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Obtaining the Synthetic Fuels from Waste Plastic and Their Effect on Cavitation Formation in a Common-Rail Diesel Injector

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Abstract: The presented paper addresses two significant issues of the present time. In general, the studies of the effect of synthetic fuels on cavitation formation and cavitation erosion prediction in the nozzle tip of common-rail diesel injectors were addressed. The first problem is plastic waste, which can have a significant negative environmental impact if not treated properly. Most plastic waste has high energy value, so it represents valuable material that can be used in resource recovery to produce various materials. One possible product is synthetic fuel, which can be produced using thermal and catalytic pyrolysis processes. The first issue addressed in the presented paper is the determination of fuel properties since they highly influence the fuel injection process, spray development, combustion, etc. The second is the prediction of cavitation development and cavitation erosion in a common-rail diesel injector when using pyrolytic oils from waste plastic. At first, pyrolytic oils from waste high- and low-density polyethylene were obtained using thermal and catalytic pyrolysis processes. Then, the obtained oils were further characterised. Finally, the properties of the obtained oils were implemented in the ANSYS FLUENT computational program and used in the study of the cavitation phenomena inside an injection nozzle hole. The cavitating flow in FLUENT was calculated using the Mixture Model and Zwart-Gerber-Belamri cavitation model. For the modelling of turbulence, a realisable $k-\epsilon$ model with Enhanced Wall Treatment was used, and an erosion risk indicator was chosen to compare predicted locations of cavitation erosion. The results indicate that the properties of the obtained pyrolytic oils have slightly lower density, surface tension and kinematic viscosity compared to conventional diesel fuel, but these minor differences influence the cavitation phenomenon inside the injection hole. The occurrence of cavitation is advanced when pyrolytic oils are used, and the length of cavitation structures is greater. This further influences the shift of the area of cavitation erosion prediction closer to the nozzle exit and increases its magnitude up to 26% compared to diesel fuel. All these differences have the potential to further influence the spray break-up process, combustion process and emission formation inside the combustion chamber.

Keywords: plastic waste; synthetic fuels; pyrolytic oils; common-rail; cavitation; erosion; transient simulation

1. Introduction

Internal combustion engines are still the main propulsion systems in the transport sector worldwide [1]. In recent decades, much focus has been on producing and developing biofuels from different raw materials [2,3]. Studies like [4] have confirmed the possible usage of biofuels in vehicles with internal combustion engines. Despite all the benefits that biofuels can bring, they will never be able to completely replace fossil fuels due to their interference with the food chain [5]. The focus has been shifted to producing low-carbon fuels (also called E-fuel) and synthetic fuels [6,7]. E-fuels are produced in several steps from hydrogen and carbon using different processes. Synthetic fuels can be produced from different solid materials, from which waste plastic has great potential.

Plastic has replaced several traditional materials and plays a significant role in everyday life. Compared to traditional materials like steel and wood, plastic's main advantages are its light weight, durability, and low production costs. In 2021, more than 390 million tonnes of plastic were produced worldwide, from which more than 90% was fossil-based plastic produced from petrochemicals [8]. The European Union (EU) accounted for 57.2 million tonnes of plastic production in 2021, from which more than 39% was used for packaging. Via mixed and separate waste collection in the EU, slightly less than 30 million tonnes of plastic were collected for further treatment in 2020. 42% of the collected plastic waste was used for energy recovery, 35% of collected plastic was recycled, and 23% was sent to landfills [8]. If we look globally, the percentage of plastic waste sent to landfills is even higher, around 40% [8]. Considering this and the fact that plastic has a limited number of cycles for its recycling due to its degradation properties, we can see that plastic waste has great potential for producing synthetic fuels. Thermal degradation of plastic through pyrolysis is a very promising process for producing synthetic fuels. Pyrolysis is a process in which long-chain polymers of plastic are decomposed into smaller, less complex molecules at elevated temperatures and in the absence of oxygen. This process generates syngas, solid residue, and pyrolysis oil (PO) as three main products [9]. The obtained PO properties and quantities can be further influenced by catalyst usage in a process called catalytic pyrolysis [10].

Jahirul et al. [11] used high-density polyethylene (HDPE), polypropylene (PP), and polystyrene (PS) for the production of pyrolytic oils in batch pyrolysis reactor at 540 °C. The obtained POs were further used in a distillation process from which diesel, gasoline, and residue were obtained. The properties of the obtained diesel and gasoline fuels were very similar to those of conventional fuel. Pakiya Pradeep and Gowthaman [12] performed thermal and catalytic pyrolysis of LDPE plastic from the packaging and printing industries. They used magnesium bentonite as a catalyst. All obtained PO from thermal and catalytic pyrolysis processes had properties similar to diesel fuel, which indicates their potential usage in internal combustion engines. A reactor with a fixed bed was used to obtain pyrolytic oils from mixed plastic in a study by Singh et al. [13]. The pyrolytic oils they obtained were high-quality fuels with physical properties similar to diesel fuel, so they concluded that they represent an excellent alternative for usage in diesel engines. A similar study was performed by Das et al. [14], where medical plastic waste was used to produce pyrolytic oils using a batch pyrolysis reactor. Singh et al. [15] used LDPE plastic to produce PO using thermal and catalytic pyrolysis in a batch pyrolysis reactor. The characterisation of the obtained pyrolytic oils indicated that they all have properties similar to conventional diesel fuel, but the oils obtained via catalytic pyrolysis had higher quality.

From the above short review of pyrolytic oils, it can be seen that plastic waste presents a suitable raw material for synthetic fuel production and has considerable potential for its usage in internal combustion engines as a substitute or additive to conventional fossil fuels. However, small differences in PO properties, compared to conventional fuels, can have an influence on internal fuel flow in diesel injectors, which will further influence spray formation, fuel combustion, and the emission formation process in modern diesel engines, where injection pressures are very high and injection times very short [16,17]. There are many studies in which the influence of different fuel properties on fuel flow

conditions in common-rail diesel injectors was studied experimentally and/or numerically. Y. Wei et al. [18] performed an experimental study in which the effect of string cavitation on real-size diesel nozzle internal flow and near-field spray characteristics was studied. They concluded that needle lift height influences flow characteristics inside the injection hole, which further influences cavitation phenomena and spray development. Kumar et al. [19] used the RANS approach with the Zwart-Gerber-Belamri cavitation model to study cavitation flow in a Bosch conical mini-sac type six-hole axisymmetric vertical multi-hole diesel injector using diesel and biodiesel fuels. The numerical results were compared to the experimental ones obtained on a 15X scaled-up replica of a used injector. The authors concluded that numerical and experimental results give a good qualitative comparison of the predicted cavitation phase. The most significant area of cavitation phase formation was at the upper edge of the nozzle injection hole. The scaled-up diesel fuel injection nozzle was also used in the experimental and numerical work of Li et al. [20], where they studied string cavitation at different needle lifts and injection pressures. They concluded that a hollow spray is formed at low needle lifts, allowing ambient air to be sucked into the injection hole. Fuel properties also influence the fuel flow in the diesel injector nozzle. It was concluded in the study of Yu et al. [21] that fuels with higher viscosity lead to lower cavitation formation inside the fuel injector. Viscosity also influences fuel spray, which is longer and narrower if the fuel viscosity is higher. Torrelli et al. [22] concluded that less viscous fluids have lower friction, resulting in higher fuel velocities and influencing their mass flow rate at the same injection pressure. Jiang et al. [23] found a higher probability of cavitation formation when fuels with lower viscosity are used in diesel injectors.

Several approaches to predicting cavitation erosion from CFD simulations have been proposed and applied to various cases of cavitating flows in the literature. Proposed approaches range from more straightforward erosion indicators proposed by Gomez et al. in [24], Mo et al. [25] and Brunhart et al. [26] to more complex and physically accurate modelling of cavitation erosion proposed by Leclercq et al. in [27], Schenke et al. [28], Arabnejad et al. [29] and Fortes Patella et al. [30].

A phenomenological cavitation erosion model, describing the transfer of initial potential energy of large cavitation structures to a solid surface, has been proposed by Fortes-Patella et al. [30] and applied to the case of predicting cavitation erosion on a hydrofoil [27]. Schenke et al. [28] provided a more detailed description of the energy transfer, termed energy focusing, which has recently been further evaluated and successfully applied to different geometries [28,31]. A different state-of-the-art approach to describe cavitation erosion based on the energy description has been developed by Arabnejad et al. [29], where the kinetic energy of the liquid surrounding the vapour cavity is considered instead of the cavity potential energy.

Development and evaluation of cavitation erosion models, particularly complex ones, is often performed on a geometry for which it is possible to conduct detailed experiments in a cavitation tunnel, for example, hydrofoils, marine propellers, venturis, or nozzles. Numerical studies of cavitation erosion in more complex engineering applications, where mesh movement is required, can be further limited by the complexity of implementing the developed cavitation erosion models in CFD software by researchers. In such instances, simpler erosion indicators have been used, and some were found to be appropriate for predicting cavitation erosion.

