Numerical simulation of hydrocarbon fuel combustion processes in a burner with axial injection of steam jet

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Abstract. A pilot 10 kW burner of novel design using a concept of hydrocarbon fuel combustion enhancement by axial injection of superheated water steam jet is considered. Numerical simulation of turbulent reacting flow and heat transfer, including the radiative heat transfer, soot and NOx formation processes, during combustion of vaporized diesel fuel in this burner has been performed in 2D axisymmetric formulation. As a combustion model, the conserved scalar approach with constrained-equilibrium chemistry model has been used with account for 3 inlet streams and 32 species. The field distributions of velocity, temperature, concentrations of gas species and soot have been obtained from numerical predictions. The numerical results allow to conclude that the effect of combustion intensification, observed in the burner outer flame, arises from the fuel gasification process enhanced by the influence of steam jet.

1. Introduction
The needs to increase the efficiency of autonomous heating devices stipulate the interest in scientific research of innovative techniques. One of the promising trends is the development of small-scale burners operating at sub-standard liquid hydrocarbon fuels (and waste). Practical use of such fuels, despite their availability, is yet complicated because a number of problems related to their low reactivity and negative environmental impact remain unresolved. In this regard, of particular importance is the fundamental research aimed at the search and substantiation of physical-chemical mechanisms for drastic intensification of combustion and environmental safety.

The presented work is devoted to numerical study of steam-enhanced regime of combustion of heavy-weight hydrocarbon fuel in a pilot burner. It is recognized that ad hoc supply of water steam into reaction zone can improve the performance and ecological aspects of heavy-fuel combustion process. Such principle of the fuel combustion enhancement by superheated water steam jet (thus called a steam-enhanced combustion regime) has been implemented in a pilot ~10 kW burner developed at the Institute of Thermophysics SB RAS [1, 2].

The pilot burner consists of a cylindrical body with the furnace, fuel pipe, air duct, built-in steam generator with the nozzle (sprayer) and the gas generation chamber (see figure 1). The steam generator has a form of annular chamber and includes three separate units: the tank, evaporation tank, steam separator, and steam superheater [2, 3]. The vertical cylindrical chamber of gas generation, being the main channel, is located in the center (along the burner axis), and the steam nozzle is mounted coaxially. There is a separate supply of fuel, air and superheated steam in the burner. The diesel fuel has been used in laboratory tests [3]. At the initial stage of burning in the absence of a steam jet, one
can observe a sooting flame which is typical for diesel fuel combustion in a pool-fire regime [3]. With this, water is heated and pressure in the evaporation tank increases. The heat released during combustion is partially consumed in the steam superheater by increasing the water steam enthalpy. The superheated steam discharges from the nozzle, forming a steam jet evolved into the zone of combustion of products of the fuel thermal decomposition. Then a steady-state regime is reached, being the autonomous and self-sustained operational mode of the burner – this regime can be characterized by the formation of bright and short flame (see figure 1) with drastic intensification of combustion and significantly smaller soot emission [3].

In a series of experimental research works [1–6] the possibility of ecologically safe utilization of heavy-weight or low-grade liquid hydrocarbon fuels, also including some combustible industrial wastes, in this type of burner has been demonstrated. With this, a number of regime variants for diesel fuel combustion has been studied (using the controlled feeding of fuel and steam at varied ratio of their flowrates, as well as by varying the steam temperature) as reported in [4]. Similarly, another series of regime variants in case of burning the waste oil of car transmission as fuel has been studied in [5]. The experiments on a modified pilot burner design (but following the same principle of steam-enhanced combustion) with results of calorimetric measurements have been reported in [6]. The intensified combustion process with bright flame and significantly lower emissions of CO, NOx and soot from the burner has been observed and measured in the aforementioned experimental studies. However, to reveal the conditions and mechanisms leading to such improved performance of the studied burner, detailed aerothermochemical structure of reacting flow and its analysis are necessary, especially inside the burner body (because of known difficulties to apply the field measurement techniques there). With this goal, the numerical simulation of aerodynamics, heat transfer and combustion processes inside the pilot burner with axial injection of superheated steam jet (and in the outer flame) has been performed and its results are presented herein.

2. Mathematical model

Due to axial symmetry of the burner, the problem is formulated in 2D cylindrical coordinates (x, r). The reacting flow of multicomponent gas-phase mixture is assumed to be steady-state incompressible and, within RANS framework, the Favre-averaged governing equations are closed with “realizable” modification of $k-\varepsilon$ turbulence model [7].

