Numerical analysis of the water steam jet gasdynamic parameters influence on the hydrocarbon fuel combustion in a pilot burner

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Abstract. On the basis of the conserved scalar approach with constrained-equilibrium chemistry model, variant numerical simulation of aerodynamics, heat transfer and the vaporized diesel fuel combustion processes, including soot formation and its effect on radiative heat transfer, has been performed in the pilot burner designed according to a concept of a hydrocarbon fuel combustion enhancement by axial injection of superheated water steam high-speed jet. The aerothermochemical structure of multicomponent reacting flow inside the burner has been analysed for the three cases of numerical study, including two regimes of the water steam axial injection with different jet velocity, and one regime of air injection through the same axial nozzle. The dependencies of the burner flame characteristics and its ecological performance on the given gasdynamic parameters of the discharged steam or air jet have been obtained. Also the numerical study has confirmed the low-NOx features of the burner operational regimes with water steam injection.

1. Introduction

It is known that ad hoc injection of water steam towards a reaction zone can improve the performance and ecological aspects of combustion of heavy-weight hydrocarbon fuels. This principle of the fuel combustion enhancement by superheated water steam jet has been implemented in a laboratory-scale 10 kW burner device developed at the Institute of Thermophysics SB RAS [1, 2]. In this novel-design device the steam nozzle is mounted at the burner axis, and the vertical cylindrical chamber (main channel of the burner) is located coaxially. The experimental research reported in [1–4] have demonstrated the appearance of intensified low-soot bright flame discharged from the studied burner. This burner device, fed with diesel fuel and, separately, with water steam generated in a boiler unit, reaches autonomous steady-state regime when the steam pressure inside the boiler grows up to ~3 bar or higher. Then, owing to axial injection of high-speed steam jet, the performance of combustion process in the burner changes distinctly (compared to an absence of water steam), with substantially smaller soot and NOx emissions in the burner torch [1, 2]. The detailed description of the burner design and its operational principle has been given in [3, 4].

With aim to investigate the conditions and mechanisms leading to improved performance of this novel burner, the processes of the vaporized hydrocarbon fuel combustion in this burner have been recently studied numerically in [5] with mathematical description based on the conserved scalar approach with constrained-equilibrium chemistry model. The presented paper is devoted to further development of numerical study [5] with an emphasis on comparative analysis of the influence of the water steam high-speed jet gasdynamic parameters on the diesel fuel combustion in the novel burner.
2. Mathematical model and inlet conditions

The reacting flow of multicomponent gas-phase mixture is assumed to be steady-state. Within RANS framework, the Favre-averaged governing equations are closed with “realizable” k-ε turbulence model [6]. To describe 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 at each point of the flow is determined from values of independent variables: mixture fraction \( \xi \) and its variance for which the corresponding transport equations are solved. Enthalpy \( H \) equation is also solved to account for heat loss. The chemical constrained-equilibrium model [7] has been used. To add the water steam jet as a separate stream, the secondary conserved scalar (denoted as \( \xi_2 \) herein) submodel [8] has been applied, therefore the space of independent variables has been specified as \( \{ \xi, \xi_2, H \} \) in computations. The lookup table of dependent quantities constructed for 32 species has dimensions 40×25×128 in this space [5].

The radiation energy transport equation is based on the known \( P-I \) approximation of the spherical harmonics method, with this the no-soot gas mixture absorption coefficient \( \alpha_s \) is calculated according to WSGGM model [9]. The effect of soot on radiative heat transfer is very important because of soot particles’ influence on the total absorption coefficient defined as \( \alpha_s = \alpha_s + \alpha_i \) where for soot absorption \( \alpha_i \) the approximation [10] has been used. The two-step non-equilibrium model [11] has been applied for the soot processes modelling.