Brunhart et al. [26] used a dynamic mesh method within ANSYS Fluent to simulate fluid flow with the occurrence of cavitation in a diesel fuel pump. They considered several erosion risk indicators and concluded that the most accurate results were obtained with the maximum value of the squared total time derivative of pressure, the maximum value of potential power density by Fortes-Patella et al. [30], and the maximum value of total time derivative of pressure. In a numerical study to predict cavitation erosion in GDI injectors by Santos et al. [24], three erosion indicators were compared in the case of a URANS and an LES simulation. They concluded that accumulated (time integral) total

time derivative of pressure and accumulated cavitation potential energy by Fortes-Patella et al. [30] gave accurate erosion prediction in both URANS and LES cases. To numerically predict vibration-induced cavitation erosion in high-speed gears, Mo et al. [25] used and assessed different erosion risk indicators in a moving mesh CFD simulation. They concluded that modified erosion indicators that consider the vapour volume fraction improved the prediction of cavitation erosion in comparison with erosion indicators based only on pressure derivatives.

The short review above indicates that numerical simulations are appropriate for studying internal fuel flow, cavitation phenomena, and erosion prediction in modern diesel injectors when using fuels with different properties. Since modern synthetic fuels are gaining in their usage, the present study focuses on cavitation erosion prediction in a common-rail diesel injector when different pyrolytic oils are used. This work is divided into two main parts. In the first part, HDPE and LDPE plastic wastes were collected and used to produce pyrolytic oils using thermal and catalytic pyrolysis in a batch reactor, where ZAP USY zeolite was used as the catalyst. The obtained oils were further characterised, and their properties were compared to conventional fuels. In the second part of the paper, the obtained POs were used to predict cavitation erosion in a Denso common-rail diesel injector. The numerical study was performed using Ansys FLUENT at actual engine operating conditions, considering full needle movement for which the dynamic mesh layering method was applied. The simulations were done using the Reynolds Averaged Navier Stokes approach (RANS), the phase change was calculated using the Zwart-Gerber-Belamri (ZGB) cavitation model, the flow was considered incompressible and realisable k-epsilon model was used for turbulence calculation. The Eulerian mixture multiphase model was used to calculate one set of conservation equations for mass, momentum, and energy for the fluid and vapour phases. Based on the previous studies, where a moving mesh has been used in a CFD simulation to predict cavitation erosion, we selected an erosion risk indicator to predict possible locations of cavitation erosion in the injector nozzle.

2. Materials and Methods

2.1. Plastic Material

In the present paper, plastic waste material collected from municipal waste at the Faculty of Mechanical Engineering at the University of Maribor, Slovenia, was used for pyrolytic oil production. After the plastic waste collection, it was separated into different types, and only LDPE and HDPE plastics were used in the pyrolytic process. Later, it was cut into smaller pieces and washed before being used for further treatment.

2.2. Catalyst

ZAP USY zeolite, produced by SILKEM d.o.o., was used as the catalyst in the catalytic pyrolysis process. The main characteristics of used zeolite are presented in Table 1.

Table 1. Used ZAP USY catalyst properties.

SiO ₂ /Al ₂ O ₃ [mol/mol]	13
BET surface area [m ² /g]	540
Na ₂ O [wt %]	0.13
Average particle size D50 [µm]	2.25
Pore volume [cm ³ /g]	0.1
Pore width [nm]	4.4

2.3. Pyrolysis

The pyrolysis process was done using a fixed-bed batch reactor. The schematic presentation of the pyrolysis process is presented in Figure 1. First, the used plastic waste was inserted into the reactor chamber. In catalytic pyrolysis, the catalyst was previously

mixed with plastic in a ratio of 10:1 and then inserted into the reactor chamber. The mass of the plastic in each experiment was 100 g, while the mass of the catalyst was 10 g. After the plastic insertion, the reactor chamber was sealed, and the electric heater was turned on. For the first 10 min, the reactor chamber was heated using the reduced power (50%) of the electrical heater. After this period, the full power of the heater was applied to increase the temperature inside the reactor chamber up to 400 °C. The pyrolytic process was stopped when the time interval between oil droplets in three consecutive droplets increased above 10 s. In all experiments, a Mistral 6 System electrical heater with a power of 4.5 kW was used. The heater was controlled via the LabVIEW program using an open loop with a possible temperature gradient of 5 °C. The temperature inside the reactor chamber was monitored using a K-type thermocouple, a National Instruments DAQ carrier WLS-9163, and a NI-9219 module.

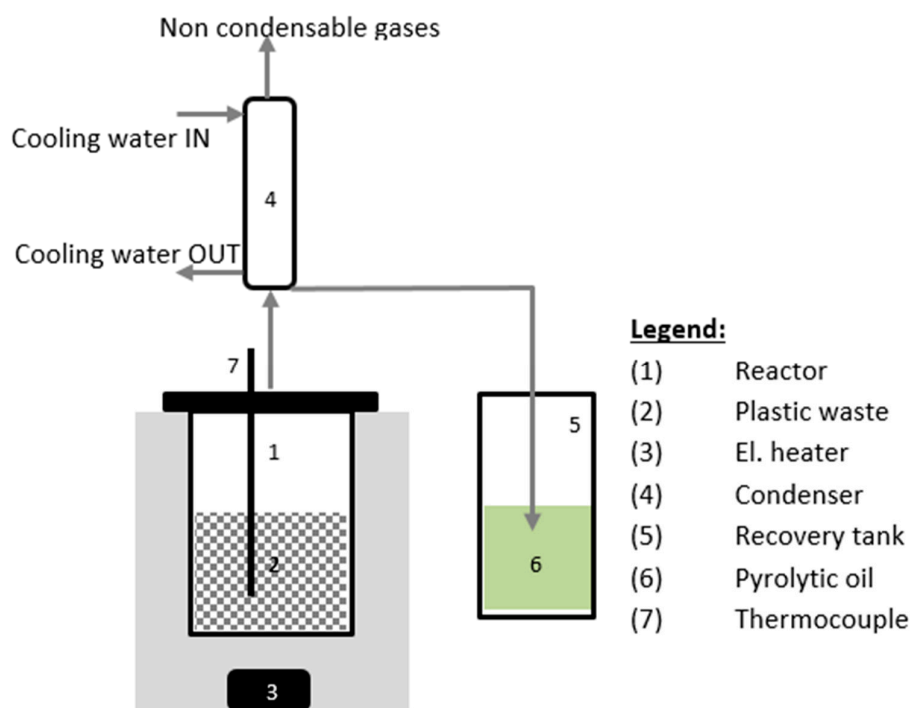


Figure 1. Schematic diagram of experimental set-up for the pyrolysis process.

The produced gases from the reactor chamber were led into the condenser. The non-condensable gases were released into the atmosphere, and pyrolytic oils were collected inside the recovery tank. The solid residue and catalyst (if used) remained in the reactor chamber and were removed after each experiment.

Table 2 presents the most relevant properties of the used pyrolysis reactor.

Table 2. Pyrolysis reactor properties.

Reactor dimensions	φ110 mm, height 190 mm
Condenser length	400 mm
Condenser pipes diameter	Inner pipe φ 12 mm/outer pipe φ 18 mm
Insulation and support	Fireclay brick pipe φ 190 mm + 100 mm glass wool

2.4. Oils Characterisation

The obtained pyrolytic oils were further analysed to obtain the required properties for numerical simulations. The results marked with the abbreviations HDPE and LDPE refer to oils obtained from thermal pyrolysis of HDPE and LDPE, while HDPE_z and LDPE_z refer to oils obtained from catalytic pyrolysis of HDPE and LDPE mixed with the catalyst (zeolite) in a ratio of 10:1. Figure 2 presents the pyrolytic oils' density, which was determined in a temperature range from 15 to 40 °C using a portable density meter, Mettler Toledo Density2Go. The density meter uses the oscillating U-tube principle in order to determine sample density.

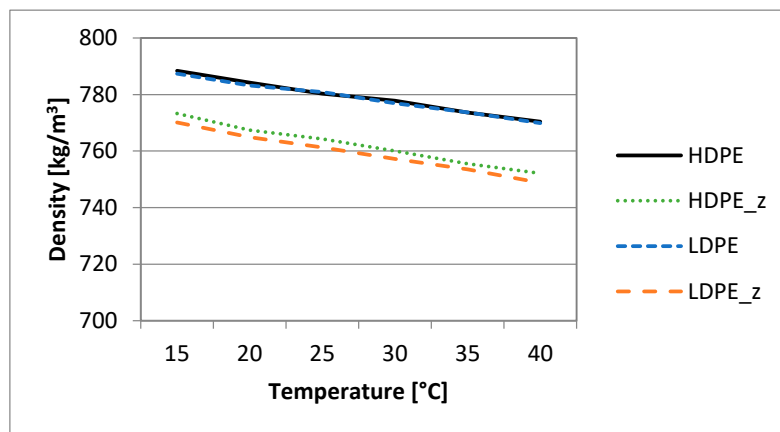


Figure 2. Obtained pyrolytic oils' density.

