Numerical study of combustion of the diesel fuel sprayed with a steam jet in a prospective burner device

D V Krasinsky¹, A I Tsepenok²

¹ Kutateladze Institute of Thermophysics SB RAS, Novosibirsk, 630090, Russia
² OOO "ZiO-COTES", Novosibirsk, 630049, Russia

E-mail: dkr@itp.nsc.ru

Abstract. A prospective laboratory-scale burner device that employs a concept of liquid fuel spraying in the high-speed superheated steam jet is considered. The presented work is devoted to numerical study of aerothermochemical processes occurring in this novel-design burner during the combustion of diesel fuel sprayed with axial jet of water steam. The mathematical model is based on Euler-Lagrange approach for two-phase turbulent reacting flow description applied in 2D axisymmetric steady-state formulation. The vaporized diesel fuel combustion is described via EDC model with chemical kinetics mechanism for \( n \)-heptane (30 species, 66 reactions). The two-step soot model is also used, as well as NOx prediction at post-processing stage. The fields of velocity, temperature, heat fluxes, gas species and disperse phase concentrations, including soot and NOx, have been obtained from numerical simulation for a typical operational mode with diesel supply rate of 1.2 kg/hour and water steam flowrate of 0.8 kg/hour. Analysis of these flowfield data has allowed to reveal the two-layer coaxial structure of reacting flow (consisting of relatively cold near-axis jet layer and the coaxial layer formed by the hot recirculation zone) inside the burner.

1. Introduction

The development of small-scale burners utilizing the low-grade liquid hydrocarbon fuels stipulates the need for fundamental research aimed at investigation of aerothermochemical processes leading to drastic intensification of combustion while matching the environmental safety standards. It is recognized that ad hoc supply of water steam into reaction zone can improve the performance and ecological aspects of heavy-weight hydrocarbon fuel combustion. Such principle of the fuel combustion enhancement by superheated water steam jet has been implemented in a pilot ~10 kW burner developed earlier at the Institute of Thermophysics SB RAS [1]. The steam nozzle is mounted at the burner axis, the vertical cylindrical chamber (main channel of the burner) is located coaxially. There is a separate supply of fuel, air and superheated steam in the burner, with atmospheric air being sucked into the burner through a row of openings made around perimeter of the steel body. The burner reaches the autonomous self-sustained operational mode when the steam pressure inside its boiler part grows up to ~3 bar or higher. In this mode, owing to the supply of steam jet, the formation of bright and short flame is observed with drastic intensification and improved performance of combustion process in the burner (compared to an absence of water steam) characterized by significantly smaller soot and NOx emissions [2]. The processes of the vaporized hydrocarbon fuel combustion in this pilot burner have been recently studied numerically in [3] with mathematical description based on the conserved scalar approach with constrained-equilibrium chemistry model.
With further elaboration of this burner’s design, carried out recently at the Institute of Thermophysics SB RAS, a novel technique of the liquid fuel spraying by the use of high-speed steam jet has been suggested and studied in experiments [4–6]. In this technique the liquid fuel flows down from the fuel-supply pipe inclined at 30° to horizon, ending with a needle located in the vicinity over the steam nozzle orifice, thus appears a hanging fuel drop releasing the liquid that is sprayed by the steam jet stream. It has been noted in [4] that due to this way of liquid fuel feeding into the burner, as there’s no direct contact between the fuel and the nozzle body, the surface of steam nozzle is not subject to carbonization or coke deposition. As a result, the gas-droplet reacting turbulent flow is formed inside the chamber of this modified burner with liquid fuel spraying technique. The body of this novel-design laboratory-scale burner is comprised of the vertical cylindrical chamber of 97 mm height and internal diameter ∅51 mm. A sketch of the burner geometry and its operational principle is given in [5, 6]. The manifold of heat-mass transfer processes takes place there, including the following: the high-temperature vaporization of diesel fuel droplets, the multistage non-equilibrium chemistry reactions in gas-phase multicomponent mixture including soot, the convective and radiative heat transfer. The presented work is devoted to numerical modelling of two-phase aerodynamics, heat transfer and combustion, with account for the aforementioned complex of processes, in the considered novel-design burner and its outer flame.

