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Nanomaterials and Their Use in Low-Cost Technologies for Reducing Harmful Emissions from the Combustion of Liquid Fuels in Injection Systems †

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Abstract: In this paper, the combustion processes of liquid fuels under conditions of high turbulence are investigated using mathematical modelling methods and the determination of the effective combustion by detecting the concentration of combustion products formed in the combustion chamber. The paper presents a numerical study of the effect of the injection rate on the combustion of liquid fuels by solving differential equations describing turbulent inter-acting flows and comparing nanoscale solutions with changes in the structural solutions of the combustion chamber.

Keywords: combustion; nanotechnology; injection systems; harmful emissions

Today, the development of nanotechnology successfully solves various problems in science and problems in engineering applications. The properties of nanomaterials differ significantly from their bulk materials due to the synergistic effect of various physical phenomena. Combustion processes based on chemical reactions are widespread in natural phenomena and in today's daily life, therefore their study and determination of effective conditions of combustion is of great importance for ecology and human life. It is known that physical, mathematical models, numerical methods and computational methods based on mathematical modelling make it possible to conduct numerical experiments. Based on numerical simulation of the process, they are adapted for a fairly simple explanation.

Determining the effective modes of combustion processes of liquid fuels and their use in industry and everyday life is an important problem for ensuring that the combustion products emitted into the environment correspond to the corresponding values.

Today, ensuring energy security and the use of its environmentally efficient methods directly depends on the use of digital modelling and appropriate methods of its application. For these reasons, the reduction of the release of combustion products of a chemical reaction as a result of the combustion process requires careful study not only of the combustion process itself, but also of the preparation for combustion and the processes occurring during it.

Knowing the laws of combustion processes, it is possible to explain the effect of liquid droplets on the distribution of combustion products, determined on the basis of the dependence of various physicochemical parameters in combustion reactions. The study of all stages of combustion processes is of great importance for solving problems that arise in thermal power engineering and ecology. In this paper, the study of liquid fuel combustion processes based on mathematical modelling methods based on differential equations was carried out and the effective combustion characteristics were determined taking into account the formation of carbon dioxide and oxygen in the combustion chamber.

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The modern design of technical combustion systems must take into account three important factors: heat and mass transfer, optimization of combustion efficiency and reduction of pollutant emissions. Thus, computational fluid dynamics (CFD) is a convenient, economical and reliable tool for facilitating the design of combustion systems. The structure and stability of the flame, the emission of pollutants highly dependent on the aerodynamic and mixing characteristics of the fuel and combustible air flows near the combustion zone.

1. Nanoscale Characteristics in Fuel Combustion

The creation and industrial production of technical devices with low energy consumption and nanoscale elements require an evolutionary transformation of existing approaches to the search and synthesis of materials with predetermined properties and characteristics. Methods for processing raw materials in order to form conditions for self- or forced assembly of atoms (molecules) into nano-objects, nanostructures or nano-scale elements in materials for various purposes are called nanotechnologies [1–3]. The characteristics of nanomaterials depend on their dimensional data and differ on other scales in the nanometer version [4]. Given that nanoparticles can burn and release energy much more easily due to their large surface area to volume ratio and short oxidant diffusion length, it is worth considering their effect on combustion processes in injection systems more carefully [5]. Nanoparticles are widely used as additives to fuels, lubricants and catalysts to reduce harmful emissions during combustion. Given their large surface area, they can be combustion improvers. The purpose of this study is to consider the contribution of nanomaterials in improving the properties of fuel in internal combustion engines made in previous works and compare their effectiveness with the efficiency of changing the design solutions of the combustion chamber.

2. Modeling of Chemical Kinetics of Combustion Processes

Nanoparticles can perform various important functions as an additive in combustion chambers. Previous studies have suggested that nanolubricants are used to reduce friction and wear in the tribopair6 therefore provide stability between contact surfaces and reduce friction. Research has often examined the mechanical mixed bed under various conditions and its stability during processes. Nanosized metal oxides are used as fuel additives to ensure complete combustion. They improve combustion characteristics and can provide additional oxygen to reduce harmful exhaust emissions [6].