As can be seen from the presented results, the density of pyrolytic oils is slightly lower than that of diesel fuel, which the European Standard EN590 [32] limits in the range from 820 to 845 kg/m³ at a temperature of 15 °C.

Figure 3 presents the results of pyrolytic oils' surface tension, determined using a Krüss EasyDyne K20 tensiometer in a temperature range from 15 to 40 °C. The tensiometer uses precise force-measuring probes to measure the tensile force of the submerged probe in order to determine sample surface tension.

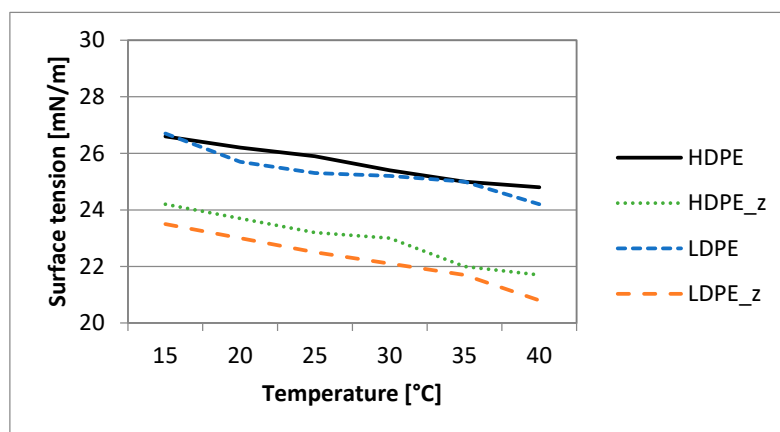


Figure 3. Obtained pyrolytic oils' surface tension.

The obtained values of PO surface tension are in good agreement with that of conventional diesel fuel determined by Ren et al. [33] and Chhetri and Watts [34].

The viscosity of pyrolytic oils was determined in the temperature range from 25 °C to 40 °C using a viscometer and a thermostatic bath. A viscometer is an instrument that

works on the principle of Poiseuille's law. It typically uses the rate of flow of liquids through a capillary tube to determine the fluid's viscosity. The results are presented in Figure 4.

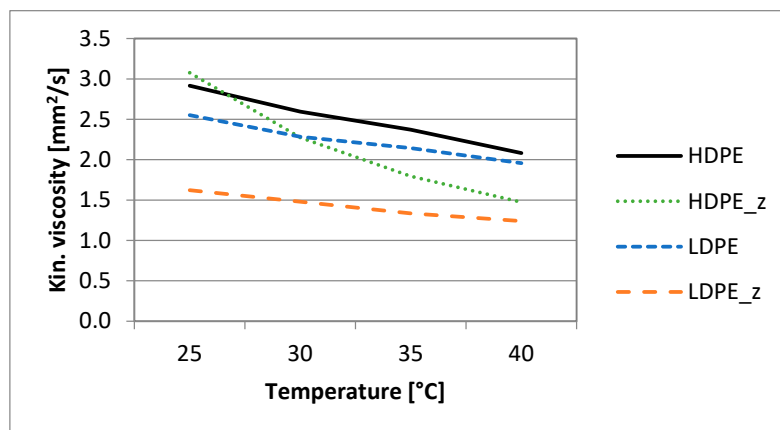


Figure 4. Obtained pyrolytic oils' kinematic viscosity.

The EN590 standard for diesel fuel limits the required kinematic viscosity range from 2 to 4.5 mm²/s at 40 °C. Comparing the results of PO kinematic viscosity to the EN590 standard, we can see that catalytic pyrolysis produces oils with lower kinematic viscosity than required.

The carbon number distribution of pyrolytic oil is presented in Figure 5. The results of carbon number distribution were determined using a Thermo Quadrupole GC–MS Model DSQ II-Trace Ultra GC analyser. It was equipped with a DB-5MS capillary column (30 m, 0.25 mm i.d., 0.25 µm film thickness) from Agilent Technologies. Helium (99.999% pure) at a constant 1.0 mL/min flow rate was used as the carrier gas.

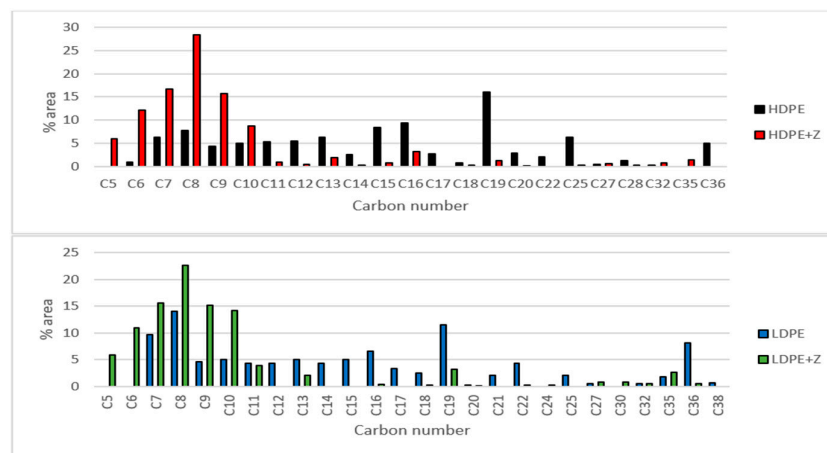


Figure 5. Obtained pyrolytic oils' carbon number distribution.

As can be seen from the presented results in Figure 5, the use of a catalyst influences a narrower range of carbon number distribution for both plastic types. The highest area percentage for HDPE was obtained for C19 (15.9%) and C8 (28.4%) for HDPE_z, while for LDPE and LDPE_z, the highest area percentages were obtained for C8, 13.9% for LDPE and 28.4% for LDPE_z.

Table 3 presents the results of the obtained pyrolytic oils elementary composition, which is important to know since the chemical composition of fuels influences its calorific value, emission formation, etc. The composition was measured using a TruSpec Micro

analyser from LECO, which uses a combination of a flow-through carrier gas system in conjunction with individual highly selective, infrared, and thermal conductivity detection systems to determine sample CHNSO composition.

Table 3. Elementary composition of pyrolytic oils.

	Nitrogen %	Carbon %	Hydrogen %	Oxygen %
HDPE	0.1880	81.0686	13.3376	5.4058
HDPE_z	0.2040	71.2566	11.3413	17.1981
LDPE	0.1877	78.9637	13.0302	7.8184
LDPE_z	0.2021	68.0774	10.8749	20.8456

From the presented results of PO elementary composition, it can be seen that the used catalyst influences the reduction of hydrogen and carbon in PO. At the same time, it increases oxygen and nitrogen content.

2.5. Fuels' Properties for Simulations

Table 4 presents the properties of the obtained pyrolysis oils and the diesel fuel used in the numerical simulations. The saturation pressure for all fuels was the same (1000 Pa) since the works in references [35,36] indicate that a sharp drop of pressure at the nozzle hole entry is so rapid that the absolute value of the fuel saturation pressure is of minor influence on cavitation occurrence

Table 4. Fuel properties used in the simulations.

Fuel Properties	D2	HDPE	HDPE_z	LDPE	LDPE_z
Density at 15 °C [kg/m ³]	830	788.4	773.3	787.4	770.1
Surface tension [mN/m]	26.8	26.2	23.7	25.7	23
Kin. Viscosity [mm ² /s]	2.14	2.08	1.47	1.96	1.24

2.6. Engine and Engine Operating Regime

The used injector was taken from a 4-cylinder Nissan YD22 engine. The engine operated at 1700 rpm, 110 NM of torque, and 6.33 bar of brake mean effective pressure (BMEP). In this regime, the injection pressure was 845 bar, and the total injection duration for diesel fuel was 1.26 ms [37].

The main properties of the engine are presented in Table 5.

Table 5. Properties of the tested engine.

Properties	Value
Engine displacement [L]	2.184
Max. power [kW]	82 (@4000 min ⁻¹)
Max. torque [Nm]	248 (@2000 min ⁻¹)
Compression ratio	16.7/1
Bore [mm]	86.5
Stroke [mm]	94

2.7. Injection System

A solenoid-operated Denso injector model 7H150 was used in the presented work. The injector has seven injection holes with a length of 0.76 mm and a diameter of 0.15 mm. A detailed description of the experimental set-up was presented in [37,38]. The back pressure during the injection measurement was 60 bar.