From analysis of experimental observations mentioned above it was concluded that the simulation of detailed chemistry is necessary to reproduce the conditions and processes taking place inside the studied burner. Therefore for detailed description of the mixture thermochemical state with account for many (>10) species, the conserved scalar approach (Shvab-Zeldovich approximation) has been used in the work. In this approach the thermochemical solution vector of dependent quantities $\phi = \{T, \rho, C_p, Y_i, \ldots\}$ at each point of the flow is determined from values of independent variables: mixture fraction $\xi$ and its variance $\xi'^2$, for which the corresponding transport equations are solved. Enthalpy $H$ equation is also solved to account for heat loss. The chemical constrained-equilibrium model [8] has been used. To add the water steam jet as a separate stream, the secondary conserved scalar (denoted as $\zeta$ herein) submodel [9] has been applied, therefore the space of independent variables has been specified as $\{\xi, \zeta, H\}$ in computations. The lookup table of dependent quantities constructed for 32 species has dimensions $40 \times 25 \times 128$ in this space.

To account for turbulent fluctuations on combustion, at each CFD iteration the pdf-averaging of the table solution vector was calculated: $\bar{\phi} = \int_0^1 \phi(\xi, \zeta, H) P(\xi, \zeta'^2, \zeta d\xi$, with this the presumed $\beta$-function has been used as pdf function $P$ with mean values $\bar{\xi}, \bar{\zeta}'^2$ as its parameters. The “runtime” averaging
done at each iteration, though taking more computational time, has allowed to limit the lookup table by three dimensions for the used model extension with secondary mixture fraction.

The radiation energy transport equation is based on the known $P-1$ approximation of the spherical harmonics method, with this the no-soot gas mixture absorption coefficient $\alpha_g$ is calculated according to the weighted sum of gray gases model [10]. The effect of soot on radiative heat transfer is very important because of soot particles’ influence on the total absorption coefficient defined as $\alpha_g = \alpha_g + \alpha_s$ where for soot absorption $\alpha_s$ the approximation [11] has been used:

$$\alpha_s = b_1 \rho_s \left[ 1 + b_2 (T - 2000) \right],$$

where $\rho_s$ is the soot “continual” density, $b_1 = 1232.4$ m$^2$/kg, $b_2 = 4.8 \times 10^{-4}$ K$^{-1}$.

Because of substantially non-equilibrium features of the soot formation, growth and oxidation processes, the aforementioned chemical equilibrium model [8] cannot be applied for description of these processes. Instead, the two-step soot model of Moss-Brookes [12] has been used. This model is based on two transport equations for the normalized radical nuclei concentration and the soot mass fraction. The source terms in these equations describe the balance of nucleation, coagulation and growth processes for soot particles, and their oxidation. Also Hall extension [13] of this model, applicable for higher hydrocarbon fuels, has been used in computations.

To predict the nitrogen oxides (NOx) emission in the burner, the transport equations for the concentrations of NO and intermediate species (HCN, NH$_3$, and N$_2$O radicals) are solved at the stage of post-processing of main solution. Within the general kinetic model [9] the following NOx formation mechanisms were taken into account: – extended “thermal” N$_2$ oxidation mechanism of Ya. B. Zeldovich; – “prompt” NO formation in reaction of N$_2$ with hydrocarbon radicals following C. P. Fenimore mechanism; – the mechanism with intermediate N$_2$O formation.

For numerical approximation of convective terms of Favre-averaged momentum equations the second-order upwind scheme [9] has been applied. The numerical solution of the governing equations at each CFD iteration is obtained according to PISO algorithm [14] which provides reliable pressure-velocity decoupling. The computational domain is schematically shown in figure 2, where numbers $1$–$3$ denote the inlet boundaries of the studied burner configuration. At the external inlet boundary 4 (surrounding the burner body at $r > 46$ mm), the air coflow velocity of 0.02 m/s has been specified to stabilize computations. The inlet boundary conditions are shown in table 1. The diesel fuel at inlet boundary 2 has been presumed to be vaporized at $T_{in} = 600$ K and represented by a mixture of the following hydrocarbon species: \{CH$_4$, C$_2$H$_2$, C$_3$H$_6$, C$_4$H$_6$, C$_6$H$_6$, C$_8$H$_2$\}.

The unstructured computational grid built for finite-volume discretization of equations consists of 85984 hexahedral cells. The average size of a mesh cell inside the main channel of the burner is about 0.5 mm and is refined to 0.3 mm nearby the axis, whereas inside channel 1 (see figure 2) of the steam
nozzle the cell size in radial direction is 0.05 mm. Computations have been performed with the use of CFD package FLUENT.

| Boundary type       | \( \xi_{in} \) | \( \zeta_{in} \) | \( T_{in} \)(K) | Mixture molar weight (g/mol) | Mass flowrate (g/s) |
|---------------------|----------------|----------------|----------------|-----------------------------|---------------------|
| 1: H\(_2\)O steam   | 0              | 1              | 500            | 18                          | 0.0417              |
| 2: fuel             | 1              | 0              | 600            | 57                          | 0.0732              |
| 3: air to burner    | 0              | 0              | 300            | 28.9                        | 0.1767              |
| 4: outer air        | 0              | 0              | 300            | 28.9                        | 18.254              |

