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TECHNOLOGY AND CODE FOR NUMERICAL SIMULATION OF DIFFERENT COMBUSTION TYPES IN HIGH-SPEED VISCOUS GAS TURBULENT FLOWS

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Abstract

The principal aim of the work is development and realization of a computationally efficient method for numerical simulation of turbulent flows with combustion that occur in perspective aircraft combustors. An original combined method is developed. It treats different combustion regimes (in the range from premixed to non-premixed diffusive combustion) without alteration of numerical algorithm. Validation of code for simulation of 3D flows on the basis of unsteady RANS equations for multi-component compressible gas with finite rate chemical reactions is described. "Laminar approximation" and classical presumed PDF approach together with flamelet model with direct calculation of mass fractions and temperature are compared with universal method where PDF approach is used only for calculation of source terms.

1 Introduction

Turbulent combustion has become an object of detailed research approximately since the middle of XX century - in particular works [1-5] et al. Much attention was given to the structure of turbulent flame and combustion mechanisms. In turbulent combustion several principally different combustion regimes were distinguished: regions of distributed combustion (where chemical reaction time is large compared to the biggest characteristic time scale of turbulent flow), regime of micro-flames - flamelets - when the largest time scale of chemical reaction is small compared to the smallest turbulent time scale (Kolmogorov scale) et al.. A large amount of works devoted to development of mathematical models for numerical simulation of turbulent diffusion combustion (see reviews: [6-8] et al.).

In current work the approach based on solution of RANS equations is used for turbulent combustion modelling. The first one utilizes averaged in time Navie-Stocks equations (RANS). Turbulence is described through differential models of (k-ε) class or through non-bussinesk differential models for the second moments. For turbulent combustion description the probability density function (PDF) approach is usually used together with models like flamelet [9].

Promising way for development of computationally non-expensive procedure for PDF construction is flamelet approach (FL) formulated for subsonic turbulent flames in studies of [10-12]. In this conceptual view of turbulent combustion the reaction zone is analyzed as a collection of laminar flame elements (flamelets) imbedded in the turbulent flow [13-22]. The simplification of the turbulence/chemistry interaction modeling is achieved here based on the assumption that chemical processes are mostly confined to the local vicinity of the stoichiometric surfaces. This assumption allows to reduce instantaneous conservation equations for reactive scalars to the system of ordinary differential equations (flamelet equations). An advantage of this concept is that it essentially decouples complex chemistry calculations from the turbulent flow description.

In subsonic case one can imagine all the characteristics of combustion as a function of two independent random variables - passive admixture fraction z and scalar dissipation rate N. Consequently for mean value calculation it's necessary to define joint PDF of different z and

N values realization. For supersonic diffusion combustion description one must take into account the third random variable - velocity modulus U [23]. The form of pdf(z) dependence is defined by the character of components mixing in the considered point of flow and may be defined differently.

There are two main approaches which are dominant in high-speed combustion modeling now. In the first approach, PDF form is assumed based on intuition of modeliers (see, for example, [10-12]). It's possible to choose a function depending on several parameters and on z so that it takes required form under the proper parameters choice. Such a PDF is called *presumed*. PDF form is presumed so that its form is uniquely defined by the mean value of z and mean square of its fluctuations (variance). (e.g., [24]. The second way is much more elaborate and it is based on the solution of evolution equation for PDF [25]. This approach was proposed by [26]. for incompressible flames. Recently, it was modified for modeling of compressible flames in studies of [27-30]). But its realization in CFD is extremely expensive in computations due to large multidimensionality of PDF evolution equation [31].

Joint PDF of z and N may be found from the conditions of statistical independence of z and N, and for N log-normal distribution is used. Here big difficulties arise associated with large PDF dimensionality. For this reason though these methods may be used in case of simple chemical kinetics scheme, it couldn't be easily generalized on more complex schemes. However these difficulties may be overcome with the use of Monte-Karlo method [6, 25]. The most recent works include flamelet-structures dynamics in time [32], use the theory of fast decay of uniform turbulence and Fokker-Plank equation [33].