2.8. Numerical Model

One-seventh of the whole injector (one injection hole) was considered for the numerical model in order to reduce the calculation time. A 3D geometric model was created with the 3D Computer-Aided Design (CAD) modelling software v 2021 R2 ANSYS SpaceClaim. The computational mesh for the CFD simulations was created using the ANSYS Meshing software v 2021 R2. Figure 6 shows a cross-section of the injector nozzle, a 3D CAD model of the injector nozzle, and parts of a computational mesh.

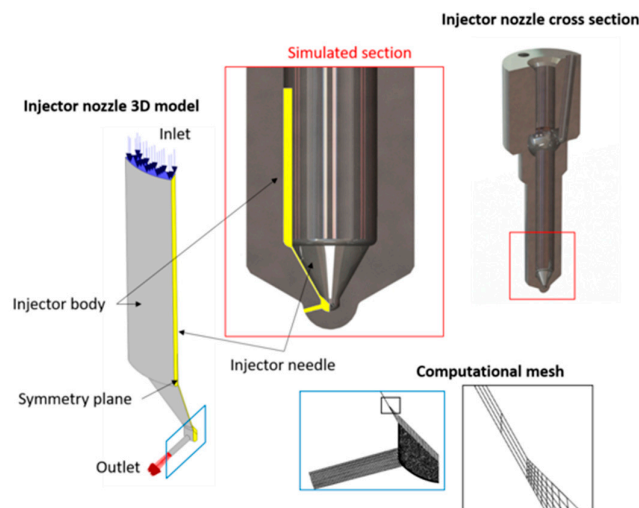


Figure 6. Injector nozzle model and computational mesh of nozzle cross-section.

2.9. Mesh Independence Study

Before analysing the results, it is necessary to perform an appropriate mesh independence study in order to estimate the numerical error. The numerical error was estimated with the grid convergence index (GCI) method, which is a recommended method for the uniform reporting of mesh refinement studies in CFD [39,40].

For the purpose of conducting a mesh independence study, the average fuel velocity at the outlet, the average turbulent kinetic energy at the outlet, and the total vapour volume in the domain were monitored. The mesh study with the calculation of GCI, presented in Table 6, was carried out with the injection needle half open.

Table 6. Mesh independence study.

Mesh	Number of Elements	Average Velocity at the Outlet [m/s]	Average Turbulent Kinetic Energy at the Outlet [J/kg]	Total Vapour Volume in the Domain [m ³]
Coarse (3)	228,777	282.54	1679.96	2.20×10^{-12}
Medium (2)	515,722	279.40	1752.87	1.92×10^{-12}
Fine (1)	1,147,432	287.46	1775.26	1.94×10^{-12}
GCI_{fine}^{21} [%]	-	2.19	0.73	0.07
GCI_{medium}^{32} [%]	-	0.86	2.33	1.18

Based on the mesh independence study, the medium mesh with 515,722 elements was selected for further analysis. The medium mesh provided a good balance between the numerical error of calculations and the calculation times. Details of the medium mesh are presented in Table 7.

Table 7. Detailed properties of the selected medium mesh.

Number of Elements	Hexahedral	Tetrahedral	Wedge	Total
	316,316	157,946	41,460	515,722
Number of Nodes	407,936			
Minimum orthogonal quality	0.22			
Maximum aspect ratio	15.1			
Maximum skewness	0.77			
Maximum y^+	43.3			

2.10. Time-Step Independence Study

For the chosen medium mesh, the time-step independence study was conducted similarly to the mesh independence study. Three time steps, separated by a factor of ten, as shown in Table 8, were selected based on our experience [16]. The total injected fuel mass per injection cycle was monitored to analyse the time-step independence. The findings of the time-step independence study are presented in Table 7.

Table 8. Time-step independence study.

Time-Step	Time-Step Size [s]	Injected Fuel Mass per Cycle [mg]
Large (3)	1×10^{-6}	27.85
Medium (2)	1×10^{-7}	27.78
Small (1)	1×10^{-8}	27.65
GCI_{fine}^{21} [%]	-	0.87
GCI_{medium}^{32} [%]	-	0.53

2.11. Simulation Set-Up

The simulations were prepared and run in a commercial CFD software ANSYS Fluent 2021 R2, which uses the Finite Volume Method. The pressure-based solver with a coupled algorithm for pressure-velocity coupling was selected for the solution of governing equations.

Gradients were computed via the Least Squares Cell-Based method. A PRESTO interpolation scheme was selected for pressure interpolation. Interpolation of momentum, volume fraction, turbulent kinetic energy, and turbulent kinetic energy dissipation rate face values was accomplished using a QUICK scheme. Since the flow under consideration was unsteady, transient simulations were performed. The Second Order Implicit method was selected to integrate the transient terms in equations.

To simulate the motion of the injector needle, the dynamic mesh model with the dynamic layering mesh update method was selected. The transient needle movement was defined via the needle velocity profile. The velocity of the needle was calculated by taking the time derivative of the experimentally determined [16] needle position over time, as shown in Figure 7. There was a small gap at the beginning of the simulation, with a minimal distance of $1 \mu\text{m}$ between the needle and the body of the injector. This was done to avoid having zero-thickness cells in the dynamic mesh zone, which is imposed by the dynamic layering method.

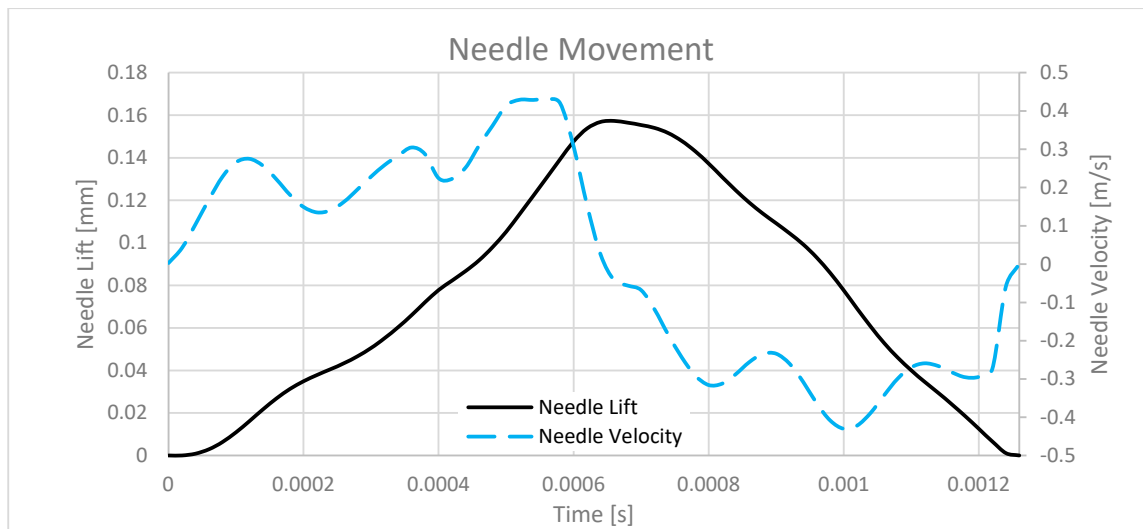


Figure 7. Needle Lift and Needle Velocity.

At the inlet (Figure 6), an injection pressure of 845 bar was prescribed. At the outlet (Figure 6), the in-cylinder back pressure of 60 bar was prescribed. The symmetry boundary condition was used on the sides of the injector body. The remaining surfaces (injector body, injector hole, and injector needle) were assigned a no-slip wall boundary condition.

The simulation time of 1.26×10^{-3} s was equal to the physical time of one injection cycle. Based on the time-step independence study, a time-step of 1×10^{-7} s was chosen. For each time step, the solution was obtained iteratively. The number of iterations per time step was limited to 100; however, a scaled residual convergence criterion of 10^{-3} was achieved before this limit.

2.12. Mathematical Models

The following section presents the basic equation of used mathematical models. All models were already implemented in FLUENT software v 2021 R2 except the model for calculating the Cavitation erosion risk indicator. Their detailed description can be found in [41]. An overview of the models used in this study, which are presented in the following, is given in Table 9.

Table 9. Overview of the used models with an explanation of underlying assumptions.

Physical Phenomena	Used Model	Assumption/Limitation
Multiphase flow	Mixture	Assumed equal pressure and velocity between the phases
Turbulence	URANS Realizable $k-\epsilon$	Assumed fully turbulent flow, isotropic and homogeneous turbulence
Cavitation	Zwart-Gerber-Belamri	Assumed simplified bubble dynamics (surface tension, viscosity, non-condensable gas and second-order effects are neglected), homogeneous liquid–vapour mixture consisting of bubbles that have the same size
Cavitation erosion	ERI	Only the collapse stage of vapour in direct contact with the wall (first cell layer) is considered to be erosive

2.13. The Mixture Model

Cavitating flow consists of a liquid and vapour phase. In the adopted mixture model, the liquid and vapour phases are considered a mixture with an assumption of equal pressure and velocity between the phases. Therefore, one set of continuity and momentum

equations is solved for the mixture, and the volume fraction equation is solved for the secondary (vapour) phase.