Due to axial symmetry of the burner, the problem is formulated in 2D cylindrical coordinates (\( x, r \)). The burner computational domain is schematically shown in figure 1, where numbers 1–3 denote the inlet boundaries of the studied burner configuration. At the external inlet boundary 4 (surrounding the burner body at \( r > 46 \text{ mm} \)), the air coflow velocity of 0.8 m/s has been specified to stabilize computations. More detailed description of the employed mathematical model and numerical algorithm is given in [5]. Computations have been performed with the use of CFD package FLUENT.

The variant numerical simulation, carried out in the work, includes two regimes of the water steam injection through the axial nozzle, denoted herein as cases ‘S-jet-1’ and ‘S-jet-2’, that differ by the steam jet velocity provided the same flowrate of steam. The boundary conditions at inlet 1 for these cases are given in table 1. Another regime, when air has been supplied through the same nozzle instead of steam, is denoted as ‘A-jet’ case, for which the air jet velocity and the flowrate are the same as in case ‘S-jet-1’, but the inlet air temperature was set to \( T_{in}=640 \text{ K} \) to compensate the molar weight inequality of air and water.

The diesel fuel at inlet boundary 2 has been represented by a mixture of the hydrocarbon species \{CH\(_6\), C\(_2\)H\(_5\), C\(_3\)H\(_6\), C\(_4\)H\(_8\), C\(_6\)H\(_{14}\), C\(_8\)H\(_{18}\)\} as a model fuel with molar weight of 58.6 kg/kmol, assumed to be vaporized (at inlet temperature \( T_{in}=600 \text{ K} \)), with stoichiometric mixture fraction value for this model fuel equal to \( \xi_{i,m} \approx 0.092 \). Other inlet boundary conditions are also specified in table 1.

**Figure 1.** Sketch of computational domain (zoom-in view of the burner body).
The flowrate of the diesel fuel feeding into burner, specified in the numerical study, was 0.81 kg/hour, and the superheated water steam flowrate has been set to 0.25 kg/hour. The mass-based ratio $\gamma = G_3/G_2$ of inlet air and fuel flowrates inside the burner volume, specified in computations, is $\gamma \approx 7.93$, with this the corresponding equivalence ratio $\varphi \approx 1.24$, thus inside the burner channels the fuel-rich conditions are formed and the combustion process completes only in the outer flame (torch) owing to further mixing with external (atmospheric) air.

Table 1. Inlet conditions for the steam jet burner regimes.

| B.C. nr. $i$ | Inlet type | $\xi_{1,in}$ | $\xi_{2,in}$ | Mass flowrate $G_i$ (g/s) | Case of steam jet regime | Inlet velocity $U_{in}$ (m/s) | Inlet temperature $T_{in}$ (K) |
|-------------|------------|--------------|--------------|--------------------------|--------------------------|-------------------------------|-------------------------------|
| 1           | H$_2$O-steam | 0            | 1            | 0.0688                   | S-jet-1                  | 637.9                         | 400                           |
| 2           | Fuel       | 1            | 0            | 0.2245                   | S-jet-2                  | 1188.2                        | 745                           |
| 3a          | Air-to-burner | 0            | 1            | 0.353                    | –                        | 0.06                          | 600                           |
| 3b          | Air-to-burner | 0            | 0            | 0.290                    | –                        | 0.4                           | 300                           |
| 3c          | Air-to-burner | 0            | 0            | 1.138                    | –                        | 0.12                          | 300                           |
| 4           | Air-external | 0            | 0            | 730.1                    | –                        | 0.48                          | 300                           |