The principal aim of current work is development and realization of a computationally efficient method for numerical simulation of turbulent flows with combustion that occur in perspective aircraft combustors. An essential problem in simulation of turbulent combustion is correct description of chemical processes in the presence of turbulent pulsations. In real combustors, different combustion regimes may occur. Two limiting cases are the premixed combustion and the non-premixed diffusive combustion. In the first limit case, it is possible to neglect the contribution of turbulent fluctuations into average rates of reactions ("laminar approximation"). In the limit of diffusive combustion, the turbulence-combustion interaction (TCI) may be taken into account using the method based on a probability density function (PDF) together with some variant of flamelet model.

An original combined method has been developed. It has advantage to treat different combustion regimes without alteration of numerical algorithm. These include limits of premixed and non-premixed diffusive combustion. Both "laminar approximation" and PDF method are applied only to calculation of source terms in equations for the components of reacting gas. In principle, PDF approach makes it possible to define immediately (directly from precalculated library) temperature and gas components fractions and thus to reduce the amount of equations to be solved – we will call it simple PDF-flamelet approach. But in this case it will describe only purely diffusive combustion limit. In developed combined method PDF approach together with some variant of flamelet model is used only for modeling source terms in equations for components of reacting gas, if the limit of diffusion combustion is locally realized. The method takes into account non-equilibrium combustion effects and turbulence intermittency effects. If the limit of premixed combustion arises, then the source terms are calculated using parameters of mean flow and usual Arrenius-like formulas. The final values of source terms are calculated as a linear combination of these two limiting cases.

This combined method was implemented into a code for simulation 3D flows on the basis of unsteady RANS equations for multi-component compressible gas with finite-rate chemical reactions. The equation system is closed by $(q-\omega)$-turbulence model and by a kinetic scheme of hydrogen-air combustion. Detailed description of the numerical method can be found in [34]. Additional differential

equations include two for mixture fraction mean value $\bar{z}$ and variance $\sigma = \overline{z'^2}$ and one for intermittency factor. Numerical method has the 2nd approximation order in all variables.

Original numerical technology for fast and correct computations of non-stationary viscid gas flows [35] has been incorporated into the code. It includes fractional time stepping (In the case of rational programming, this procedure diminishes the total time of computation (because small quantity of time steps is performed in large cells)) and an approximate "wall law" boundary condition (it allows to place small amount of cells inside the boundary layer). It has been verified by comparison with the calculations based on standard no-accelerated technology. This methodology gives the possibility to perform 3D calculations of practical combustor geometry.

Some results of program validation are presented, including simulation of Evans-Schexnayder-Beach experiment [36] (combustion in axisymmetric jet), Burrows-Kurkov experiment [37] (combustion in 2D plane wall jet) and Ben-Yakar experiment [38] (combustion in transverse jet). The results obtained with taking TCI into account are compared with results obtained with neglecting TCI, with simple PDF-flamelet approach and with experimental, theoretical and computational results presented in available literature. The influence of turbulent parameters and of kinetic scheme is studied. Results of the new method adjustment and testing are demonstrated.

2 Validation of 3D code without TCI

First of all the code S3pp was created and validated for simulation 3D flows on the basis of unsteady RANS equations for multi-component compressible gas with finite-rate chemical reactions. The results of test tasks modelling obtained with the help of the S3pp code were compared with the results obtained with other available programs including its 2D prototype, with experimental and theoretical data available in literature. The most interesting results include simulation of experiment with combustion of a transverse jet of hydrogen in supersonic crossflow of air is also regarded (fig. 1 a)). It is widely-used scheme for combustion realization in high-speed combustors. This test demonstrates the ability of new code to simulate essentially 3D flows with turbulent combustion. In fig. 1 b) one can see OH mass fraction with superimposed isolines of heat release rate θ, due to similarity of the contours we could conclude that *OH* mass fraction is a good parameter, indicating heat release during combustion process. In fig. 2 the obtained Mach number and fuel mass fraction (H_2) fields are compared with experiment by Ben-Yakar (2006) [38].