Since the mixture consists only of a liquid and vapour phase, a relation for the volume fraction of liquid (α_l) and vapour phase (α_v) is written as follows:

$$\alpha_l + \alpha_v = 1 \quad (1)$$

The properties of the mixture are then obtained via the mixing rule. The density of the mixture is calculated as follows:

$$\rho = \alpha_v \rho_v + (1 - \alpha_v) \rho_l \quad (2)$$

Similarly, the dynamic viscosity of the mixture is calculated as follows:

$$\mu = \alpha_v \mu_v + (1 - \alpha_v) \mu_l \quad (3)$$

where ρ_l and ρ_v are the liquid and vapour density, respectively, and μ_l and μ_v are the liquid and vapour dynamic viscosity.

The continuity and the momentum equations for the mixture are:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (4)$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} \quad (5)$$

where $\mathbf{u}$ is the mixture velocity, p is the pressure of the mixture, and $\boldsymbol{\tau}$ is the mixture shear stress tensor.

Additionally, the vapour phase volume fraction equation is:

$$\frac{\partial (\alpha_v \rho_v)}{\partial t} = \nabla \cdot (\alpha_v \rho_v \mathbf{u}) = R_e - R_c \quad (6)$$

where R_e and R_c are mass transfer source and sink terms, respectively, which represent evaporation and condensation.

2.14. Turbulence Modelling

The URANS approach was used, and the Realizable $k-\varepsilon$ model with Enhanced Wall Treatment (EWT), which is y^+ insensitive, was chosen based on the recommendations found in the literature [42,43]. The realisable $k-\varepsilon$ model introduces an additional transport equation for the turbulent kinetic energy (k)

$$\frac{\partial (\rho k)}{\partial t} + \nabla \cdot (\rho k \mathbf{u}) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] + G_k - \rho \varepsilon \quad (7)$$

and an additional transport equation for the turbulent kinetic energy dissipation rate (ε)

$$\frac{\partial (\rho \varepsilon)}{\partial t} + \nabla \cdot (\rho \varepsilon \mathbf{u}) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] + \rho C_1 S \varepsilon - \rho C_2 \frac{\varepsilon^2}{k + \sqrt{\nu \varepsilon}} \quad (8)$$

where μ_t is turbulent viscosity and G_k represents the generation of turbulent kinetic energy. σ_k is the turbulent Prandtl number for k with a value of 1.0, σ_ε is the turbulent Prandtl number for ε with a value of 1.2, and C_2 is a model constant with a value of 1.9. C_1 is calculated as follows:

$$C_1 = \max \left[0.43, \frac{\eta}{\eta + 5} \right] \quad (9)$$

$$\eta = S \frac{k}{\varepsilon} \quad (10)$$

$$S = \sqrt{2SS} \quad (11)$$

where $\mathbf{S}$ is the mean rate of the strain tensor. The turbulent viscosity is calculated in the same way as in the standard k - ε model as follows:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \quad (12)$$

where C_μ is a function of the mean strain and rotation rates, the turbulent kinetic energy, and the turbulent kinetic energy dissipation rate. For conciseness, equations to calculate C_μ [41,44] and G_k [41,45] are omitted here and are available in the referenced literature.

2.15. Cavitation Modelling

The mass transfer cavitation models are based on a simplified version of the Rayleigh-Plesset equation to account for bubble growth and collapse. Bubble dynamics is expressed via the bubble radius (R_B) as follows:

$$\frac{dR_B}{dt} = \sqrt{\frac{2}{3} \frac{p_v - p_\infty}{\rho_l}} \quad (13)$$

where p_∞ is the far-field pressure, which is replaced with the local pressure (p) in the cell centre for practical purposes.

The Zwart-Gerber-Belamri cavitation model assumes that all bubbles in a liquid-vapour mixture have the same size. Zwart, Gerber, and Belamri expressed the total inter-phase mass transfer rate per unit volume as [46]

$$R = N_B \frac{dm_B}{dt} = N_B \left(4\pi R_B^2 \rho_v \frac{dR_B}{dt} \right) = \frac{3\alpha_v \rho_v}{R_B} \sqrt{\frac{2}{3} \frac{p_v - p}{\rho_l}} \quad (14)$$

where N_B is the number of bubbles per unit volume of the fluid mixture, and the vapour volume fraction is expressed as follows:

$$\alpha_v = V_B N_B = \frac{4}{3} \pi R_B^3 N_B \quad (15)$$

Equation (14) has been derived for the bubble growth phase; a general form to include condensation is given as follows:

$$R = \frac{3\alpha_v \rho_v}{R_B} \sqrt{\frac{2}{3} \frac{|p_v - p|}{\rho_l}} \text{sign}(p_v - p) \quad (16)$$

The authors in [46] noticed that the model worked well for condensation but was numerically unstable and physically incorrect for vaporisation. To account for the decrease in nucleation site density with increasing vapour volume fraction, α_v in Equation (14) was replaced with $\alpha_{nuc}(1 - \alpha_v)$. The final form of the ZGB cavitation model is as follows:

If $p \leq p_v$ then

$$R_e = F_{vap} \frac{3\alpha_{nuc}(1 - \alpha_v)\rho_v}{R_B} \sqrt{\frac{2}{3} \frac{p_v - p}{\rho_l}} \quad (17)$$

If $p > p_v$ then

$$R_c = F_{cond} \frac{3\alpha_v \rho_v}{R_B} \sqrt{\frac{2}{3} \frac{p - p_v}{\rho_l}} \quad (18)$$

where F_{vap} and F_{cond} are empirical calibration coefficients for vaporisation and condensation, respectively. The original authors in [46] reported the following model parameters: $R_B = 10^{-6}$ m, $\alpha_{nuc} = 5 \times 10^{-4}$, $F_{vap} = 50$, and $F_{cond} = 0.01$.

2.16. Cavitation Erosion Risk Indicators

Cavitation erosion prediction from numerical simulations of cavitating flow is an active research topic. Different approaches have been suggested and investigated in the literature. Based on previous investigations in the literature, an erosion risk indicator (ERI) was chosen to compare predicted locations of cavitation erosion for different fuels.

Fortes-Patella et al. [30] proposed an energy cascade model where cavitation erosion is related to the initial potential energy of cavitation structures. For an arbitrary shape of the cavity, the potential energy per unit volume is:

$$e_{pot} = \alpha_v(p_d - p_v) \quad (19)$$

where p_d is the pressure driving the cavity collapse, then by taking a total derivative, the radiated power is expressed as:

$$\dot{e}_{rad} = \frac{De_{pot}}{Dt} = \left(\frac{D\alpha_v}{Dt}\right)^- (p_d - p_v) \quad (20)$$

where $\left(\frac{D\alpha_v}{Dt}\right)^-$ represents that only the negative values of the total derivative are considered. This is in accordance with the model's basic assumption that only the collapse stage is considered.

Melissaris et al. [31] derived two alternative formulations for $\left(\frac{D\alpha_v}{Dt}\right)^-$ and concluded that the formulation where the total derivative of vapour volume fraction is expressed with the cavitation sink term is the most accurate, which was also confirmed by our previous work [47].

Finally, the radiated cavitation power, expressed with the cavitation sink term, is:

$$\dot{e}_{rad} = \frac{\rho}{\rho_l} \frac{R_c}{\rho_v} (p_d - p_v) \quad (21)$$

and ERI is:

$$ERI = \int_0^t \dot{e}_{rad} dt \quad (22)$$

where the integral in Equation (22) is taken from the beginning of the needle motion cycle (time $t = 0$ s) to the end of the needle motion cycle (time $t = 1.26 \times 10^{-3}$ s).

3. Results

In the following section, cavitation development and cavitation erosion in the injection hole of the nozzle are presented for different fuels.

A general overview of the in-nozzle flow for all the fuels under consideration is presented in Figure 8. Cavitation development in the injection hole for all the fuels under consideration is presented in detail in Figures 9 and 10. The corresponding cavitation erosion prediction is presented in Figure 11. Finally, a quantitative comparison of cavitation erosion for different fuels is presented in Figure 12.

