Calculation and analysis of the flamelet library for numerical modelling of the non-premixed combustion of natural gas in a pilot burner

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Abstract. The flamelet modelling concept has been employed for numerical simulation of the non-premixed combustion of natural gas in a pilot burner of novel type. This prospective laboratory-scale burner device is featured by axial supply of high-speed jet of flue gases, while the fuel (natural gas) and the oxidizer (air) are supplied radially and separately inside the burner chamber. With the use of chemical kinetics mechanism for natural gas (62 species, 398 reactions) the flamelet library has been generated, from its analysis the flame quenching has been determined at the scalar dissipation rate limit of 42 (1/s). From this library the lookup-table of thermochemical solution has been pre-calculated with the presumed beta-function pdf averaging. On this basis the numerical simulation of aerodynamics, heat transfer and the natural gas combustion processes, including soot formation and its effect on radiative heat transfer, has been performed in the considered pilot burner run at the thermal load of 8.8 kW and air excess coefficient of 0.85 (inside the burner body). The distributions of gas species are presented. The predicted NOx emission in exhaust gases is 48.8 mg/m³ for the studied burner regime.

1 Introduction

The need to diminish the effects of environmental pollution during the combustion of organic (and fossil) fuels stands in a row of major scientific and technological problems nowadays. A principle of ad-hoc supply of water steam into reaction zone of a hydrocarbon fuel appears to be a promising technology to improve ecological aspects of combustion in the burner devices. Based on this principle, a series of novel laboratory-scale burners have been developed at the Institute of Thermophysics SB RAS [1-3]. It has been demonstrated in our studies that the axial blowing of high-speed jet of superheated water steam into the burner chamber leads to substantially reduced soot and nitrogen oxides (NOx) emissions in the burner torch [1-5]. The description of the pilot burner design and its operational principle has been given in [2-5].

The use of other inert gas mixtures (except the H₂O steam), blown in a high-speed jet through the axial nozzle, has been found in our recent studies [6, 7] to provide a qualitatively similar effect of emissions reduction in a burner.

The present numerical study aims to continue the research conducted recently on the performance of this novel burner, with emphasis on the simulation of natural gas combustion taking into account the detailed chemistry by the use of the flamelet modelling approach. The chosen composition of the axial high-speed jet corresponds to the products of complete combustion in the burner torch – this would allow to mimic the effect of flue gases recirculation back into the burner chamber. The work presents analysis of the flamelet library obtained for the natural gas – air diffusion flame. Then the numerical simulation of aerodynamics, heat transfer and the natural gas combustion processes has been performed in the considered pilot burner.

2 Mathematical models and numerical solution

2.1 The burner flow and heat transfer modelling

The reacting flow of multicomponent gaseous mixture is assumed to be steady-state. Within RANS framework, the Favre-averaged governing transport equations for the flow momentum and enthalpy are closed with “realizable” modification of k-ε turbulence model [8]. Radiative heat transfer is modelled according to P-I approximation of the spherical harmonics method, with WSGGM [9] and soot absorption models taken into account. The two-step non-equilibrium model of Moss-Brookes [10] has been applied for the soot processes modelling.

An axial symmetry of the burner allows to formulate the problem in 2D cylindrical coordinates (r, z). The burner device geometry and a zoom-in part of...
computational domain are schematically shown in Figure 1, where the inlet boundaries of the studied burner configuration are enumerated from 1 to 4. The mixture composition specified at these inlets is given in Table 1. The mass flowrate of the natural gas supplied through inlet 1 has been set to 0.64 kg/h. The lower calorific value of this gas fuel equals to 49.53 MJ/kg, so the given fuel flowrate corresponds to the burner thermal load of ≈8.8 kW. The mass flowrate of air supplied through the inlets 3a and 3b (in total, see Figure 1) corresponds to the burners of combustion in the fuel and air. Therefore, the jet mixture composition 0.85 inside the burner body. The conditions of prescribed air excess coefficient, which is set to the value of 0.85 inside the burner body. The conditions of atmospheric pressure (1 atm) are assumed. The Dirichlet boundary conditions for temperature at the inlets 1, 3a, 3b and 4 are all set to the value of 300 K.

![Fig. 1. Sketch of computational domain and boundary types (zoom-in view of the burner body).](image)

Table 1. Mixture composition at inlet boundaries.

