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Energetic Efficiency of Turbulent Biofuel Combustion for Advanced Bioenergy Technologies

Abstract. The combustion processes of biodiesel droplets in a combustion chamber using numerical modeling of two-phase reacting flows and complex turbulent currents are investigated in this study. The focus is on analyzing temperature fields, aerodynamic characteristics, and soot particle distribution at varying Reynolds numbers. The results show that optimal combustion conditions for biodiesel are achieved at Reynolds numbers between 20 000 and 25 000, where the greatest combustion temperatures can attain levels of up to 2700 K, signifying both high energy effectiveness and strong combustion stages. Furthermore, this extent of Reynolds number results in a notable decrease in soot particles (75-50 g/g), indicating a more thorough fuel combustion process and enhanced oxidative conditions. The outcome data affirms that expanding Reynolds numbers elevate combustion temperatures and improve biodiesel's environmental efficiency by diminishing the emanations of solid burning byproducts. This inquiry highlights the biodiesel promise as a sustainable and eco-friendly substitute for conventional hydrocarbon fuels, offering optimal combustion characteristics under high turbulence conditions.
Keywords: biodiesel, combustion, numerical modeling, soot emissions, turbulent flow.

Introduction

Liquid hydrocarbon fuels, including gasoline and diesel, continue to serve as the primary power sources for transportation and various manufacturing processes, owing to their high-capacity storage, widespread accessibility, and convenience in distribution and energy storage systems. Nonetheless, their utilization is related with several major biospheric and market-related issues, primarily the release of carbonic acid gas (CO_2) and other climate-altering gases that exacerbate Earth's warming trend, in addition to contributing to atmospheric and aquatic pollution. These factors considerably heighten the difficulties encountered by contemporary society regarding long-term sustainable progress [1, 2].

In light of worldwide initiatives aimed at decreasing carbon emanations and decarbonizing energy supply and transport networks, significant emphasis is placed on the shift towards carbon-free and non-polluting renewable energy systems. With growing concerns about the environment, biodiesel is becoming an increasingly popular alternative to traditional fossil fuels. Produced from renewable organic sources, biodiesel is a sustainable solution that reduces carbon emissions (COx), improves ambient air quality, and can be easily integrated into existing fuel infrastructure [3, 4].

Reducing the use of fossil fuels and actively developing alternative energy is a strategically important step to strengthen the country's energy security and decarbonize the extractive industries of the economy. This not only reduces the negative impact on the environment but also reduces dependence on energy imports, making the country's economy less vulnerable to fluctuations in world prices and more resilient to external challenges [5]. This article explores both the environmental and economic dimensions of hydrocarbon liquid fuel utilization, while also assessing the potential prospects and impediments linked to their substitution with biofuels, with a focus on the role of biodiesel in the process of decarbonization and the transition to sustainable energy systems [6].

The distinctive components of the global energy system experienced varying growth rates in 2024, highlighting the influence of both immediate factors and more profound basic patterns. Renewable energy sources represented the most significant portion of the increase in overall energy supply, contributing 38%. This was taken after by natural gas at 28%, coal at 15%, oil at 11%, and nuclear energy at 8% (Fig. 1) [7]. The energy demand relative to economic growth experienced only a 1% improvement, reflecting the ongoing deceleration observed over the last few years. The increase in CO_2 emanations associated with energy has decelerated to 0.8%, in contrast to the 1.2% rise observed in 2023 [8].

