Numerical simulation of liquid hydrocarbon fuel burning in a direct-flow evaporation burner in a jet of superheated steam

Ar A Dekterev¹, A V Minakov¹², I S Anufriev¹

1 Institute of Thermophysics SB RAS, 1 Acad. Lavrentiev pr., Novosibirsk, 630090, Russia
2 Siberian Federal University, 79 Svobodny pr., Krasnoyarsk, 660041, Russia

E-mail: dek_art@mail.ru

Abstract. In this work, the process of diesel fuel combustion in a laboratory sample of an original evaporation-type burner with superheated steam supply to the reaction zone was investigated by numerical simulation. Fuel burning in such a burner occurs in a steam jet flowing through the nozzle. In the framework of research, a mathematical model was developed, the influence of various models of turbulence, approaches to simulation of combustion, and response schemes were investigated.

1. Introduction

Currently, disposal of huge amounts of liquid hydrocarbon wastes accumulated at the oil industry enterprises (waste engine and transmission oils, lubricants, oil sludge, oil production, and refining waste) is an urgent task. Much of this waste is not suitable for regeneration, but it can be incinerated. Solving this problem is important both in terms of improving the environmental situation and expanding the fuel and raw material base of the energy sector through the use of substandard liquid hydrocarbon fuel.

In this work, the process of diesel fuel combustion in a laboratory sample of an original evaporation-type burner [1-2] with superheated steam supply to the reaction zone was investigated by numerical simulation.

The main elements of the burner are as follows (figure1): cylindrical body, combustion chamber with a pre-chamber, steam nozzles, gas generation chamber, and output nozzle. The design of the used burner provides for a natural air flow from the atmosphere into the reaction zone through the openings in the lower part of the combustion chamber. Standard diesel fuel is fed into the combustion chamber through the fuel line. Two steam nozzles (opening angle of 17°) connected to the external steam generator are installed coaxially above the combustion chamber at the base of the gas generation chamber; they are oriented vertically (output diameter of 0.5 mm). The lower one is directed downwards into the prechamber (with an internal cavity in the form of a hemisphere with a conical outlet) located at the bottom in the center of the combustion chamber. The upper nozzle is directed upwards into the gas generation chamber. The evaporating components of the fuel are ignited in the combustion chamber. The products of thermal decomposition and incomplete combustion of fuel are gasified in the gas generation chamber with mixing with an upward jet of superheated steam. The resulting combustible mixture of CO and H₂ burns in a flame, mixing with oxygen from the outer atmosphere.
2. Mathematical model

As part of the work, a mathematical model of this process was developed. The simulation was based on the RANS approach. When performing the computations for modeling the turbulent flows, a wide range of modern models was considered: popular URANS models with vortex viscosity ($k-\varepsilon$ realizable, $k-\omega$ SST), non-stationary model of Reynolds stresses RSMLRR (Launder-Reece and Rodi). To simulate turbulent combustion in the gas phase, several popular approaches were considered: EBU vortex breakage model, hybrid model, EDC model (Eddy Dissipation Concept), FGM model (Flamelet generated manifold) with equilibrium kinetics.

Diesel fuel was presented in the form of surrogate n-heptane (C$_7$H$_{16}$) fuel. To simulate the kinetics of combustion in the gas phase, several kinetic mechanisms were considered, containing: 1, 42, and 60 reactions. Radiation heat transfer was simulated using the discrete ordinate (DO) model, and the absorption coefficient was calculated using the weighted sum of gray gases model (WSGGM).

To take into account soot formation, the Moss-Brooks model with two transport equations for concentrations of soot nuclei and its mass fraction was used. The soot affects the radiative transfer significantly, since the soot particles are taken into account in the total coefficient of medium absorption.

A complete spatial geometry of the computational domain, representing the inner part of the burner and surrounding space, was constructed. Since the geometry is axisymmetric with an accuracy of up to the holes for air inflow, in order to reduce the estimated time, a sector of 30°, containing 1/12 of the geometry with one hole, was taken. The diameter of the area, where the flame expands after exiting the burner, is 500 mm, its length is 600 mm. The dimensions are chosen to exclude the influence of the side and exit boundaries on the flow (see figure 2).
During the research, calculations were carried out for several values of the relative mass flow rate of steam. The paper presents the calculation options corresponding to the values of the relative mass flow rate of steam equal to $\Phi = 0.5$ and $\Phi = 1$. The boundary conditions corresponding to these conditions are presented in the table.