<table>
<thead>
<tr>
<th>B.C. nr.</th>
<th>Inlet flow type</th>
<th>Mixture composition</th>
<th>Mixture fraction ( \xi_m )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>species</td>
<td>mole fraction, %</td>
</tr>
<tr>
<td>1</td>
<td>Fuel</td>
<td>CH₄</td>
<td>93.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>C₂H₆</td>
<td>4.7</td>
</tr>
<tr>
<td></td>
<td></td>
<td>C₄H₁₀</td>
<td>2.1</td>
</tr>
<tr>
<td>2</td>
<td>Axial jet</td>
<td>CO₂</td>
<td>9.77</td>
</tr>
<tr>
<td></td>
<td></td>
<td>H₂O</td>
<td>18.57</td>
</tr>
<tr>
<td></td>
<td></td>
<td>N₂</td>
<td>71.66</td>
</tr>
<tr>
<td>3a, 3b, 4</td>
<td>Air</td>
<td>O₂</td>
<td>21.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>N₂</td>
<td>79.</td>
</tr>
</tbody>
</table>

An axially-mounted nozzle has the diameter of 0.5 mm (inlet 2), through this orifice a high-speed jet is released and evolves along the burner axis. The specified jet velocity at inlet 2 is 680 m/s, corresponding to Mach number M=1.68 (at the temperature of 414 K). The mixture fraction value at inlet 1, 3a and 3b are all set to the value of 300 K.

![Fig. 1. Sketch of computational domain and boundary types (zoom-in view of the burner body).](image)

2.2 Flamelet modelling of the natural gas – air diffusion flame

From an earlier analysis of experimental observations [2, 3] it was concluded that the simulation of detailed chemistry is important to reproduce accurately the conditions and processes taking place inside the studied burner [4, 5]. Thus, for a description of the mixture thermochemical state with account for many species (e.g. \( N_s>10 \)), the conserved scalar approach for diffusion flames (non-premixed combustion systems) known as the 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 a set of independent variables, with mixture fraction \( \xi \) being the principal one. Thus, the corresponding transport equations are solved for mixture fraction \( \xi \) and its variance \( \xi^2 \) (which represents the 2nd moment of turbulent pulsations in \( \xi \)). Also the enthalpy \( \mathcal{H} \) transport equation is considered to take into account the effects of non-adiabaticity (radiative and convective heat loss).

Within the conserved scalar modelling framework, basically two routes to a treatment of the chemical reactions kinetics can be mentioned: as the first one, the chemical constrained-equilibrium model [12] is well-known. It is based on an assumption of chemical equilibrium for all species (with special constraints), therefore a chemical kinetics mechanism is not used in that model. As the second route, the flamelet models [13] are known as a general approach to include detailed flame chemistry (reactions kinetics) with account for non-equilibrium effects.

In a laminar steady-state flamelet model [14] the balance equations for the temperature \( T \) and concentrations of gas species (mass fractions \( Y_k \)) are formulated in the mixture fraction space \((0 \leq \xi \leq 1)\) as follows:

\[
\frac{1}{\rho} \frac{\partial C_p \rho \xi}{\partial \xi} \frac{\partial^2 T}{\partial \xi^2} = -\frac{\sum_{k=1}^{N_s} H_k \dot{w}_k}{\xi_m} \\
\frac{1}{\rho} \frac{\partial C_p \rho \xi}{\partial \xi} \frac{\partial^2 Y_k}{\partial \xi^2} = -\dot{w}_k
\]

where \( \rho \) is the mixture mass density, \( C_p \) – the mixture specific heat at constant pressure, \( H_k \) – enthalpy of species \( k \), \( \dot{w}_k \) – rate of chemical production of species \( k \), and the species index \( k=1...N_s \). The quantity \( \chi \) appearing in equations (1)-(2) is called the scalar dissipation rate \((s^{-1})\), with definition:

\[
\chi = 2D|\nabla \xi|^2
\]

where \( D \) is the diffusion coefficient (assumed in the model as a single quantity for all species), and the next term in the product in (3) is the magnitude of gradient of \( \xi \). The scalar dissipation rate \( \chi \) can be interpreted as the
inverse of a representative diffusive time that limits the reacting system from attaining a chemical equilibrium [15]. Therefore, quantity $\chi$ is used in the flamelet model to characterize a departure of reactions from equilibrium.

With this it should be noted that the definition of $\chi$ via formula (3) is not used in the calculations; instead, the quantity $\chi^*$ is considered as a parameter of the system of ordinary differential equations (1)–(2). Thus, in flamelet calculations, for each specified value of $\chi^*$, the solution of ODEs (1)–(2) is obtained. As a result of this solution process with $\chi^* = \text{var}$, the flamelet library can be built up from the obtained set of 1-D thermochemical solutions. After the flamelet library is created in the form of a lookup-table, the thermochemical data can be retrieved from it (at any given point $(\tilde{\xi}; \tilde{\chi}^{ stars }; \tilde{\chi}_c; \Delta H)$ in the library) during iterative solution procedure in CFD code. To link the CFD-solution flowfield with flamelet library data, the scalar dissipation rate in CFD flowfield is modelled as:

$$\tilde{\chi}_e = C_x \tilde{\chi}^{ stars } $$

(4)

where $C_x \approx 2$ is a recommended value, see e.g. [15].