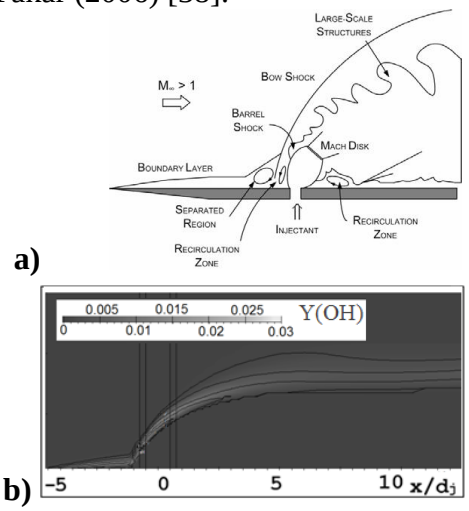


Fig. 1 a) Schematic of an underexpanded transverse injection into a supersonic crossflow [38];

b) OH mass fraction with superimposed isolines of heat release rate at the plane of symmetry

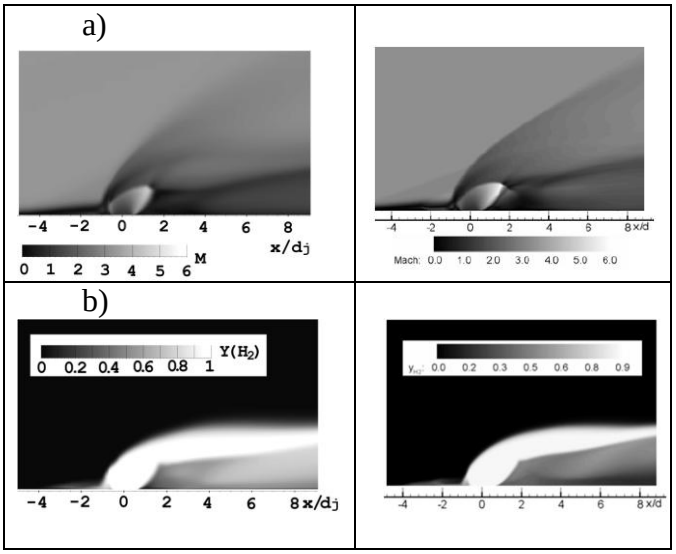


Fig. 2 Mach number (a) and hydrogen mass fraction (b) fields in the symmetry plane of transverse jet, obtained in RANS calculation by the authors (left) and in averaged DES calculations [39] (right)

3 Realization of "simple flamelet" approach

As the final developed model includes usage of flamelet libraries, it was decided to realize first "simple flamelet" approach. We'll remind that in this case the gas components fractions (and possibly temperature) during the calculation are extracted directly from precalculated library and it permits to reduce the amount of equations to be solved. Reactive species mass fractions Y_i or temperature T are found from the solution of the following system of the ordinary differential equations:

$$\begin{gathered}\frac{\partial Y_i}{\partial t} - \overline{N}_t^s \frac{d^2 Y_i}{dz^2} - R_i = 0, \;\; i = 1, 2, \ldots, N_{comp} \\ \frac{\partial\, \rho H}{\partial t} - Sc \cdot \rho \cdot \overline{N}_t^s \frac{d^2 H}{dz^2} = 0\end{gathered} \qquad (1)$$

where t is time, ρ is density, z - mixture fraction, $H = \sum_{i=1}^{N_{sp}} h_i + \frac{\left(\vec{U} \cdot \vec{U}\right)}{2}$ - total enthalpy of the mixture, h_i - specific enthalpy of mixture component i), R_i - chemical production term of Y_i; Sc - Schmidt number. The conditionally averaged value of scalar dissipation at the stoichiometric surface is approximated as: $\overline{N}_t^s = \frac{\overline{N}\big|_{\bar{z}=z_{st}}}{\gamma\big|_{\bar{z}=z_{st}}}$, where $\overline{N}\big|_{\bar{z}=z_{st}}$ and $\gamma\big|_{\bar{z}=z_{st}}$ are the mean value of the scalar dissipation N and intermittency factor γ calculated under the condition that mean value of mixture fraction $\bar{z} = z_{st}$. While creating the flamelet library we find the stationary solution $(t \to \infty)$ of the system (1) with the time-marching method.

The verification of this part of work was based on the reports [40-41] (it will be linked as "Report" in pictures further) and the first aim on this stage was to repeat the methodology as much as possible and to obtain results possibly closer to the ones obtained by the authors of [40-41]. The next aim was to explore the influence of different parameters in the calculation and choose the most appropriate for the class of tasks under consideration.