This paper considers the KIVA software package for modeling the chemical kinetics of combustion processes in diesel and aircraft engines. This software package is adapted to the proposed problem of burning liquid fuels in highly turbulent combustion chambers. This made it possible to calculate the flow aerodynamics, injection mass, oxidizer temperature, pressure distribution, flow turbulence characteristics, concentrations of combustion products, and other combustion characteristics of fuel vapors and liquid fuels throughout the volume of the combustion chamber [7].

Two RSTMs have been implemented in the KIVA code. Comparison with available, albeit limited, experiments shows that the RSTM results are more realistic. RSTM is able to fix most recirculation structures, including those arising due to the anisotropy of turbulent stresses [8].

The results of changing the injection angle in the spray system showed results from 2 to 10 degrees and the effective parameters of injection in fuel combustion were studied. Figure 1 shows the results of the temperature distribution. As can be seen in the figure, the maximum temperature value at 8 degrees shows 2691 K, and the minimum value is 691 K. Figure 2 shows the distribution of carbon dioxide when the injection angle changes. Figure 3 shows the octane distribution and oxygen evolution. Figure 4 shows the distribution of the minimum and maximum values of fuel release as a result of the combustion process in the combustion chamber.

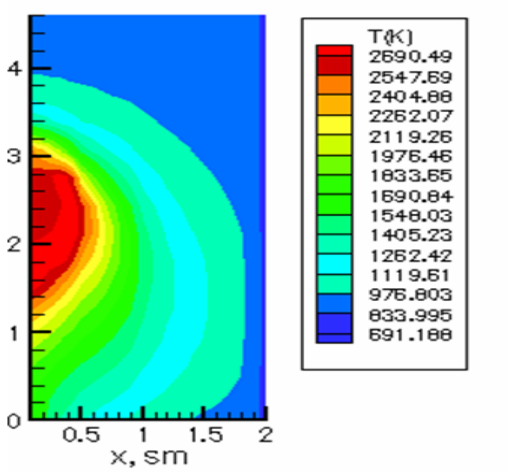

Figure 1. Temperature distribution.

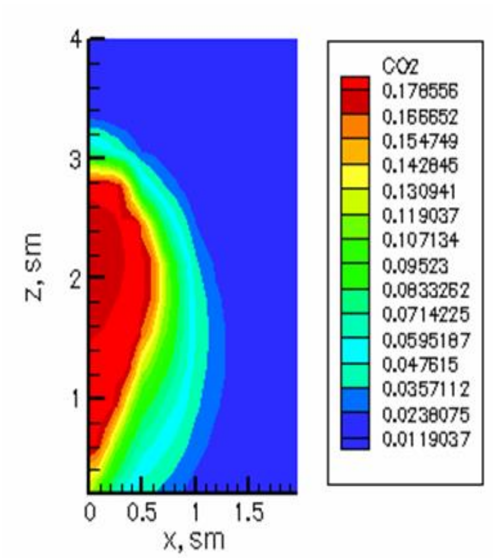

Figure 2. Distribution of carbon dioxide.

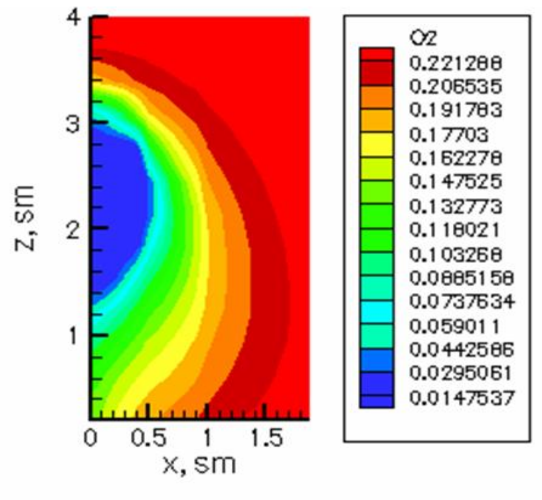

Figure 3. Distribution of oxygen.