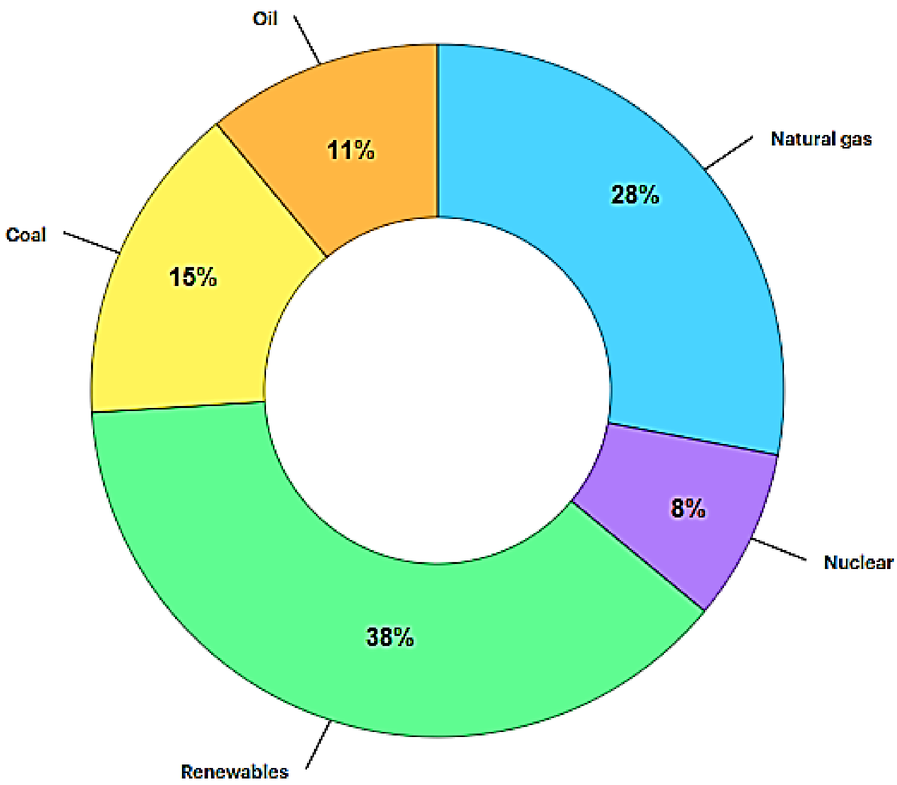


Figure 1 - Share of energy demand growth by source in 2024

The transition to biofuels is becoming an important step in the fight against global climate change and the depletion of traditional energy resources. Biofuels produced from renewable sources such as vegetable oils, agricultural and livestock waste can significantly reduce carbon dioxide emissions and other pollutants. This process contributes not only to environmental sustainability, but also to the creation of new jobs, stimulating the development of green technologies and energy independence [9].

Biodiesel, as an alternative to traditional carbon fuels, has specific combustion characteristics that require more in-depth study to ensure maximum environmental friendliness and cost-effectiveness of its use. Modeling heat and mass transfer processes during its combustion allows us to accurately predict the behavior of the fuel during combustion, improve combustion processes and reduce pollutant emissions. Such studies contribute to the improvement of combustion technologies and ensuring their safe operation, which is important for the development of bioenergy and the transition to sustainable energy solutions.

The liquid particles sputtering and combustion numerical model

The mathematical modeling of liquid fuel sputtering and combustion relies on equations that describe droplet dynamics, evaporation processes, and the transport of mass and energy within the system [10–16]. The accuracy of these models is highly dependent on the proper specification of initial and boundary conditions.

The conservation equation for the chemical species participating in the combustion process is governed by their flux densities, which represent the rate of mass transfer per unit area [10]:

$$\frac{\partial \rho_m}{\partial t} + \vec{\nabla}(\rho_m \vec{u}) = \\ = \vec{\nabla}\left[\rho D \vec{\nabla}\left(\frac{\rho_m}{\rho}\right)\right] + \dot{\rho}_m^c + \dot{\rho}^s \delta_{m1}, \quad (1)$$

where ρ_m signifies the mass volumetric density of the reactive chemical entities participating in the energy release process, ρ means the density of mass at a spatial location of the substance contained within a specified flow domain, and u represents the velocity vector associated with the transport of liquid fuel droplets within the reacting medium

The continuity equation (1) for the liquid phase can be derived by integrating the conservation equations corresponding to its individual constituent components:

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}(\rho \vec{u}) = \dot{\rho}^s. \quad (2)$$

The equation governing the motion of the liquid phase is expressed as [11, 12]:

$$\frac{\partial(\rho \vec{u})}{\partial t} + \vec{\nabla}(\rho \vec{u}\vec{u}) = \\ = -\frac{1}{a^2}\vec{\nabla}p - A_0 \vec{\nabla}\left(\tfrac{2}{3}\rho k\right) + \vec{\nabla}\vec{\sigma} + \vec{F}^S + \rho\vec{g}. \quad (3)$$

The coefficient of A_0 is zero for laminar flows, whereas for turbulent flows, A_0 is equal to one.