The flow parameters are obtained with the use of joint PDF of mixture fraction z and scalar dissipation at the stoichiometric surface N^s by the relation:

$$\begin{aligned}\bar{f}_i = \gamma \int_0^1 f_i^{\,flamelet}\left(z, \bar{p}, \overline{N}_t^s\right) \mathrm{pdf}(z)\,dz + \\ + (1-\gamma)\left((1-\bar{z})\cdot (f_i)_O + \bar{z}\,(f_i)_F\right),\end{aligned} \qquad (2)$$

where f_i is any flow parameter (mass fraction Y_i or temperature T), $f_i^{\,flamelet}$ correspond to the values obtained from solution of eq. (1), $(f_i)_O$ stands for oxidizer and $(f_i)_F$ for fuel parameters, γ is the intermittency factor, δ is Dirac function, P_t is the mixture fraction probability density function in a turbulent mixing layer. In current work so far we neglect scalar dissipation fluctuations in averaging procedure as in [40-41]. The scalar dissipation rate N is modeled in turbulent flow field using the semi-empirical relation $N = C_N \frac{\overline{z'^2}}{k} \cdot \varepsilon$, where k and ε are mean turbulent kinetic energy and its dissipation rate respectively, C_N is the model constant and usually it is selected as $C_N = 2$.

Different PDF functions were regarded. In engineering applications the β-function is the most popular presumed PDF function used to model the probability density function for the mixture fraction. It is also taken as the basic in this work. In this case $\mathrm{pdf}(z)$ is approximated by the formula $\mathrm{pdf}(z) = \frac{z^\beta (1-z)^\gamma}{\int_0^1 z^\beta (1-z)^\gamma\, dz}$.

We will call it *pdf1*. Coefficients β and γ define the maximum of $\mathrm{pdf}(z)$ and they may be defined by the conditions:

$$\begin{cases}\int_0^1 z \cdot \mathrm{pdf}(z)\,dz = \bar{z} \\ \int_0^1 (z-\bar{z})^2 \cdot \mathrm{pdf}(z)\,dz = \overline{z'^2}\end{cases}.$$

In order to reproduce the methodology from [40] the PDF used in that work was also regarded - it has the Gaussian form in the non-intermittent $\gamma = 1$ part of the mixing layer (deeply inside the mixing layer):

$pdf(z)=\frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{(z-\bar{z})^2}{2\sigma^2}\right)$ and the form of Airy function in the intermittent $\gamma<1$ regions: $pdf(z)=\frac{1.404}{z_t}Ai\left(1.788\frac{z}{z_t}-2.338\right)$ (we'll link it further as pdf_2), where $z_t=\frac{\bar{z}}{\gamma}$ is the mixture fraction value conditionally averaged over the moments when the turbulent mixing layer is observed in a given point.

What is kept in the final library used during calculations is not the values $f_i^{flamelet}$ obtained from solution of eq. (1), but the values $\tilde{f}_i$, obtained by averaging $f_i^{flamelet}$ with PDF through (1). So the library is tabulated with the values of $\overline{N}_t^s$, $\bar{p}$, $\bar{z}$, $\overline{z'^2}$ as parameters.

We solve a differential equation for γ from [42]:

$$\frac{\partial\gamma}{\partial t}+\frac{\partial(\gamma u_i)}{\partial x_k}+\frac{\partial}{\partial x_k}\left[(1-\gamma)\frac{\nu_t}{\sigma_g}\frac{\partial\gamma}{\partial x_k}\right]=S_g,$$

where $\sigma_g=1$, ν_t is kinematic coefficient of turbulent viscosity. In addition the approximate relation used in [40] was regarded:

$$\gamma=\begin{cases}\dfrac{1.31}{1+(\sigma/\bar{z})^2}, & \sigma/\bar{z}>0.555\\ 1, & \sigma/\bar{z}\le 0.555\end{cases}.$$

3.1 Test 1: Evans-Schexnayder-Beach experiment modeling

In fig. 3 one can see the scheme of Evans-Schexnayder-Beach experiment [36]. In this experiment hydrogen combustion in a round supersonic jet is investigated. Hydrogen was injected through supersonic axisymmetric nozzle with Mach number *M=2* into cocurrent flow of heated air containing water vapor with Mach number *M=1.9*. Composition measurements were done at the cross section $x/d=15.5$.