2. Mathematical model

The 2D axisymmetric steady-state formulation in cylindrical coordinates is employed for mathematical model that is based on Euler-Lagrange approach for two-phase flow description and on RANS approach with the use of “realizable k-ε” turbulence model [7]. Radiative heat transfer is modelled according to P-1 approximation with WSGGM [8] and soot absorption taken into account. The two-step soot model of Moss-Brookes [9] has been used. The Eddy Dissipation Concept of Magnussen [10] (EDC-model) has been applied as turbulent combustion model. To represent a real diesel fuel, the n-heptane (chemical formula nC7H16) has been chosen as a commonly used model (or surrogate) fuel. The thermophysical properties of n-heptane as liquid fuel, including temperature-dependent expressions for the latent heat of evaporation and for the saturated vapour pressure, needed to model vaporization rate of a fuel droplet, are given in [11]. The size distribution of droplet particles at their initial injection points (located near the steam nozzle exit) was taken from measurements [4]. The chemical kinetics mechanism adopted in the present work and describing the non-equilibrium reactive processes during combustion of n-heptane, is based on the one developed in [12] and contains 30 species (including inert nitrogen N2) and 66 reactions. The numerical solution procedure is generally similar to the one described in [3], computations have been performed using CFD package ANSYS Fluent.

3. Numerical results

The burner operational mode with diesel fuel feeding rate of 1.2 kg/hour and superheated water steam flowrate of 0.8 kg/hour, that was used as a typical regime in experimental works [5, 6], has been considered in the numerical study. The performed numerical modelling of the whole range of aerothermochemical processes in the studied burner has allowed to obtain a detailed flowfield information including the fields of velocity, temperature, radiated heat fluxes, species and disperse phase concentrations, including soot and NOx, in the burner and its outer flame (torch). These results are shown in figures 1–6 (it should be noted that the field values are represented there with mirror reflection at burner symmetry axis for clearer view) and are also analysed as profile distributions along the burner axis in figures 7–9. The field of velocity magnitude (see figure 1) shows the burner aerodynamic structure formed by the high-speed jet of water steam released from the axially-mounted steam nozzle (orifice ∅0.6 mm). Due to the conditions (temperature Tt=250°C and pressure Pt=7.8·105 Pa) of superheated steam supplied at the input tube (internal diameter ∅3 mm) that feeds the nozzle, the steam jet discharged from the nozzle orifice becomes supersonic with Mach number Mn~1.2 (at nozzle exit plane). Then velocity of the supersonic expanding jet stream grows further, so within the jet initial region (up to the distance of about 12 nozzle diameters, i.e. ~ 7.2 mm from the steam nozzle
exit) $M \approx 1.47$ and the corresponding axial velocity is $U_x \approx 721$ m/s, as found from the obtained velocity and Mach number profiles along the axis. Further downstreams the jet velocity decays (with transformation to subsonic flow regime) and the jet spreading inside the burner chamber causes the entrainment of external air (see figure 1) that is sucked into the chamber through the air supply openings located along the perimeter of chamber wall. The presence of upper lid (with internal orifice $\varnothing 25$ mm and width of 5 mm – seen as white rectangle in figure 1), covering the chamber top, results in partial inclination and attachment of the flow towards the lid wall and the chamber wall, thus leading to recirculation of the flow formed between a shear layer of the central jet and the chamber and lid walls. This
The distribution of fuel droplets concentration is shown in figure 2 where the locations of initial droplets “seeding” (applied in numerical simulation as 5 injection rakes in a framework of Lagrangian tracking for disperse phase) can be noticed as a region of maximum concentration of disperse phase that “hangs” over the steam nozzle exit. The initial size distribution for the injected fuel droplet particles was specified in the range of 12–35 μm, following the data from experimental study [4]. It is seen from figure 2 that the largest concentration of droplets is reached at the axis line – a more detailed analysis indicates that air entrainment effect can be the cause for such behaviour. Because of evaporation process, the region where the droplets are seemingly present is bounded (note a logarithmic scale of legend in figure 2). Part of the model diesel fuel (n-heptane) evaporated inside the burner chamber enters the recirculation zone (mentioned above) as gaseous species n-C₇H₁₆ and undergoes the reaction processes there. Another part of n-heptane in gaseous or disperse phase is moved out of the burner along an axial jet, thus fuelling the torch (i.e. outer flame region).