The equation described below represents the viscous stress tensor [11]:

$$\sigma = \mu\left[\vec{\nabla}\vec{u} + (\vec{\nabla}\vec{u})^T\right] + \lambda\vec{\nabla}\vec{u}I. \quad (4)$$

Droplet sputtering necessitates phase transitions in order to satisfy the internal energy conservation principle [13]:

$$\frac{\partial(\rho \vec{I})}{\partial t} + \vec{\nabla}(\rho \vec{u}\vec{I}) = -\rho\vec{\nabla}\vec{u} + \\ +(1 - A_0)\vec{\sigma}\vec{\nabla}\vec{u} - \vec{\nabla}\vec{J} + A_0\rho\varepsilon + \dot{Q}^c + \dot{Q}^s. \quad (5)$$

The relation is responsible for calculating the heat flux vector J [14]:

$$\vec{J} = -K\vec{\nabla}T - \rho D \sum_m h_m \vec{\nabla}(\rho_m/\rho), \quad (6)$$

where T is the local temperature of the liquid phase, h_m is the enthalpy of the reaction components, $\dot{Q}^c$ is the amount of heat generated by physical and chemical transformations occurring within the system, $\dot{Q}^S$ is the portion of the heat introduced by the injection of fuel droplets into the system.

Using models based on two mathematical equations is advantageous for estimating velocity and turbulence intensity in engineering applications. The two-equation model is commonly preferred for technical flow analysis. By employing two equations, this model facilitates the calculation of turbulent kinetic energy and the rate at which it dissipates [15, 16]:

$$\rho\frac{\partial k}{\partial t} + \rho\frac{\partial \overline{u}_j k}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]\frac{\partial \overline{u}_i}{\partial x_j} + \\ +G - \frac{2}{3}\rho k \delta_{ij}\frac{\partial \overline{u}_i}{\partial x_j} - \rho\varepsilon, \quad (7)$$

$$\rho\frac{\partial \varepsilon}{\partial t} + \rho\frac{\partial \overline{u}_j \varepsilon}{\partial x_j} - \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] = \\ = c_{\varepsilon_1}\frac{\varepsilon}{k}G - \left[\left(\frac{2}{3}c_{\varepsilon_2} - c_{\varepsilon_3}\right)\rho\varepsilon\delta_{ij}\frac{\partial \overline{u}_i}{\partial x_j}\right] - c_{\varepsilon_2}\rho\frac{\varepsilon^2}{k}. \quad (8)$$

These are standard k-ε equations. The wide application of this model in the problems of complex turbulent flows' simulations is due to its relative simplicity, high efficiency, and reliability. This empirical turbulence model is easy to implement, requires little computational resources, and provides an accurate description of the flow, even without combustion. Besides, the model is well-suited for problems involving chemically reacting flows and demonstrates high accuracy, especially in conditions of high turbulence and at high Reynolds numbers.

The experimental results were employed to determine the constant values of the coefficients c_{ε_1},

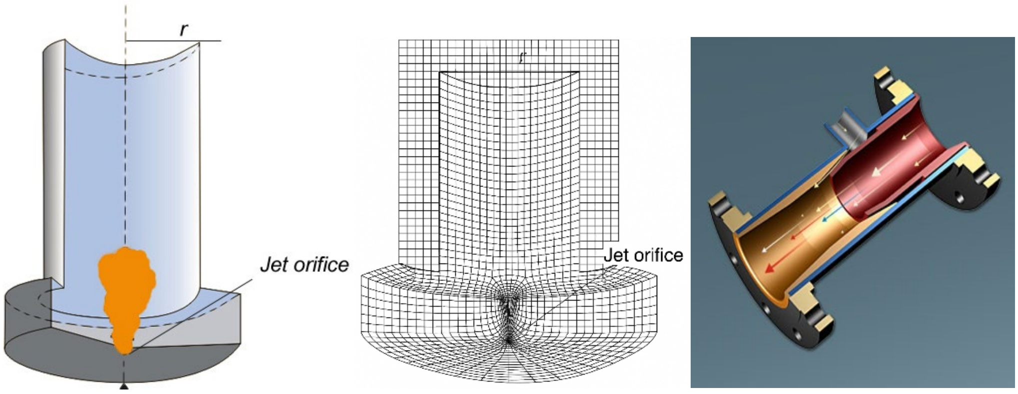
c_{ε_2}, c_{ε_3}, σ_k, σ_ε [10, 14]. The empirical derivation of the default values for these constants is commonly used in engineering calculations.