Parameters of hydrogen jet: Y_{H_2}=1, M=2, T=251K, p=105 Pa. Parameters of air flow: Y_{H_2}=0, Y_{O_2}=0.241, Y_{H_2O}=0.281, Y_{N_2}= 0.478, M=1.9, T= 1495K, p= 105 Pa, where Y_i is mass fraction of *i* mixture component.

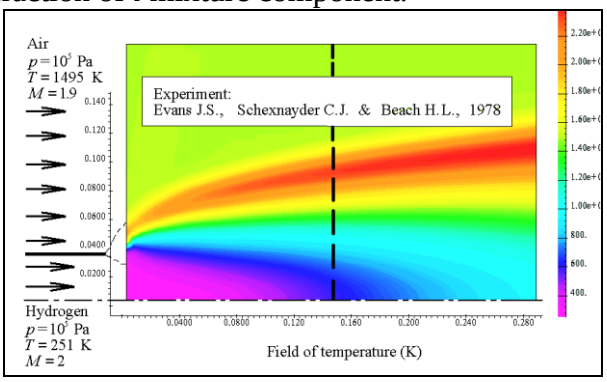


Fig. 3 The scheme of Beach et al. experiment

In fig. 4 author's first results of Beach et al. experiment modeling are presented. Here one can compare results, obtained with the use of: quasi-laminar and simple PDF-flamelet model; equilibrium and non-equilibrium flamelet approximation; different shapes of presumed PDF function - 1) beta-function (pdf_1) – "Flamelet 1" in fig. 4 a) and 2) Gaussian form together with Airy function (pdf_2) – "Flamelet 2" in fig. 4; different intermittency factor modeling - 1) with the use of approximate relation [43] – "Flamelet 1" and 2) by solving additional differential equation for intermittency factor – "Flamelet 2".

For this task we managed to obtain results that are close to presented in [40-41]. Thus the first main goal was reached. The use of flamelet approach allowed to approach the experimental results. Besides it occurred that the form of used PDF has essential influence on obtained results.

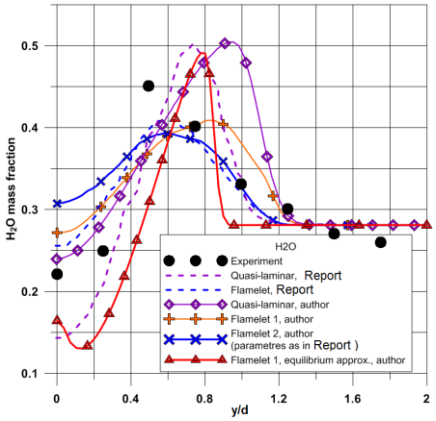


Fig. 4 Comparison of flamelet and quasi-laminar predictions together with experimental data in experiment Evans & others. Transversal H_2O mass fraction distributions in the section x/d=15.5

The next series of calculations were held with improved version of flamelet library and its

integration precalculation (clustering to z_{st} in z variable, dependence of definition domain and step in library in σ variable on z variable, larger amount of values in the library in scalar dissipation variable N). In fig. 5 one can see the influence of empirical coefficients (Sc_T^z, Pr_T^Ψ, C_N and C_Ψ) used in additional differential transport equations for the mixture fraction mean value $\bar{z}$ and variance $\sigma = \overline{z'^2}$. It should be mentioned that the influence is great. The best results (thick line with round markers) were obtained with Pr_T^t=1, Sc_T^z=1, Pr_T^Ψ=1, C_Ψ=2, C_N=0.1.

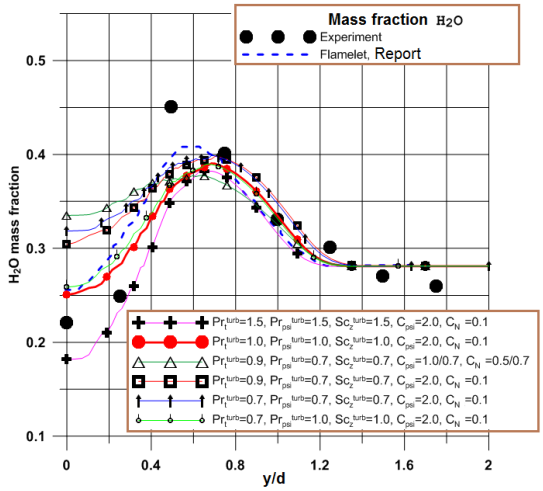


Fig. 5 Parametric flamelet calculations in Evans & others experiment. Transversal H_2O mass fraction distributions in the section x/d=15.5