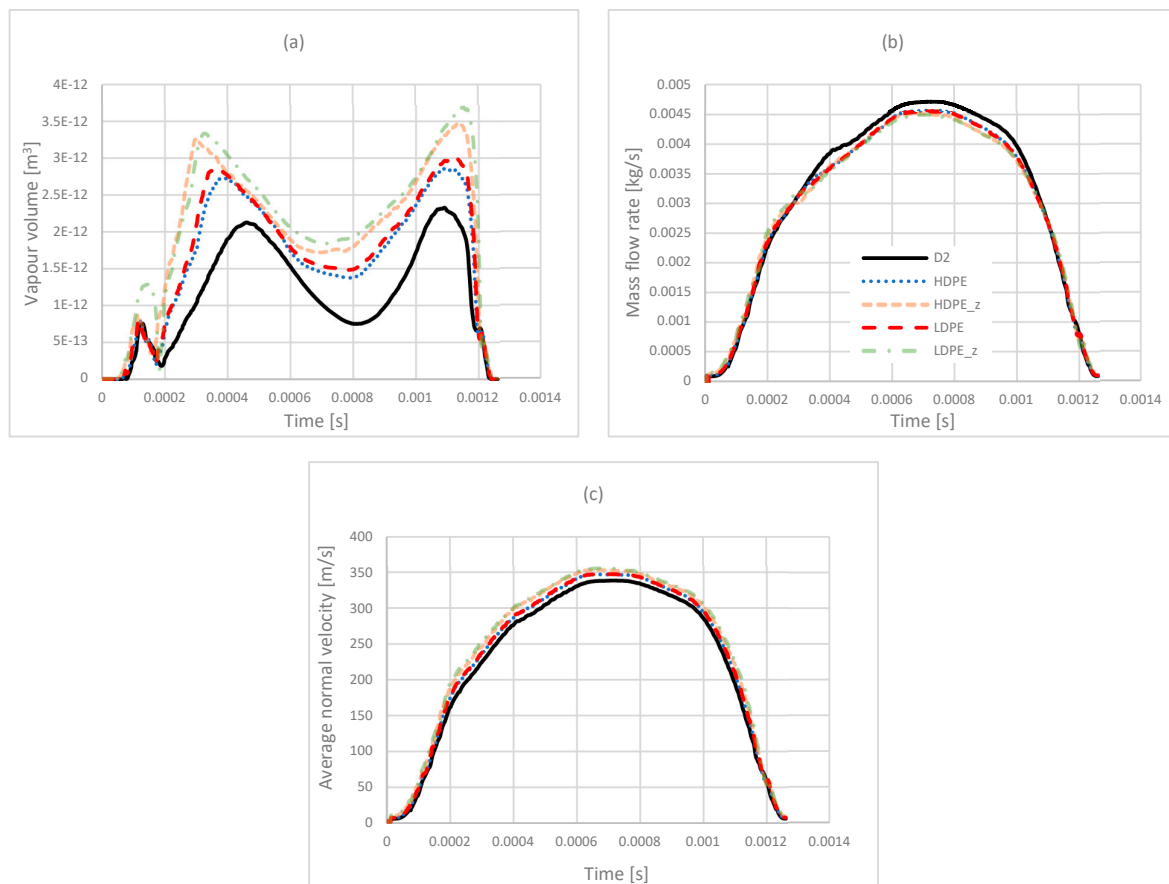
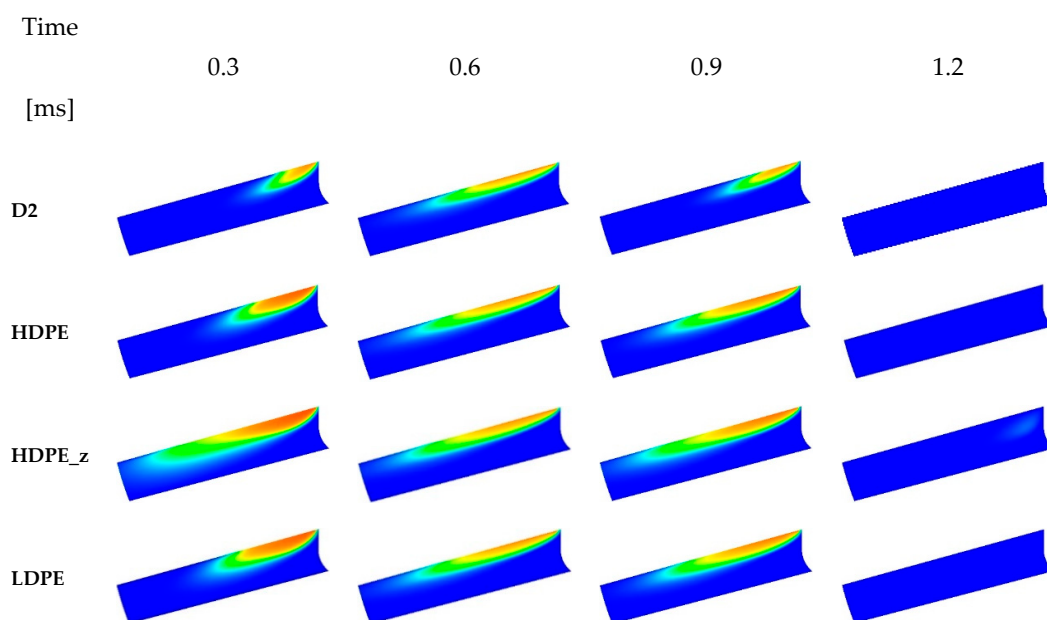


Figure 8. Integral quantities for one injection hole over one injection cycle for different fuels (a) Total vapour volume in the domain; (b) Mass flow rate at the outlet; (c) Average normal velocity at the outlet.



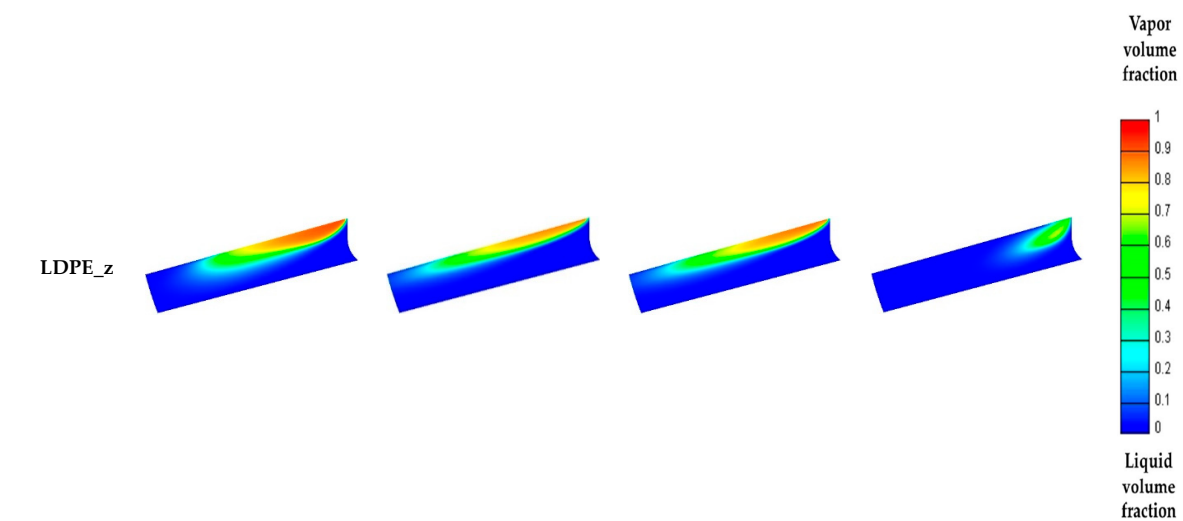
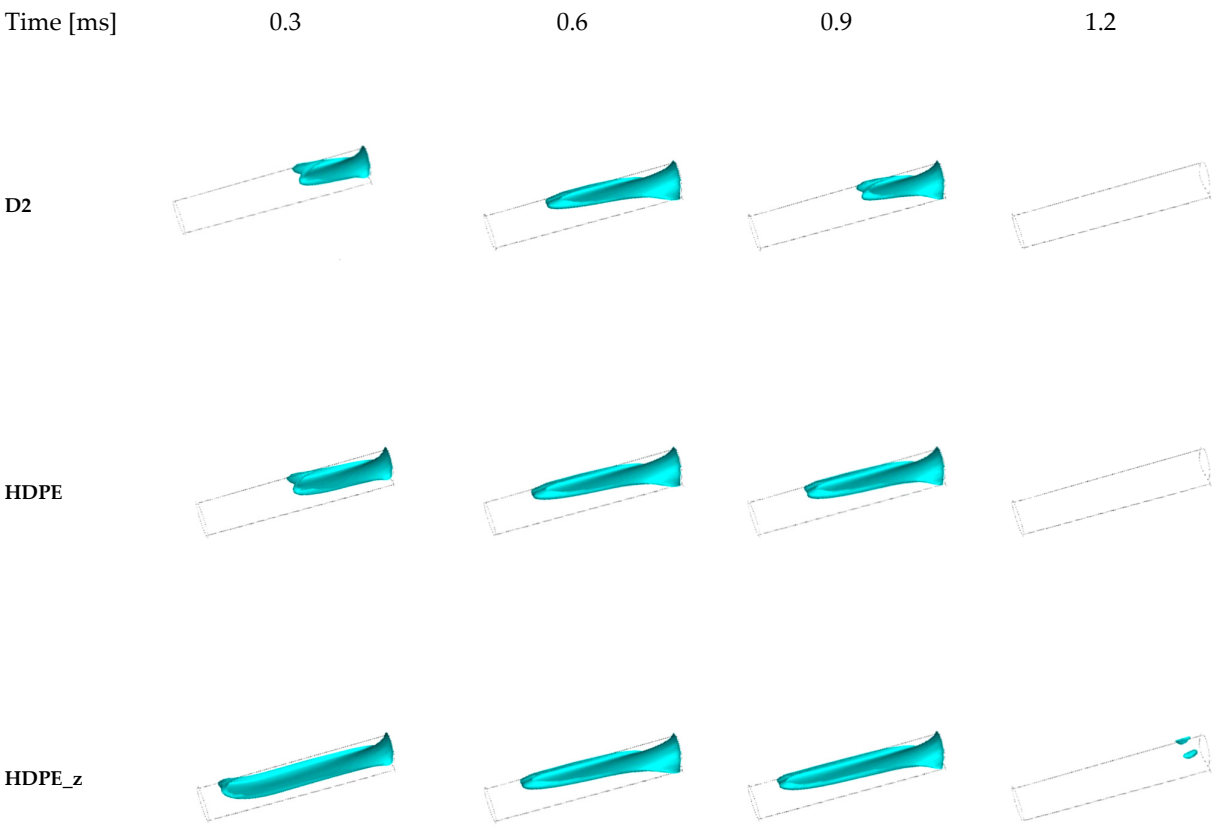