3. Numerical results

The results of variant numerical modelling (including the cases ‘S-jet-1’, ‘S-jet-2’ and ‘A-jet’) of the flow and the vaporized diesel fuel combustion processes in the studied burner are demonstrated in figures 2–9. The field of mixture fraction $\xi_1$ distribution inside the burner channels is shown in figure 2 (for the case ‘S-jet-2’). The $\xi_1$ scalar essentially determines the thermochemical state of the mixture (excluding soot). The field of secondary conserved scalar $\xi_2$, denoting the evolution of the water steam jet is shown in figure 3 (in logarithmic scale, case ‘S-jet-2’). It can be seen from figure 3 that the steam axial jet, due to its momentum effect, is streaming through the main channel, thus forming aerodynamic structure of reacting flow inside the burner. As it has been concluded in [5], a reacting flow inside the main channel of this burner is characterized by a three-layer coaxial structure, with its near-axis layer featuring the low-oxygen zone with conditions facilitating the process of the fuel gasification there, and its middle layer representing the conical flame front. Because the near-axis layer is directly formed by the high-speed axial jet of scalar $\xi_2$ (water steam), it is evident that the given gasdynamic parameters of the steam jet can exert a substantial influence on an overall aerothermochemical structure in the burner. Quantitative estimation of this influence is analysed in

Figure 2. Field of mixture fraction $\xi_1$ in the burner (case ‘S-jet-2’).
figures 4–9 representing the profiles of variables along the burner axis for the three compared cases. Here it has to be noted that abscissa value $X=0$ denotes the burner exit plane in these figures, and $X<0$ relates to inner part of the burner, while $X>0$ relates to external region of burner torch (outer flame).

As indicated in table 1, the jet inlet velocity (prescribed at the steam nozzle orifice) is ~1.86 times larger in case ‘S-jet-2’ than in two other cases (provided the same flowrate) – this difference is clearly seen from the profiles of axial velocity component in figure 4. Then in case ‘S-jet-2’ the near-axis values of corresponding mixture fraction $\xi_1$ (see figure 5) and soot concentration $C_{soot}$ (see figure 6) appear to be lower inside the burner main channel because of more pronounced air entrainment (due to higher jet velocity) from the bottom chamber into the main channel. Decreasing the values of mixture fraction $\xi_1$ there effectively implies approaching to the stoichiometric value $\xi_{1,\text{st}}$, i.e. to the reaction front – this leads to increasing the flow temperature inside the near-axis layer of main channel in case ‘S-jet-2’ (compared to case ‘S-jet-1’), as seen from figure 8. Another factor of importance is the soot influence on radiative heat transfer and, consequently, on the temperature field, because the presence of soot provides the largest contribution to the total absorption coefficient $\alpha_{\Sigma}$. One can see from figure 7 that the profiles of $\alpha_{\Sigma}$ are similar to the soot concentration profiles plotted in figure 6. Therefore, when soot concentration is lower (in cases ‘S-jet-2’ and ‘A-jet’), decreasing the values of $\alpha_{\Sigma}$ results in temperature rising due to weakening the heat removal (by radiative heat transfer) from the reaction front. It should be noted that the temperature maximum in case ‘S-jet-2’ takes place inside the burner main channel (at $X<0$, see figure 8) – this is a qualitative distinction to the case ‘S-jet-1’ with lower inlet velocity of steam jet.

In the case ‘A-jet’, when air is supplied through the axially-mounted nozzle instead of steam, the temperature level along the burner axis becomes notably higher (see figure 8), because in presence of $O_2$ from air jet the vaporized fuel is directly oxidized there (instead of the fuel gasification process at low-$O_2$ conditions in case of steam jet), and also the effect of weakening the radiative heat transfer (see figure 7) plays its role in increasing the temperature in case ‘A-jet’. Therefore, as the nitrogen oxide NO formation in the burner and its outer flame torch primarily follows the “thermal” mechanism of Ya.B.Zeldovich, the level of NO emission in case ‘A-jet’ appears to be an order of magnitude higher (see figure 9), than in the steam jet cases, because of the effects of increasing the temperature and presence of $O_2$ mentioned above. This rise of NO emission in the burner is a principal drawback of the regime ‘A-jet’ with axial jet of air.

