# Computer simulation of liquid fuel combustion in developed turbulence using the soot formation and oxidation model

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This paper presents the results of computer simulations of the combustion of various types of liquid fuel in a combustion chamber in developed turbulence. When performing a computer experiment, the Shell global chemical reaction model was used which takes into account the formation and oxidation of soot. In the work, a model of a combustion chamber in the form of a cylinder was used, the height of which is 15 cm, diameter 4 cm. This model shows that when fuel interacts with an oxidizing agent, radicals are formed that participate in further reactions and lead to the formation of branching agents and intermediates. The paper presents the results of computer simulation of the combustion of three types of fuel, taking into account the formation and oxidation of soot in developed turbulence, and investigated the average concentration fields of the reaction components, as well as the temperatures in the combustion chambers.

Keywords: numerical investigation, internal combustion engines, turbulent flow, soot, carbon oxides.

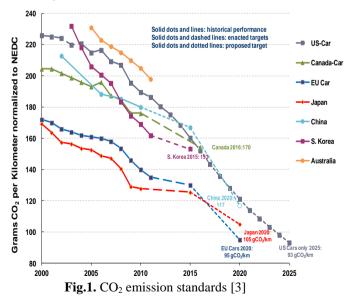
#### INTRODUCTION

The regulations on pollutant emissions are becoming tougher over time, for example, until 2025, as a result of the basic rules established around the world, it is planned to reduce the carbon dioxide emission of CO2 from cars to about 100 mg/km (Fig.1.). Although carbon dioxide is not a toxic gas, it still poses an environmental hazard due to the greenhouse effect. The annual carbon dioxide emissions, according to estimates [1, 2], are about 30 billion tons due to various types of human activity around the world.

At the present stage of energy development, environmental problems are gaining priority. It is known that the International Energy Agency (IEA) has set the task of using renewable energy sources as an energy carrier up to 80% by 2050 and halving the emission of carbon dioxide into the atmosphere as an indicator of emissions of harmful substances [3]. Therefore, the improvement of systems and devices for burning various types of fuel is aimed at increasing the efficiency and, as a result, at reducing the emission of harmful substances into the atmosphere.

Diesel engines are characterized by increased soot emissions. Soot - a fine-dispersed amorphous carbon residue released from smoke resulting from incomplete combustion of fuel.

The formation of carbon black precursors occurs during the period of autoignition, i.e. at low temperatures, i.e. radiation does not have a strong effect on soot formation. Radiation can influence its oxidation, but due to the low concentration of soot in a diesel engine and very short oxidation times, we can ignore the effect of radiation.



## INITIAL DATA FOR COMPUTATIONAL EXPERIMENTS

In this regard, in this work, we studied the

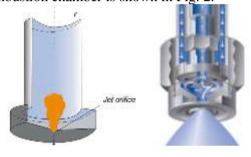
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combustion of various types of liquid fuels using the Shell global chemical reaction model taking into account the formation and oxidation of soot, which consists of the following stages [4]:

- 1. The formation of radicals in the fuel with the oxidant interacting;
- 2. Formation of branching agents and the intermediate products.

In this work, a mathematical model was used that describes the combustion of liquid fuels based on the equations of conservation of mass, momentum and energy.

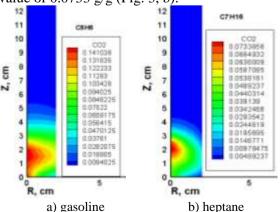
In the work, a model of a combustion chamber in the form of a cylinder was used, the height of which is 15 cm, diameter 4 cm. A general view of the combustion chamber is shown in Fig. 2.

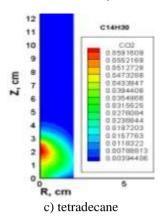


**Fig.2.** The general view of the combustion chamber and its nozzle

#### COMPUTER SIMULATION RESULTS

Fig. 3 presents the average concentration of carbon dioxide in the combustion chamber for three types of liquid fuel (gasoline, heptane, tetradecane). For the three studied types of fuel, intensive formation of carbon dioxide occurs on the axis of the combustion chamber in the region up to 2 cm in height of the chamber. The highest value of gasoline resulting from combustion is 0.1410 g/g (Fig. 3, a). While combustion of heptane, the concentration of carbon dioxide takes a maximum value of 0.0733 g/g (Fig. 3, b).





Accordingly, for tetradecane, the concentration of carbon dioxide in the combustion chamber reaches a maximum value of 0.0592 g/g (Fig. 3, c).

These figures show the results of a computer experiment on the combustion of three types of fuel, taking into account the formation and oxidation of soot in developed turbulence: the graphs show the average concentration fields of the reaction components, as well as the temperatures in the combustion chamber.

#### CONCLUSIONS

In this paper, based on a model of chemical reactions, a numerical simulation of the injection of liquid fuel into the combustion chamber was carried out. The model of chemical reactions used takes into account the formation and oxidation of soot during the combustion of liquid fuels.

As a result of the computational experiments, the distributions of the average concentrations of the reaction components and the average temperature field in the combustion chamber for three types of liquid fuel were obtained.

### **REFERENCES**

- [1] A.S. Askarova, et al. Investigation of the different Reynolds numbers influence on the atomization and combustion processes of liquid fuel. *Bulgarian Chemical Communications* **50**, 68-77, (2018).
- [2] Bolegenova S., Sh. Ospanova, et.al. 3D modelling of heat and mass transfer processes during the combustion of liquid fuel. *Bulgarian Chemical Communications* **E**, 229-235 (2016).
- [3] Richardson M., Danford A., Stewart P., Pulignano V. Employee participation and involvement: Experiences of aerospace and automobile workers in the UK and Italy. *European Journal of Industrial Relations* **16**, 21-37, (2006).
- [4] Gorokhovski M., et. al. The extended IEM mixing model in the framework of the composition PDF approach: applications to diesel spray combustion. *Combustion Theory and Modelling* **10**, 155-169, (2006).