The problem's physical setup

This study makes use of the model of the cylinder-shaped burner chamber measuring 15 cm in height and 4 cm in diameter. Figure 2 (a, b) presents an overview of the combustion chamber along with its numerical discretization grid. The computational space incorporates 650 cells. Liquid fuel droplets are infused via a nozzle positioned at the center of the chamber's lower section. The initial gas temperature in the chamber is 900 K, the pressure is 80 bar, and the fuel injection speed is 250 m/s.

Liquid nozzles are used to spray fuel oil in diesel engines, with an operating pressure of 10 to 200 bar (Fig.2, c). They create a hollow cone-shaped spray, forming "sheets" of liquid that break up into droplets [17]. As the flow increases, aerodynamic disintegration of the threads and turbulent disintegration occur, causing the liquid to break up into small droplets.

The fuel used in the work is biodiesel, which has several significant advantages. It is an environmentally friendly alternative energy source, as its combustion emits 50-80% less carbon dioxide CO_2 compared to traditional hydrocarbon fuels [18]. Produced from renewable resources, biodiesel is an environmentally friendly fuel that reduces emissions of pollutants such as soot and carbon oxides. Since biodiesel production is based on the use of renewable raw materials, its replacement of traditional fuels helps create a greener and more sustainable energy system and leads to a reduction in human impact on the environment.



a) b) c)

Figure 2 – Main structural elements used in modeling the system under study:
a) Schematic representation of combustion chamber geometry;
b) Visualization and discretization of the computational domain;
c) Illustration of an injector nozzle designed to spray fuel droplets

Biodiesel demonstrates benefits in diesel engines from both an environmental and performance standpoint. Its improved lubricating properties reduce friction between components, resulting in reduced wear and increased engine life. Additionally, biodiesel's higher cetane number allows for more efficient combustion, potentially improving power and fuel economy. The use of biodiesel results in a significant reduction in the emissions of pollutants, including toxic gas CO, nitrogen oxide compounds NOx, and non-combusted carbon-based compounds, thereby situating it as a more ecologically feasible option compared to ordinary petroleum diesel fuel. Additionally, biodiesel can be blended with traditional diesel fuels, facilitating a gradual and practical transition toward cleaner energy sources

Simulation results

In this paper, we study the combustion processes of biodiesel droplets in a combustion chamber using numerical simulation methods for two-phase reacting flows, considering complex turbulent flows. The study analyzed temperature fields, aerodynamic characteristics, and concentration distributions of the mixture at different Reynolds numbers.

Figure 3 shows the results of a numerical experiment to determine the optimal combustion mode of biodiesel fuel in a model combustion chamber depending on the Reynolds number. In the range of Re values from 5,000 to 15,000, the combustion temperature of the fuel-oxidizer mixture is about 1900–2000 K. With an increase in the Reynolds number to 20 000–25 000, an increase in the maximum temperature of the reacting flow to 2500–2700 K is observed, which indicates more efficient mixing of the components and a high intensity of the combustion processes of the droplets.

Analysis of soot particle emissions (Fig. 4) showed that at low Re values, the soot concentration is significantly higher. In the range of Re=5,000–15,000, it reaches 65–130 g/g. With increasing flow turbulence and Re growth to 25 000, a decrease in soot emissions to a level of 50–75 g/g is observed, which indicates improved oxidation conditions and more complete fuel combustion.