Figure 9. Results of cavitation in the injection hole—vapour volume fraction on the middle presentation plane.



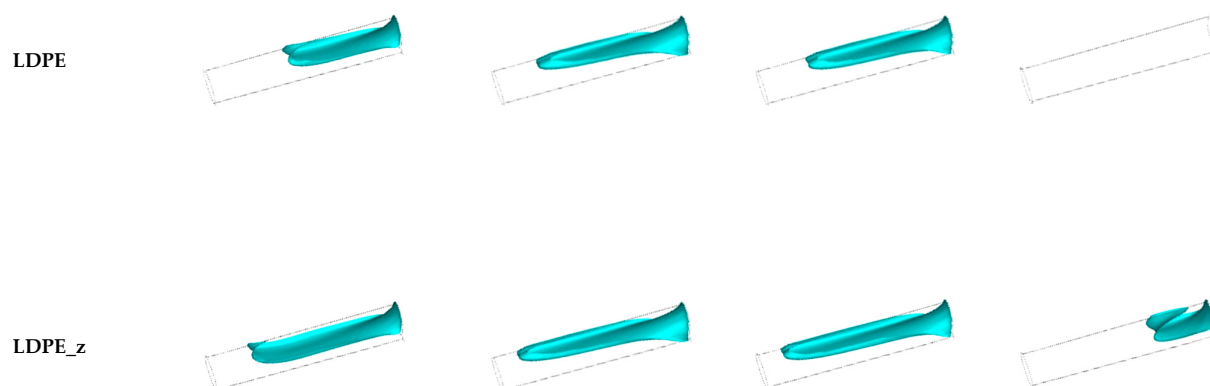


Figure 10. Results of cavitation in the injection hole—iso-surface of 20% of vapour volume fraction.

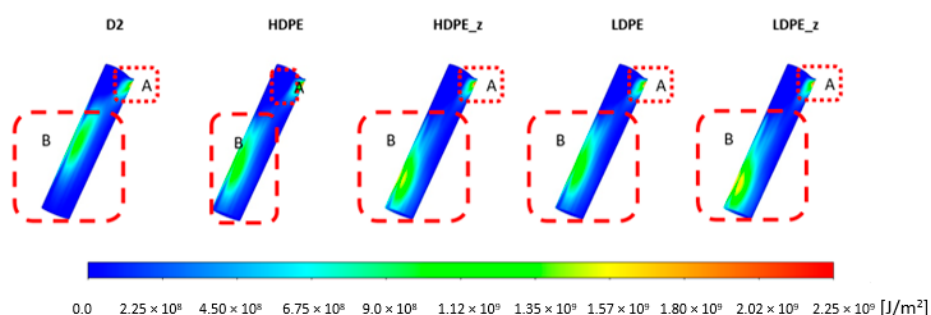


Figure 11. Results of cavitation erosion prediction—contours of ERI on the injector hole surface.

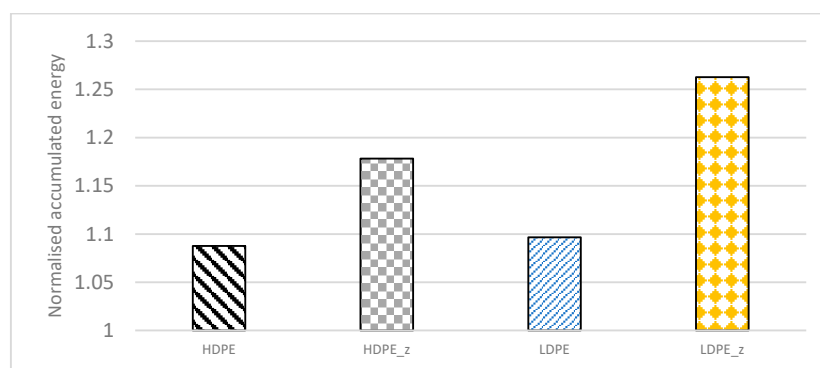


Figure 12. Results of cavitation erosion prediction—normalized total values of ERI on the injection hole surface.

3.1. In-Nozzle Flow

To better describe the flow features during an injection cycle, three distinct phases of an injection cycle are identified with respect to the motion of the injector needle. The first phase is identified and termed the needle opening phase, which starts from the closed position at time $t = 0$ s to time $t = 6 \times 10^{-4}$ s when the needle is fully open (more than 95% of maximum needle lift). This is followed by a phase when the needle is fully opened,

from time $t = 6 \times 10^{-4}$ s to time $t = 7.4 \times 10^{-4}$ s. Finally, from time $t = 7.4 \times 10^{-4}$ s, the needle begins to close until it reaches a fully closed state at time $t = 1.26 \times 10^{-3}$ s, which concludes the needle-closing phase.

From Figure 8, it can be seen that cavitation is present in all three needle motion phases for all fuels under consideration. In the needle opening phase, there is a rapid increase in the vapour volume, followed by a decrease that continues during the needle opening phase. The initial increase in vapour volume results from an increased mass flow rate due to the needle opening. Since the flow rate in the injection hole increases, there is a corresponding drop in local pressure as the velocity locally increases. However, as the vapour cavity in the injection hole grows, the liquid flow becomes more and more restricted, and the rate of increase in mass flow rate begins to drop. As the needle keeps lifting towards the end of the opening phase, the pressure in the injection hole somewhat increases, which causes a reduction in vapour cavity volume. The mass flow rate levels off when the needle reaches a fully opened phase. At the beginning of the needle closing phase, vapour volume begins to increase again due to a transient pressure drop. At first, the mass flow decreases slowly as the vapour cloud in the injection hole chokes the flow, causing a local velocity increase around the vapour cloud. In a later stage of the needle closing phase, the pressure in the injection hole increases due to a drop in mass flow rate, and vapour decreases rapidly. Finally, as the needle reaches the fully closed position, the vapour vanishes completely as the mass flow rate drops to zero.

While these general observations can be made for all fuels considered, some differences are also observed. For all pyrolytic oils, an increase in vapour volume is observed across all needle movement phases. The addition of zeolite to either HDPE or LDPE fuel shows an additional increase in vapour volume across all needle movement phases.

In the needle opening phase, all pyrolytic oils exhibited a higher rate of increase in vapour volume compared to regular diesel fuel. Also, the flow choking and a following drop in vapour volume in the needle opening phase occurred earlier for pyrolytic oils, particularly in the cases of added zeolite. This larger spread and faster formation of cavitation are explained by the lower viscosity of pyrolytic oils, which is even lower when the zeolite is added. It has previously been suggested that fuels with lower density and viscosity have less resistance to flow disturbance created by needle motion [22]. This more responsive behaviour of fuels with lower density and viscosity can be observed in the needle-closing phase. As the needle begins to close, vapour volume increases faster for pyrolytic oils with lower density and viscosity. However, towards the end of the needle closing phase, the lower viscosity of pyrolytic oils allows for higher flow velocity around the vapour cavity and longer persistence of a low-pressure region in the injection hole due to lower friction in the flow [22]. This means the final vapour collapse occurs faster and later in the needle-closing phase.

The results in Figure 8c indicate that the velocity of all pyrolytic oils is higher than that of diesel fuel. This mechanism can be explained by the lower viscosity of pyrolytic oils, which decreases the friction of fuel flow.