In the performed variant numerical simulations the following ecological characteristics of the burner exhaust have been obtained: the integral value of NOx concentration is equal to 12 mg/m$^3$ in case ‘S-jet-1’, 20 mg/m$^3$ in case ‘S-jet-2’, and 150 mg/m$^3$ in case ‘A-jet’. Thus, the comparison of the burner ecological performance for two regimes (‘S-jet-1’ vs ‘S-jet-2’) with axial injection of superheated water steam allows to conclude that the case ‘S-jet-1’ with smaller inlet velocity of axial jet appears to be more advantageous. However, compared to the regime with air supply through the axial nozzle, both regimes with water steam axial injection demonstrate a drastic reduction in NOx emission by 7 – 12 times in the studied burner.

Figure 3. Field of secondary mixture fraction $\xi_2$ (logarithmic scale) in the burner, case ‘S-jet-2’.
Figure 4. Profiles of axial velocity component $U$ along the burner axis, m/s.

Figure 5. Profiles of mixture fraction $\xi_1$ along the burner axis.

Figure 6. Profiles of soot concentration $C_{\text{soot}}$ along the burner axis, kg/m$^3$.

Figure 7. Profiles of absorption coefficient $\alpha_\Sigma$ of gas-soot mixture (along the burner axis), 1/m.

Figure 8. Profiles of temperature $T$ along the burner axis, K.

Figure 9. Profiles of NO mole fraction along the burner axis, ppm.
4. Conclusions
A pilot laboratory-scale burner of prospective design with axial injection of superheated steam jet, utilizing the concept of steam-enhanced combustion of hydrocarbon fuels, has been considered. As a continuation of previous numerical study [5] using mathematical description based on the conserved scalar approach with constrained-equilibrium chemistry model, a variant numerical modelling of aerodynamics, heat transfer and the vaporized diesel fuel combustion processes (including soot formation and its effect on radiative heat transfer) in the considered burner has been performed in 2D axisymmetric formulation. Detailed information on aerothermochemical structure of multicomponent reacting flow inside the burner channels and in its outer flame has been obtained for the three variants of numerical simulation, including two regimes of the water steam high-speed axial injection with different jet velocity, and one regime of air supply through the same axial nozzle. On the basis of comparative analysis of these numerical modelling results it has been shown that the high-speed axial jet is forming a certain aerodynamic and thermochemical structure of reacting flow inside the burner. The dependencies of the burner flame characteristics and its ecological performance on the given gasdynamic parameters of the supplied steam or air jet have been analysed. It has been concluded that, compared to the regime with air supply, both regimes with water steam injection demonstrate a drastic reduction in NOx emission – thus confirming the low-NOx feature of the studied burner.

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5. References
[1] Alekseenko S V, Pashchenko S E and Salomatov V V 2010 J. of Engineering Physics and Thermophysics 83(4) 729-41
[2] Patent RU2219435 (F23C11/00, F23L7/00) Method for sootless combustion of fuel 2003 Vigriyanov M S, Salomatov V V, Alekseenko S V Institute of Thermophysics SB RAS
[3] Alekseenko S V, Anufriev I S, Vigriyanov M S, Dulin V M, Kopyev E P and Sharypov O V 2014 Thermophys.&Aeromech. 21(3) 393-6
[4] Anufriev I S, Arsentyev S S, Agafontsev M V, Kopyev E P, Loboda E L, Shadrin E Yu and Sharypov O V 2017 J. Phys.: Conf. Ser. 925 012014
[5] Krasinsky D V 2018 J. Phys.: Conf. Ser. 1105(1) 012035
[6] Shih T-H, Liou W W, Shabbir A, Yang Z, Zhu J 1995 Computers&Fluids 24(3) 227-38
[7] Bilger R W and Starner S H 1983 Combustion and Flame 51, 155-176
[8] ANSYS Fluent User’s Guide. 2018 ANSYS Inc.
[9] Smith T F, Shen Z F, Friedman J N 1981 Proc. XX-th Nat. ASME-AIChE Heat Transfer Conf.
[10] Sazhin S S 1994 An approximation for the absorption coefficient of soot in a radiating gas Manuscript (Fluent Europe, Ltd.)
[11] Brookes S J and Moss J B 1999 Combustion and Flame 116, 486-503