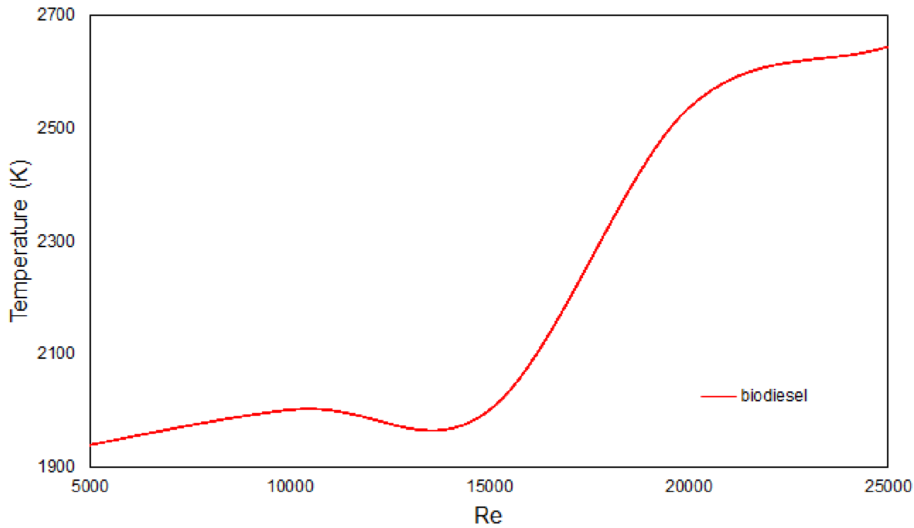


Figure 3 – Distribution of maximum combustion temperature of biodiesel depending on the Reynolds number

The obtained data indicates a direct dependence of the intensity of soot particle formation on the characteristics of the flow turbulence. At low Reynolds numbers, under conditions of less effective blending of the fuel with the oxidizing agent, a limited to a particular area accumulation of the mixture is seen, contributing to the formation of incomplete combustion zones and, consequently, increased soot formation.

On the contrary, at higher Re values, causing intensive mixing and a more uniform distribution of the mixture components, the oxidation process proceeds fully, which leads to a noticeable reduction in soot emissions. Thus, an increase in the Reynolds number contributes not only to an increase in combustion temperatures but also results in a more environmentally benign process through a decrease in the generation of solid combustion products (Fig.4).

The numerical simulation indicates that the most effective chemical reaction mode for biodiesel droplets within the burner chamber is achieved at Reynolds numbers in the range of 20 000–25 000. Within these limits, the highest burning temperature is recorded (reaching up to 2700 K), which signifies efficient energy transfer. Additionally, there is a notable reduction in the soot particles amount (down to from 75 to 50 g/g), demonstrating total oxidation and a diminished environmental impact. Thus, this Re range provides the best balance between thermodynamic efficiency and environmental friendliness of the combustion process.

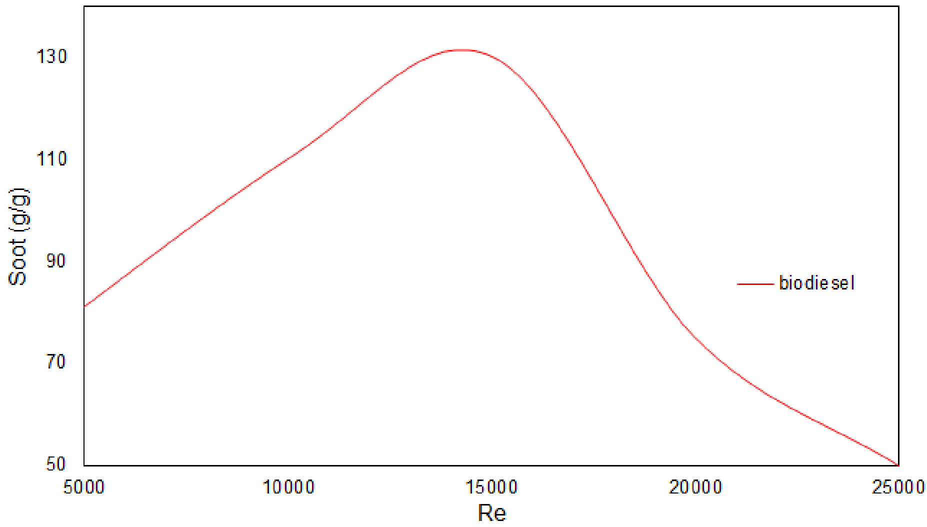
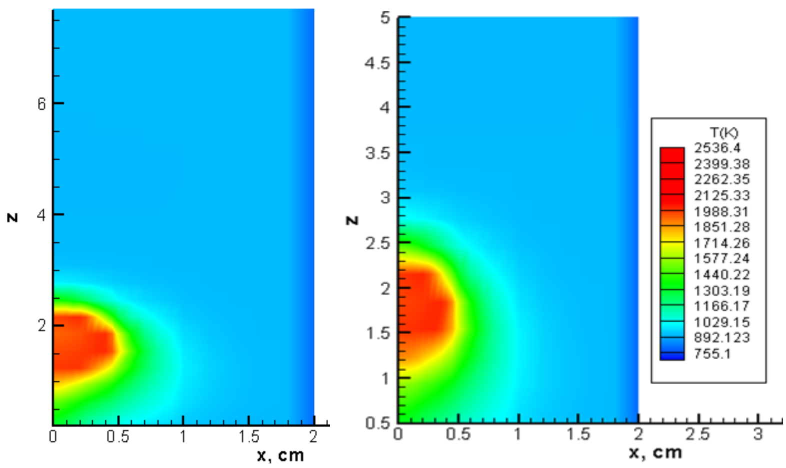