It should be noted that a principal limitation of the flamelet modelling stems from the mapping of physical space into mixture fraction space, so the boundary conditions for the chemical species have to be expressed in terms of mixture fraction. This implies that one inlet boundary can be set to an “oxidizer” type (with $\tilde{\xi}=0$) and one another inlet can be set to a “fuel” type (with $\tilde{\xi}=1$). Therefore, in general the applicability of this modelling approach is limited to only two types of boundary conditions for the species. An ad-hoc case with the third inlet type can be considered by setting an intermediate value of $\tilde{\xi}$. Such case is employed in the present study with stoichiometric mixture fraction value $\tilde{\xi}_0$ prescribed at inlet 2 (see Section 2.1 and Table 1), so that the jet (inlet 2) mixture composition corresponds to the products of complete combustion in the burner torch.

According to the modelling technique described above, the laminar flamelet library has been generated in the present study for the natural gas – air diffusion flame. In these calculations the scalar dissipation rate was varied in the range: $10^{-3} \leq \chi \leq 42$ (s$^{-1}$), with number of flamelets $n_e = 54$. The used chemical kinetics mechanism for natural gas is comprised of 62 species and 398 reactions [16]. To account for turbulent fluctuations on combustion, the pdf-averaging of the lookup-table solution vector was calculated, with this the presumed $\beta$-function pdf has been used with mean values $\tilde{\xi}, \tilde{\chi}^{ stars }$ as its parameters. As a result, the pdf-averaged lookup-table of thermochemical solution, employed in the CFD-solution process, has been pre-calculated with dimensions $64 \times 20 \times 54 \times 100$ ($n_e \times n_e \times n_e \times \Delta H$) in the present study.

### 3 Computational results

The set of solutions of ODE system (1)–(2) in mixture fraction $\xi$ space has been obtained, as described above, with the use of chemical kinetics mechanism for natural gas (containing 62 species and 398 reactions), with parameter $\chi^*$ varied from 0.001 to 42 (s$^{-1}$). This range is discretized in $n_e = 54$ nodes with variable stepping – thus, the flamelet library consisting of 54 laminar flamelet solutions has been calculated.

To analyse the thermochemical solution contained in this library, the profiles of temperature $T$ and mass fractions of some species ($Y_{OH}, Y_{CO2}$ as examples) are presented in Figures 2–5. With this, in Figures 2 and 5 the solution profiles are demonstrated versus mixture fraction $\xi$ for different values of the scalar dissipation rate $\chi$, whereas in Figures 3–4 the profiles are plotted versus $\chi$ for different values of $\xi$. From Figure 2 (where the mixture fraction $\xi$ is given in logarithmic scale for a better resolution of the near-stoichiometry range) it is clearly seen that increasing the scalar dissipation rate leads to essentially lower maximal temperatures of profiles – this is a general trend for all the profiles of $T$ in the library.

When the scalar dissipation rate is increased up to a certain value $\chi_q$, the flamelet “quenching” occurs. Nearing this effect is manifested by the dashed curve at $\chi = 40$ s$^{-1}$ in Figure 2. And Figures 3–4 indicate a pronounced downward trend in the temperature and $Y_{OH}$ profiles at $\chi > 40$ s$^{-1}$. Eventually the “quenching” value estimate $\chi_q \approx 42$ s$^{-1}$ has been obtained in the performed laminar flamelet calculations for the natural gas – air diffusion flame. For higher rates $\chi > \chi_q$, any non-trivial solution across a flame in mixture fraction space could not be found, which means that the imposed nonequilibrium effect leads to extinguishing of burning reactions.

![Flamelet profiles of temperature $T$ (K) vs mixture fraction ($\xi$ in logarithmic scale) plotted at different values of the scalar dissipation rate $\chi$ (1/s).

Fig. 2. Flamelet profiles of temperature $T$ (K) vs mixture fraction ($\xi$ in logarithmic scale) plotted at different values of the scalar dissipation rate $\chi$ (1/s).

It is interesting to note that a lower “quenching” value of $30$ s$^{-1}$ has been earlier reported in [15] (though the natural gas was approximated by a mixture of 98% CH$_4$ and 2% N$_2$ in that work). Nonetheless, the “quenching” value $\chi_q \approx 42$ s$^{-1}$ found in the current study can be considered as improving the accuracy of this estimate.
Fig. 3. Flamelet profiles of temperature $T$ (K) vs the scalar dissipation rate, at different values of mixture fraction $\chi$.