The temperature field shown in figure 3 demonstrates a complicated thermal structure inside the burner and in the outer torch region. High temperature level is seen inside the chamber recirculation zone where several spots of reaction heat release can be noticed. However the stream of entrained air separates the central jet from hot flame fronts (occurring in the recirculation zone), therefore the near-axis steam jet remains relatively cold, with temperature less than 485°C along axis inside the chamber. 

As observed from figure 3, the flow exiting the burner chamber through the lid orifice (Ø25 mm) towards the torch is comprised of two layers: the near-axis “cold” jet layer, and coaxial layer of hotter stream leaving from recirculation zone. These two layers provide different composition of reactive mixture that fuels the outer torch: the near-axis “cold” jet is carrying mostly n-C₇H₁₆, H₂O and O₂ (see curves 1, 2, 7 in figure 7), while the coaxial layer is carrying the species of gasification process H₂ and CO (as seen from figures 5–6) mixed together with complete combustion products H₂O and CO₂. The two-layer structure of the flow and chemical composition exiting the burner forms a peculiar feature of outer torch: from temperature field it can be seen that the flame front in the torch is horseshoe-shaped.

The aforementioned aerothermochemical structure in the burner and its torch can also be observed from figures 4–6 representing the fields of O₂, H₂ and CO mole fractions. It is seen that O₂ is consumed inside the chamber recirculation zone and within the horseshoe-shaped bounds of the outer torch. In these low-oxygen zones the fuel gasification prevails, therefore the concentrations of H₂ and CO reach ~10% (by volume) there. Profiles of the species mole fractions along the burner axis plotted in figure 7 provide quantitative details for analysis of reactive mixture composition in the torch. It should be noted that in figures 7–9 the value x=0 of axial coordinate denotes the burner exit plane (i.e. x<0 relates to the region inside the burner chamber and lid, while x>0 relates to the outer region). It can be seen from figure 7 that mass fraction of gaseous fuel n-heptane (curve 2) is gradually decreasing along axis and diminishes to almost zero at x≈98 mm. As opposite, the concentrations of intermediate reactants – CH₄, H₂ and CO (curves 3, 4, 5) – are increasing and reaching their maxima at similar location x≈100–118 mm. Further downstreams these species concentrations start decreasing, while CO₂ mole fraction (curve 6) grows till x≈201 mm; after that the torch flame zone cools down because of entrainment of outer air – see the rise of O₂ mole fraction (curve 1) at x>200 mm. It is worth to note that H₂O mole fraction (curve 7) remains significant (up to 18%) for the whole range of combustion zone plotted in figure 7, thus enhancing conditions for gasification process.

Profiles of the soot and NO emissions (in mole fraction ppm) along the burner axis are depicted in figure 8. A nonmonotonic behaviour seen in the soot profile (curve 1) can be attributed to the nonlinear processes of formation (primarily due to the fuel decomposition), growth, coagulation and oxidation of soot. The nitrogen oxides (NOx) in the burner and its torch are mainly formed via the extended “thermal” N₂ oxidation mechanism of Ya.B.Zeldovich, as it has been estimated in computations performed at a post-processing stage of main numerical solution. The computed integral value of NO emission in exhaust gases from the burner equals to 44.7 ppm – this value corresponds very well (with 2% accuracy) to NO emission measured in [6] for the studied operational mode of the burner.
**Figure 5.** Field of H₂ mole fraction in the burner and torch, %.

**Figure 6.** Field of CO mole fraction in the burner and torch, %.

**Figure 7.** Profiles of the species fractions along the burner axis, %
(curve 2 represents the mass fraction of n-heptane, other curves represent the mole fractions).