3.2. Cavitation Development

The development of cavitation is presented in Figure 9 as the vapour volume fraction contour in the middle presentation plane and Figure 10 as an iso-surface of 20% vapour volume fraction. Apart from the previously presented general development of the total vapour volume over an injection cycle, spatial development of cavitation is apparent in Figures 9 and 10. It is noted that, for all the fuels under consideration, the attached cavitation cloud expands in length and width. Lengthwise, the vapour is in contact with the top of the injection hole surface over the entire injection cycle. By observing the change from time $t = 3 \times 10^{-4}$ s to time $t = 6 \times 10^{-4}$ s, it can be seen that vapour extends along the width of the injection hole near the entry of the injection hole and comes in contact with the sides of the injection hole surface.

As discussed in the previous section, fuels with lower density and viscosity show a greater extent of cavitation. At any moment presented in Figure 9, the fuels with the addition of zeolite show the largest vapour cavity, while the conventional diesel fuel produced the smallest vapour cavity. Differences in final vapour collapse during the needle closing phase can be seen for time $t = 1.2 \times 10^{-3}$ s, where the fuels containing zeolite, particularly for the LDPE-derived fuel, still contain a small vapour cavity.

3.3. Cavitation Erosion Prediction

In Figure 11., the cavitation erosion prediction is presented as ERI contours, given by Equation (22). Two distinct erosion zones can be seen: a smaller one (zone A) on the sides near the entry of the injection hole and a larger one (zone B) on the top of the injection hole. The smaller erosion zone is similar in shape and size for all considered fuels. Fuels derived from HDPE and LDPE show larger maximum values of ERI in the smaller erosion zone, with the highest values recorded for fuels with added zeolite. This is a consequence of the faster final collapse of fuels with lower density and viscosity, which results in higher condensation rates.

The location of the larger erosion zone depends on the fuel. For conventional diesel fuel, it is positioned in the middle between the injector hole entry and the outlet. For other fuels considered, it is positioned further downstream; for HDPE and LDPE with added zeolite, it is present near the injector hole outlet. This can be explained by the fact that cavitation extends further downstream for HDPE and LDPE fuels and even further for fuels with zeolite. Similarly, as for the smaller erosion zone, maximum values of ERI are obtained in the case of HDPE and LDPE with zeolite. This is again explained by a higher condensation rate due to a faster collapse of cavitation in fuels with lower density and viscosity.

The occurrence of both erosion zones coincides with an unsteady closure line of the attached cavitation cloud for all used fuels. This area was previously connected with cavitation erosion due to the formation of a stagnation point in which the pressure rises from nearly vapour pressure to stagnation pressure, which causes the flow separation. The higher pressure at the stagnation point causes the violent collapse of smaller cavities, which results in erosion. The mechanism was studied in detail by Dular et al. [48].

Additionally, in the case of an attached cavity, finger-like streaks are sometimes formed. Such cavities are prone to irregular instabilities, where the streak structure collapses and re-cavitates. This has also been proposed as a mechanism for cavitation erosion at the cavity closure line [49].

ERI is integrated across the injection hole surface to assess the cavitation erosion more quantitatively. This gives a representation of the total erosion that might occur in the injector hole. In Figure 12, integrated values of ERI normalised by the value for conventional diesel are plotted for pyrolytic oils. Both HDPE and LDPE are predicted to produce around 9% more erosion. A larger increase of 18% is observed for HDPE with zeolite. The most significant increase in erosion is predicted for LDPE with zeolite, with 26% more erosion predicted than in the case of conventional diesel.

4. Discussion and Findings

In the present paper, the influence of pyrolytic oils on cavitation erosion in a common-rail diesel injector was tested numerically. In the first part of the study, waste plastic was collected, cleaned, and further used to produce pyrolytic oils. PO were produced in a batch reactor using thermal and catalytic pyrolysis processes. ZAP USY zeolite was used as a catalyst in the catalytic pyrolysis process. The obtained oils were further characterized, and their properties were compared to conventional diesel fuel. Finally, the obtained fuel properties were implemented in the ANSYS FLUENT computational program and used in the numerical study of cavitation erosion prediction. From the obtained results, we can see that the physical–chemical properties of pyrolytic oils are very similar to conventional diesel fuel. The density, surface tension and kinematic viscosity of PO are

slightly lower compared to diesel fuel, which further influences conditions inside the injection nozzle of tested common-rail injector. The lower viscosity and density of pyrolytic oils advance the formation of cavitation in the injection hole of a common-rail diesel injector. The lower viscosity and density of pyrolytic oils also influence the more rapid spread of cavitation structures in the injection hole of a common-rail diesel injector, Figures 8–10.

The pyrolytic oils' velocity and mass flow rate are influenced by their lower viscosity. The lower viscosity of the POs reduces their friction in the injection hole, which leads to a higher fuel velocity and a further increase in the mass flow rate of PO despite their lower density, as seen in Figure 8. The difference in pyrolytic oil properties further influences the length of cavitation structures in the injection hole, which is promoted by the lower viscosity of pyrolytic oils, Figures 9 and 10.

The longer cavitation structures further influence the location of the predicted cavitation erosion, which is shifted more towards the injection hole exit. Lower fuel viscosity and density increase the cavitation condensation rate, further increasing the predicted cavitation erosion damage. Cavitation erosion zones coincide with the closure of the attached cavity for all used fuels. Therefore, following the same cavitation erosion pattern, it can be concluded that the cavitation erosion mechanism is the same for all fuels analyzed in this work. The cavitation erosion mechanism is that of an attached cavity, which pulsates over time. This mechanism comprises violent cavitation collapses due to stagnation of the flow at the pulsating closure line of the cavitation cloud and instabilities connected to the formation of streak cavities. Both qualitative and quantitative results of cavitation erosion prediction from numerical simulations indicate that all synthetic fuels considered in this study could be more erosive than conventional diesel fuel.

With an erosion risk indicator implemented in a commercial CFD code FLUENT, it is possible to predict and analyze cavitation erosion for different fuels in the diesel injector both qualitatively and quantitatively.

During the presented work, only conditions inside the injection nozzle were studied. These conditions further influence spray development, spray break-up process, fuel combustion, etc. Since PO influences more extensive cavitation inside the injection hole, we can assume that the change in fuel properties will further influence spray characteristics, which will be numerically and experimentally studied in the following work. The authors will also work on upscaling the PO production capacities, which will enable further experimental testing of PO usage in internal combustion engines. Pyrolytic oils have been successfully used as an additive to diesel fuel in ratios up to 50% [13,14]. In both studies, higher brake thermal efficiency and lower specific fuel consumption were obtained. The results of emission when using pyrolysis oils as an additive were not conclusive. In the work of Singh et al. [13], higher exhaust emissions were obtained on all operating regimes, while Das et al. [14] obtained lower exhaust emissions of NO_x and HC when using PO at lower loads and higher at higher engine loads. Das et al. also concluded that adding pyrolysis oils from waste plastic increases the length of ignition delay, which further influences the combustion and emission formation process. So, we believe that additional research in the mechanism of spray break up and combustion can give more insight into the phenomena of PO combustion and emission formation.

The presented study indicates the high potential of plastic waste for further use in resource recovery. This can help to reduce the pollution and environmental impact of waste plastic. Furthermore, using proper processes, the waste plastic can be successfully converted into synthetic fuel, which can be further used as a substitute or additive for conventional fuels. According to life cycle assessment studies, fuels (oils) acquired from waste plastic emit fewer emissions compared to fuels produced from primary fossil resources [50] and can decrease the environmental effect in comparison to landfilling of plastic waste [51]. The cost of pyrolysis highly depends on the type of pyrolytic reactor used. According to Andooz et al. [52], current waste treatment systems can economically

benefit from the integration of pyrolytic processes for resource recovery (like pyrolytic oil production for usage in internal combustion engines, ethylene production, etc.).

5. Conclusions

Based on the presented findings and results, the following conclusions can be made for the numerical study of the usage of synthetic fuels from waste plastic in common-rail diesel injectors:

- Obtained pyrolytic oils have properties similar to conventional diesel fuel.
- The cavitation erosion mechanism is the same for all fuels analyzed in this work.
- The lower viscosity and density of pyrolytic oils advance the formation of cavitation and influence the more rapid spread of cavitation structures.
- The lower viscosity of the PO reduces their friction in the injection hole, which leads to a higher fuel velocity and a further increase in the mass flow rate of the PO.
- The lower viscosity of pyrolytic oils influences the length of cavitation structures.
- The length of cavitation structures influences the location of the predicted cavitation erosion.
- Lower fuel viscosity and density increase the cavitation condensation rate and increase the predicted cavitation erosion damage.
- Cavitation erosion zones coincide with the closure of the attached cavity.
- Implemented erosion risk indicator enables numerical prediction of cavitation erosion.
- The synthetic fuels considered in this study show more erosion potential compared to diesel fuel.

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