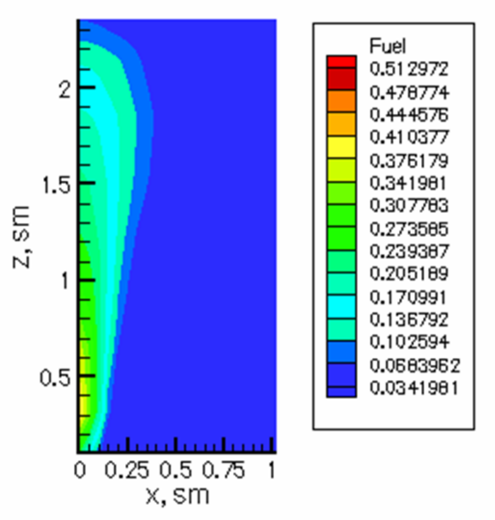

Figure 4. Fuel distribution.

The purpose of this work is to compare in the future methods for reducing harmful emissions in terms of efficiency using computer programs. In this paper, aspects of reducing harmful emissions from fuel combustion by changing the angle of fuel injection during combustion processes are studied. In the future, in my work, planning to compare combustion processes when using nanomaterials and draw a conclusion that it is more efficient to change the initial combustion processes or change combustion designs using nanomaterials for the combustion chamber and for cars. Kiva is a family of programs for studying combustion processes and chemical reactions. The KIVA family of Computational Fluid Dynamics (CFD) software predicts complex fuel and airflows as well as ignition, combustion, and pollutant-formation processes in engines. The KIVA models have been used to understand combustion chemistry processes, such as auto-ignition of fuels, and to optimize diesel engines for high efficiency and low emissions.

Considering the colossal harm of exhaust gases, attention should be paid to related solutions to this issue, which can reduce the harm of displaced substances due to nanomaterials and mechanisms for changing the design solutions of the combustion chamber for different types of fuel.

References

1. Khan, S.; Dewang, Y.; Raghuwanshi, J.; Sharma, V. Nanoparticles exceptional properties: Applications in internal combustion engines. *AIP Conf. Proc.* **2019**, *2100*, 020146.
2. Boles, M.A.; Ling, D.; Hyeon, T.; Talapin, D.V. The surface science of nanocrystals. *Nat. Mater.* **2016**, *15*, 141–153.
3. Roduner, E. Size matters: Why nanomaterials are different. *Chem. Soc. Rev*. **2006**, *35*, 583–592.
4. Sharma, V.; Kumar, B.V.M. Issues in determining size of nano-crystalline ceramic particles by X-ray diffraction. *Mater. Today Proc.* **2015**, *2*, 3534–3538.
5. Burda, C.; Chen, X.; Narayanan, R.; A. El-Sayed, M. Intestinal subepithelial myofibroblasts support the growth of intestinal epithelial stem cells. *Chem. Rev*. **2005**, *105*, 1025–1102.
6. Kuo, K.K.; Risha, G.A.; Evans, B.J.; Boyer, E. Potential usage of energetic nano-sized powders for combustion and rocket propulsion. *MRS Proc.* **2003**, *800*, 39–50.
7. Smith, M.; Crotty, J. Environmental regulation and innovation driving ecological design the UK automotive industry. *Bus. Strategy Environ.* **2008**, *17*, 341–349.
8. Yang, S.L.; Siow, Y.K.; Teo, C.Y.; Hanjalic, K. A KIVA code with Reynolds-stress model for engine flow simulation. *Energy* **2005**, *30*, 427–445.