**Figure 8.** Profiles of the soot and NO mole fractions along the burner axis, ppm.

**Figure 9.** Profile of temperature along the burner axis, °C. Solid line: numerical modelling, dots: thermocouple measurements [6].
In addition to analysis of the temperature field structure (figure 3), the temperature profile plotted along the burner axis is compared in figure 9 versus the in-flame thermocouple measurements data reported in [6]. One can see that, notwithstanding some shift in the positions of temperature maxima between two profiles, the values of these maxima are almost equal (~1334°C), and the shapes of both experimental and numerical profiles are similar. Therefore the performed comparison on the level of NO emission and on the temperature profile data indicates to adequacy of the used modelling description and the obtained numerical prediction of thermochemical conditions inside the burner torch.

4. Conclusions
The results of numerical investigation of the whole complex of aerothermochemical processes taking place in the novel-design laboratory-scale burner during the combustion of diesel fuel sprayed with a high-speed jet of water steam have been presented. The mathematical model, applied in 2D axisymmetric steady-state formulation, is based on Euler-Lagrange approach for two-phase flow description and allows to take into account the turbulent aerodynamics, the convective and radiative heat transfer processes, the vaporization of liquid fuel droplets, and the combustion of multicomponent gas mixture (with EDC turbulent combustion model using the chemical kinetics mechanism for 30 species and 66 reactions, and also the two-step soot model).

The numerical simulation, performed for the burner operational mode with diesel supply rate of 1.2 kg/hour and water steam flowrate of 0.8 kg/hour, has allowed to obtain and analyse the detailed flowfield information in the burner and its torch, including the fields of velocity, temperature, radiated heat fluxes, species and disperse phase concentrations, including soot and NOx. It has been concluded that the flow inside the burner chamber (and further exiting the chamber towards the torch) is comprised of two layers: the near-axis relatively cold jet layer, and the coaxial layer of hotter stream leaving from the chamber recirculation zone. These two layers also differ in their mixture composition, with near-axis jet layer formed mainly by three components (the injected water steam, the sprayed n-heptane (as model diesel fuel) and the entrained air), while the coaxial layer is carrying the syngas species H$_2$ and CO and the combustion products H$_2$O and CO$_2$. The comparison of the obtained numerical results versus the measurements data [6], performed on NO emission (~45 ppm) and on the temperature profile data, has shown an agreement between experimental and numerical results, thus indicating to adequacy of the used modelling description.

The presented numerical investigation forms the scientific basis for further development of the studied burner device employing a concept of liquid fuel spraying in the high-speed water steam jet.

Acknowledgements
The studies were carried out with the financial support of the RF Ministry of Education and Science, RFMEFI60417X0185.

References
[1] Alekseenko S V, Pashchenko S E, Salomatov V V 2010 J. Eng. Phys. and Thermophys. 83(4) 729-741
[2] Alekseenko S V, Anufriev I S, Vigiryanov M S, Kopyev E P and Sharypov O V 2016 Combust. Expl. & Shock Waves 52(3) 286-293
[3] Krasinsky D V 2018 J. Phys.: Conf. Ser. 1105(1) 012035
[4] Anufriev I, Kopyev E and Shadrin E 2017 MATEC Web of Conf. 115 05010
[5] Anufriev I S et al 2018 J. Phys.: Conf. Ser. 1105 012036
[6] Anufriev I S, Kopyev E P 2019 Fuel Processing Technol. 192 154-169
[7] Shih T-H, Liou W W, Shabbir A, Yang Z, Zhu J 1995 Computers & Fluids 24(3) 227-238
[8] Smith T F, Shen Z F, Friedman J N 1981 Proc. XX-th Nat. ASME-AIChE Heat Transfer Conf.
[9] Brookes S J and Moss J B 1999 Combustion and Flame 116 486-503
[10] Gran I R and Magnussen B F 1996 Combust. Science and Technol. 119 191-217
[11] Sazhin S S 2006 Progr. Energy and Combust. Science 32(2) 162-214
[12] Patel A, King S-C and Reitz R D 2004 SAE Tech. Paper Ser. 2004-01-0558