| Boundary condition       | Type of boundary condition | Parameters                      |
|-------------------------|----------------------------|---------------------------------|
| Region of steam supply  | Mass flow rate             | 260°C, 0.4-0.8 kg h\(^{-1}\)    |
| Region of fuel supply   | Mass flow rate             | 260°C, 0.8 kg h\(^{-1}\)        |
| Region of air inflow    | Fixed pressure             | 25°C, 101325 Pa                 |
| Co-current flow         | Fixed velocity             | 25°C, 0.1 m s\(^{-1}\)         |

The unstructured computational grid, in the basic version containing 2.16 million computational cells, was used for calculations (figure 3). In the zone of the flame, in the mixing zone and near the steam nozzles, the computational grid was significantly thickened for more detailed resolution of the processes. A series of calculations for grid convergence was carried out, and as a result, a grid, containing about 2.1 million calculated cells, was selected.
To verify the numerical model, the simulation results were compared with experimental measurements of temperature distribution along the burner axis.

A detailed study of the effects of turbulence models was carried out. The most popular RANS models of turbulence were considered: \( k-\epsilon \), \( k-\omega \) SST and RSM for two regimes with \( \Phi = 0.5 \) and \( \Phi = 1 \). The temperature distributions are shown in figure 4. According to analysis of simulation results, the choice of a turbulence model does not significantly affect reliability of description of the flame structure under consideration. According to the temperature distribution along the burner axis, all models gave similar results. In this case, the use of a more sophisticated RSM model compared to linear vortex viscosity models did not improve the simulation results. For further calculations, the well-proven \( k-\omega \) SST model was chosen.

![Temperature distribution](image)

**Figure 4.** The effect of turbulence models for two regimes, \( \Phi = 0.5 \) (left) and \( \Phi = 1 \) (right)

The presence of soot affects the value of the absorption coefficient. The neglect of soot formation in calculations leads to a significant underestimation of the absorption coefficient. However, according to comparison of calculations with the experiment, the formation of soot does not significantly affect temperature distribution over the burner (figure 5).

![Temperature distribution](image)

**Figure 5.** Effect of soot formation, \( \Phi = 0.5 \) (left) and \( \Phi = 1 \) (right)
3. Simulation results
The processes inside the burner were studied with the help of the developed numerical method. The simulation results in the form of distribution of the main gas-dynamic parameters inside the burner are shown in figure 6. Analysis of simulation results shows that the steam supply has a significant influence on the process of diesel fuel combustion. An increase in the relative steam flow rate leads to more intense fuel combustion inside the burner. This is clearly seen from the comparison of the temperature field for two regimes. This leads to the fact that most of part of fuel burns inside the burner. In this regard, with an increase in steam supply, underburning, amount of produced soot, and value of nitrogen oxides decrease significantly. Analysis shows that the flow structure inside the burner is quite complex. A high-speed steam jet ejects the co-current flow causing formation of several large toroidal recirculation zones. One of the recirculation zones is located behind a pinch at the burner exit and serves as a flame stabilizer.

4. Conclusions
A mathematical model of the process of diesel fuel burning in a jet of superheated steam has been developed. The model takes into account the real spatial geometry of the burner and features of its operation. The model is based on the RANS approach for modeling turbulence and on chemical reaction models that allow consideration of the finite rates of chemical reaction for detailed kinetic mechanisms.

The developed mathematical model and numerical methods were tested in detail. The results of numerical simulation were compared with the experimental data obtained. Comparison with the experiment was carried out using temperature distribution at the burner exit. Good agreement with the experiment is shown. Due to numerous tests and verification calculations, the main sub-models of the developed methodology for calculating the process of diesel fuel burning in a jet of superheated steam were finally determined.

The structure of the flow and flame outside and inside the burner is investigated in detail with the help of the developed numerical method.

Acknowledgments
The study was funded by the grant of the Russian Science Foundation (project No. 18-79-10134).

References
The study was funded by the grant of the Russian Science Foundation (project No. 18-79-10134).

[1] Alekseenko S V, Pashchenko S E and Salomatov V V 2010 J. Eng. Phys. Thermophys. 83(4) 729-741
[2] Alekseenko S V, Anufriev I S, Vigiyanov M S, Kopyev E P and Sharypov O V 2016 Combust., Expl., Shock Waves 52(3) 286-293
[3] Anufriev I S, Alekseenko S V, Sharypov O V and Kopyev E P 2019 Fuel. 254 115723.