Figure 4 – The effect of different Reynolds numbers on soot particle dispersion during biodiesel droplets combustion

The following figures 5-7 show the results of 3-D numerical simulation experiments of the biodiesel fuel particles combustion thermal processes and visualization of three-dimensional fields of temperature, concentration and velocity characteristics.

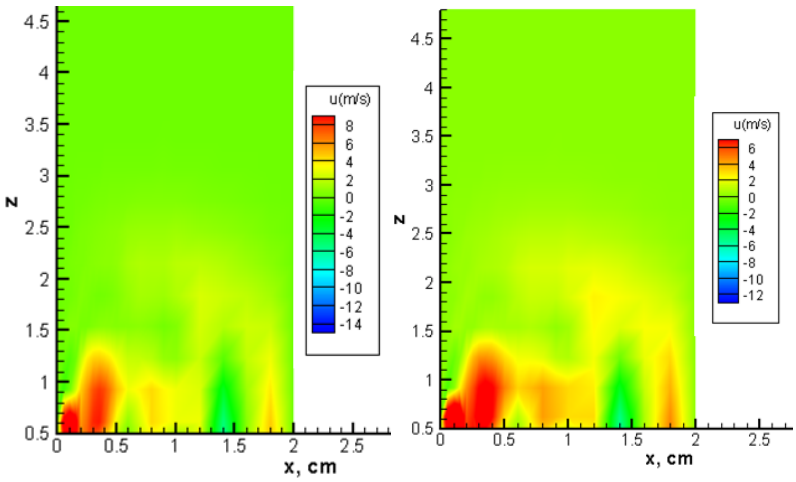
Figure 5 shows the temperature profiles of the reacting flow at a Reynolds number of 20 000 at different rime moments, representing the spatial arrangement of the temperature field and the characteristics of high thermal intensity area formation beneath conditions of strongly turbulent blending. The data reveals that the torch core develops within a height range of 1 to 2.5 cm in the combustion chamber, achieving high-temperature extremes as high as 2700 K. In the remaining part of the chamber the temperature is distributed in the range of 1300–1700 K, which indicates a pronounced localization of the intense combustion zone and an effective thermal regime in the central part of the flame.



