.; Alsaiani, A.O. Influence of hydrogenated diesel/H₂O₂ blend fuel on diesel engine performance and exhaust emission characterization. *Sci. Rep.* **2023**, *13*, 836.
32. Milojević, S. Reconstruction of existing city buses on diesel fuel for drive on hydrogen. *Appl. Eng. Lett.* **2016**, *1*, 16–23.
33. Grzejda, R. Modelling nonlinear preloaded multi-bolted systems on the operational state. *Eng. Trans.* **2016**, *64*, 525–531.
34. Grzejda, R. Thermal strength analysis of a steel bolted connection under bolt loss conditions. *Eksplot. Niezawodn. — Maint. Reliab.* **2022**, *24*, 269–274.
35. Osipowicz, T.; Koniuszy, A.; Taustyka, V.; Abramek, K.F.; Mozga, Ł. Evaluation of Ecological Parameters of a Compression Ignition Engine Fueled by Diesel Oil with an Eco Fuel Shot Liquid catalysts. *Catalysts* **2023**, *13*, 1513.
36. ☉are, A.; Toghraei, S.M.M.; Hosseini, A. Development of an emulsifier with sodium caseinate-gallic acid-bitter almond gum ternary conjugate: Focusing on structural, antioxidant, and functional properties. *Food Res. Int.* **2025**, *222*, 117659.
37. ISO 8178-1:2020; Reciprocating Internal Combustion Engines: Exhaust Emission Measurement. International Organization for Standardization: Geneva, Switzerland, 2020. Available online: <https://www.iso.org/standard/79330.html> (accessed on 30 October 2023).
38. PN-EN ISO 5165:2021-02; Petroleum Products—Determination of the Ignition Quality of Diesel Fuels—Cetane Engine Method. Polish Committee for Standardization: Warsaw, Poland, 2021.
39. Migliaccio, M.; Beatrice, C.; Briani, M.; Fraioli, V. Numerical simulations of Diesel engine combustion by means of OpenFOAM CFD ToolBox. In Proceedings of the SAE Technical Papers Conference: 9th International Conference on Engines and Vehicles, Naples, Italy, 13 September 2009.
40. Jena, A.; Agarwal, A.K. Strategical Evolution of Clean Diesel Combustion. In *Advanced Combustion for Sustainable Transport Energy, Environment, and Sustainability*; Springer: Singapore, 2022; pp. 9–42.
41. Frassoldati, A.; D’Errico, G.; Lucchini, T.; Stagni, A.; Cuoci, A.; Faravelli, T.; Onorati, A.; Ranzi, E. Reduced kinetic mechanisms of diesel fuel surrogate for engine CFD simulations. *Combust. Flame* **2015**, *162*, 3991–4007.
42. Kamimoto, T.; Kobayashi, H. Combustion processes in diesel engines. *Prog. Energy Combust. Sci.* **1991**, *17*, 163–189.

43. Peng, H.S.; Cheng, D.; Hang, F.; Hong, T. Effects of hydrogen peroxide on the low-temperature ignition delay times of ethylene/air/Ar mixtures in an RCM. *Fuel* **2024**, *358*, 130282.
44. DelVescoco, D.; Kokjohn, S.; Reitz, R. The Development of an Ignition Delay Correlation for PRF Fuel Blends from PRF0 (n-Heptane) to PRF100 (iso-Octane). *SAE Int.* **2016**, *9*, 520–535.
45. Hu, S.; Wang, H.; Yang Ch Wang, Y. Burnt fraction sensitivity analysis and 0-D modelling of common rail diesel engine using Wiebe function. *Appl. Therm. Eng.* **2017**, *115*, 170–177.
46. Imbert, B.; Lafosse, F.; Catoire, L.; Paillard, C.E.; Khasainov, B. Formulation reproducing the ignition delays simulated by a detailed mechanism: Application to n-heptane combustion. *Combust. Flame* **2008**, *155*, 380–408.
47. Mohan, S.; Dinesha, P. Performance and emissions of biodiesel engine with hydrogen peroxide emulsification and cerium oxide (CeO₂) nanoparticle additives. *Fuel* **2022**, *319*, 123872.
48. Liu, L.; Shao, W.; Yan, Y.; Liu, D.; Hang, J. Intelligent self-adaptation of marine engine degradation based on a digital-Twin model. *Energy Convers. Manag.* **2025**, *341*, 119995.
49. Duarte, E.P.; Viegas, E.K.; Santin, A.O. A machine learning-based digital twin model for pressure prediction in the fuel injection system. In Proceedings of the IECON 2022—48th Annual Conference of the IEEE Industrial Electronics Society, Brussels, Belgium, 17–20 October 2022.
50. Fuller, A.; Fan, S.; Day, C.; Barlow, C. Digital Twin: Enabling technologies, challenges and open research. *IEEE Access* **2020**, *8*, 108952–108971.
51. Magnotti, G.; Battistoni, M.; Saha, K.; Som, S. Evaluation of a new cavitation erosion metric based on fluid-solid energy transfer in channel flow simulations. In Proceedings of the Engineering, Environmental Science, Physics 14th Triennial International Conference on Liquid Atomization and Spray Systems, Chicago, IL, USA, 22–26 July 2018.
52. Magnotti, G.; Som, S. Assessing Fuel Property Effects on Cavitation and Erosion Propensity Using a Computational Fuel Screening Tool. In Proceedings of the ASME Internal Combustion Engine Division Fall Technical Conference 2019, Chicago, IL, USA, 20–23 October 2019.

Disclaimer/Publisher's Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.