Fig. 4. Flamelet profiles of OH mass fraction vs the scalar dissipation rate, at different values of mixture fraction (substituted by shifted values $\Delta \chi = \chi - \chi_{st}$ on the legend).

On the left side of the $\chi$-range, for the smallest value $\chi = 10^{-3}$ s$^{-1}$ the flamelet profiles are obviously approaching the state of chemical equilibrium – see red curves in Figures 2 and 5. And, considering Figure 5, it is observed that the profile $Y_{CO2}$ at $\chi = 10^{-3}$ s$^{-1}$ resembles an analytical form given by the full-equilibrium model for CH$_4$ – air flame [17]. Also the qualitative differences of $Y_{CO2}$ profile at $\chi = 10^{-3}$ s$^{-1}$ (red curve) from the other profiles (at $\chi \geq 1$ s$^{-1}$) are evident. The above elucidation proves that the calculated laminar flamelet library covers the whole range of thermochemical states (at adiabatic condition): from fully-equilibrium to a set of non-equilibrium states, with transformation to the flame quenching.

Through the procedure of presumed $\beta$-function pdf-averaging of laminar thermochemical solution, the flamelet library has been converted (adding two more dimensions to account for the turbulent fluctuations and the non-adiabaticity effects) into the lookup-table (see Section 2.2) to be employed in the CFD-solution process.

On this basis the numerical modelling of the turbulent multicomponent reacting flow, taking into account the whole complex of heat and mass transfer processes during the natural gas combustion, has been performed in the studied burner in 2D axisymmetric formulation. The obtained mass fraction $Y_k$ distributions are presented in Figure 6 along the burner axis, including the fuel and the sum of its intermediate decomposition species, as well as H$_2$, CO, and O$_2$.

It can be observed from Figure 6 that inside the burner body (with $x = 0$ denoting the burner exit plane, see Figure 1) a low-O$_2$ zone is formed, providing the conditions for the fuel gasification process. Indeed, at the beginning of the burner torch (i.e. near the plane $x = 0$) the fuel mass fraction is reduced to $Y_F \approx 0.015$ (see brown curve in Figure 6), but the presence of CO is much larger: $Y_{CO} \approx 0.053$. Also it can be noted that at a distance $x > 150$ mm from the burner exit plane the CO concentration diminishes.

Fig. 5. Flamelet profiles of CO$_2$ mass fraction vs mixture fraction, at different values of the scalar dissipation rate $\chi$ (1/s).

Fig. 6. Profiles of the species mass fractions $Y_k$ along the burner axis.
For an assessment of ecological performance of the burner torch in the studied regime, the field of nitric oxide concentration has been computed at the post-processing stage of numerical simulations, from it the integral value of NOx emission equal to 48.8 mg/m³ in exhaust gases from the burner has been found.

4 Conclusions

In the performed numerical study the laminar flamelet library has been generated for the natural gas – air diffusion flame, using the chemical kinetics mechanism for natural gas, comprised of 62 species and 398 reactions. In these calculations the scalar dissipation rate was varied in the range: 10⁻³ ≤ χ ≤ 42 (s⁻¹). The flamelet library profiles of temperature and some of the species are presented in mixture fraction ξ space, with the scalar dissipation rate χ varied. Also the orthogonal slices (versus χ, at ξ=var) of the flamelet library are plotted. Analysis of these profiles clearly shows the effect of the flame solution “quenching”, which appears at the scalar dissipation rate χ_q ≈ 42 s⁻¹. On the other side, for the smallest value χ = 10⁻³ the flamelet profiles are seen to approach the chemical equilibrium.

Then the procedure of presumed β-function pdf averaging of the laminar flamelets has been done (to account for the turbulent fluctuations and the non-adiabaticity effects), so the lookup-table of thermochemical solution, employed in the CFD-solution process, has been pre-calculated with dimensions 64×20×54×100.

On this basis the numerical simulation of aerodynamics, heat transfer and the natural gas combustion processes, including soot formation and its effect on radiative heat transfer, has been performed in the considered pilot burner (the composition of the axially-blown jet corresponds to the products of complete combustion in the torch) run at equivalent thermal load of ≈8.8 kW and air excess coefficient of 0.85. The integral value of NOx concentration equal to 48.8 mg/m³ in exhaust gases from the burner has been found in the numerical predictions.

References

16. ANSYS Fluent User’s Guide (ANSYS Inc., USA, 2018)