3. Numerical results

The results of numerical simulation of aerodynamics and combustion processes in the studied burner are demonstrated in figures 3–10 (it should be noted that the field values are represented there with mirror reflection at symmetry axis for clearer view). As seen from figure 3, velocity field inside the burner is formed under the momentum effect of high-speed steam jet which is “transpiercing” the main channel of the burner. In the gradient region of this jet the mixing and chemical reaction processes are intensified due to increased level of turbulent pulsations there. From iso-contours of the temperature field and the species concentrations, presented in figures 4–8, the coaxial three-layer structure of reacting flow inside the main channel can be seen. The temperature maximum is achieved in the middle layer of this structure where the conical flame front takes place – see figure 4. While along the axis and nearby it (inside the central steam jet, i.e. in the axial layer of three-layer structure) a low-oxygen zone is formed (see figure 5) thus providing the conditions to facilitate the gasification process of vaporized fuel (which spreads towards the axial layer because of ejection). Owing to such conditions in the axial layer, the fuel gasification takes place there producing CO and \( H_2 \) in high concentrations (reaching ~30% by volume) as can be seen from figures 6–7. With this, figure 8 shows that concentration of water steam is relatively large only near the steam nozzle orifice, i.e. at the bottom edge of the main channel along the axis.

![Figure 3](image3.png)  
**Figure 3.** Field of axial velocity component inside the burner, m/s.

![Figure 4](image4.png)  
**Figure 4.** Temperature field in the burner, K.

![Figure 5](image5.png)  
**Figure 5.** Field of \( O_2 \) mole fraction (logarithmic-scale legend), %.

![Figure 6](image6.png)  
**Figure 6.** Field of \( CO \) mole fraction, %.
The use of water steam has received a lot of interest in many research works as a way to improve combustion efficiency and even facilitate auto ignition. The addition of superheated steam jet at high velocity promotes distributing the fuel throughout the combustion gases and accelerating the mixing of fuel and air at small length scales. In a number of works (see e.g. [15]) it has been shown from equilibrium calculations that at conditions of lack of air and presence of steam, the syngas (CO and H₂) formation is thermodynamically more favourable than that of atomic hydrogen and hydroxyl group. These observations are fully confirmed by results of the performed numerical simulations.

The contours of soot “continual” density $\rho_s$ obtained in numerical simulations with the use of Moss-Brookes-Hall model [13] are shown in figure 9 (note the logarithmic scale) indicating the features of soot formation and oxidation processes in the burner. It can be seen that the processes of soot particles’ nucleation and concentration growth take place primarily inside the fuel vaporization chamber during the fuel pyrolysis.

The field of NO emission obtained at the post-processing stage of numerical simulations is presented in figure 10, demonstrating that the NO mole fraction does not exceed 15 ppm near the burner exit. With this, the integral value of NOx concentration equal to 12 mg/m³ in exhaust gases from the burner has been found – this value is substantially smaller than the NOx levels typical to conventional burners.

4. Conclusions

The results of numerical modelling of aerothermochemical processes during the diesel fuel combustion in the pilot burner of prospective design (developed earlier in experimental research works [1–3]) have been presented. The distinctive feature of the studied burner is the self-sustained regime of injection of superheated water steam jet into the reaction zone, called a steam-enhanced combustion regime. With the use of comprehensive mathematical model of the turbulent flow, the heat transfer processes and the combustion of multicomponent gas mixture, with constrained-equilibrium detailed chemistry approach and soot formation processes (including soot oxidation and also the effect of soot on radiative heat transfer) taken into account, the numerical simulation of the vaporized diesel fuel combustion inside the studied burner and in its outer flame region has been performed in 2D axisymmetric formulation.

The fields of velocity, temperature, concentrations of gas species, soot and NOx have been obtained from numerical modelling, their analysis has allowed to conclude on the presence of the three-layer coaxial structure of reacting flow inside the main channel of the burner, with its middle layer representing the conical flame front. Furthermore, from numerical results it has been revealed...
that the hydrocarbon fuel undergoes the gasification process in presence of steam jet inside the burner, which leads to the formation of syngas (with mole fractions of CO and H₂ reaching 30%) inside the axial layer of thermochemical structure in the burner main channel. This conclusion corresponds well to experimental observation of drastic intensification of combustion with bright and short flame from the burner. Also the low-NOx performance of the burner has been found in the numerical predictions. The obtained numerical results confirm good prospects of this burner as ecologically clean device for effective combustion of wide-range heavy-weight hydrocarbon fuels.

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