a) t=1 ms b) t=2 ms

Figure 5 – Temperature profiles during combustion of biodiesel at Re=20 000

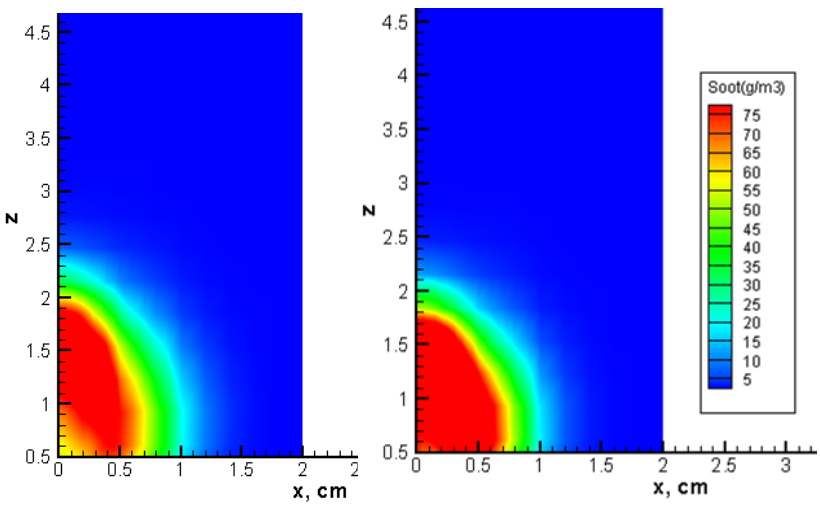
Figure 6 shows the distributions of the aerodynamic characteristics of biodiesel droplets in the combustion chamber at a Reynolds number of 20 000 at different times. Analysis of the results shows that at the bottom of the chamber, the droplet velocity is between 4 and 8 m/s, while at the exit of the chamber, a decrease in their velocity to approximately 2 m/s is observed. This indicates an intense interaction of the droplets with the surrounding flow and a gradual loss of kinetic energy during the combustion process.



a) t=1 ms b) t=2 ms

Figure 6 – Visualization of the biodiesel droplets' velocity distribution in the axial section of the combustion chamber Reynolds number of 20 000

The spatial gradient of the soot particles concentration in biodiesel-fueled combustion are illustrated in Figure 7. The maximum soot content is observed in the central axial zone, within 0.7–1.8 cm along the height of the chamber, where the soot dispersion varies between 65 g/g and 75 g/g. As one moves away from the axis and approaches the exit of the chamber, there is a marked reduction in the quantity of soot particles, ultimately falling to levels between 5 g/g and 25 g/g. This distribution indicates the localized nature of incomplete combustion and subsequent oxidation of solid particles in the residual combustion zone.



a) t=1 ms b) t=2 ms

Figure 7 – Concentration fields of soot during the biodiesel droplets combustion at Reynolds number of 20 000

The simulation data confirms that the best conditions for energy-efficient and green combustion of biodiesel droplets are achieved at high Reynolds numbers, in the range of 20 000 to 25 000. In this range, favorable temperature conditions with maximum values of up to 2700 K, uniform distribution of the thermal field, efficient mixing of components and intensive oxidation of fuel droplets are observed. In addition, a significant decrease in the concentration of soot particles is noted due to more complete combustion. Thus, combustion modes at Reynolds numbers of 20 000 and higher provide an optimal combination of thermodynamic efficiency and environmental friendliness.

Conclusions

In this paper, a numerical study of biodiesel combustion processes in a combustion chamber was performed using two-phase reacting flow and complex turbulent flow modeling methods. The main attention was paid to the analysis of temperature fields, aerodynamic characteristics and distribution of soot particles at different Reynolds numbers.

The modeling results showed that optimal conditions for biodiesel combustion are achieved at Reynolds numbers in the range from 20 000 to 25 000. High maximum temperatures (up to 2700 K) are observed in this range, indicating high heat transfer efficiency and combustion intensity. Moreover, this range of Reynolds numbers ensured a significant decrease in the concentration of soot particles (up to 75-50 g/g), indicating more complete fuel combustion and improved oxidation conditions.

These data confirm that increasing the Reynolds number both increases combustion temperatures and improves the environmental friendliness of the process by reducing particulate emissions. These results demonstrate the high potential for biodiesel to be used as an environmentally friendly alternative to traditional hydrocarbon fuels, with the ability to improve combustion performance under optimal turbulence conditions. Thus, the study showed that under highly turbulent flow conditions, biodiesel can provide an optimal combination of thermodynamic efficiency and environmental friendliness, making it a promising fuel for use in diesel engines and other energy systems.

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CRediT author statement

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