3.2 The influence of PDF form and its definition domain

The influence of PDF form with other fixed parameters was also studied (pdf_1 with beta function and pdf_2 with Gaussian and Airy function - as in Flamelet 1 and 2 described above). The results obtained with the use of these two different PDFs were varied essentially as it seemed firstly (red and green lines in fig. 6). But it occured that it's not the form of PDF that gives most difference. Using a PDF one must keep in mind its definition domain (in variables $\bar{z}$ and σ). For the β-function it comes directly from the condition on its coefficients $\beta > 0, \gamma > 0$. For the Gaussian function it might be derived from the condition known from mathematical statistics: $0 \le \bar{z} \pm k\sqrt{\sigma} \le 1$, (where $1 \lesssim k \lesssim 3$). These conditions lead to:

$$\textit{gauss}: \begin{cases} \sqrt{z'^2} \le \dfrac{z}{k} \\ \sqrt{z'^2} \le \dfrac{1-z}{k} \end{cases}, \qquad \textit{beta}: \begin{cases} \sqrt{z'^2} \le \dfrac{z^2(1-z)}{1+z} \\ \sqrt{z'^2} \le \dfrac{z(1-z)^2}{2-z} \end{cases}.$$

In fig. 7 one can see these regions depicted in $(\bar{z}, \sigma)$-plane. Taking $k = 1$ they vary greatly. As we're constrained in number of points in pre-calculated library the steps in σ differ and for Gaussian function we don't have detailed library for low values of σ especially for $\bar{z}$ close to $\bar{z} = 0.5$. But the change of library values is great here. The thing is that we need to fit the domain according to the values of σ in regarded task. We also organized a calculation with pdf_2 but with definition domain as for pdf_1. The results are close to the ones obtained with pdf_1 (line with marked crosses in fig. 6).

It must be mentioned that we might have got wrong level of σ values in our calculations due to semi-empirical eq. for σ. Previously, this equation was verified mostly for round jet configurations and for low Mach numbers. This equation requires additional verification and improvement for complex flow configurations (compressible flows, wall jets, etc.).

Dependence of obtained results on the values of σ is great and thus the model needs thorough parameters adjustment for every particular class of tasks.

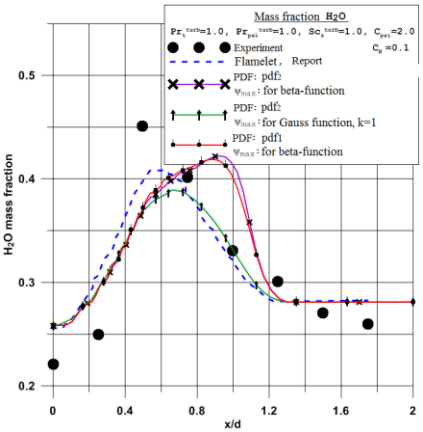


Fig. 6 The influence of definition domain of PDF and its form on the obtained results in Beach et al. task

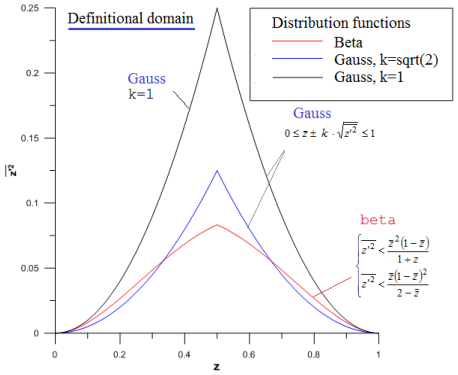
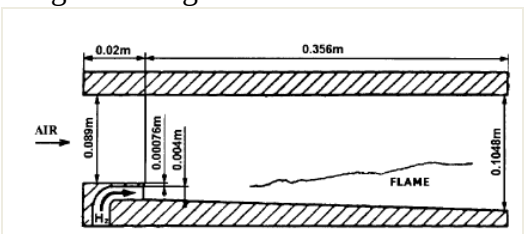


Fig. 7 Definition domains for Gauss and beta functions

Also we see a strong dependence of results on empirical coefficients in equations for parameters of. However we understand that changing these parameters we may spoil the description of classical tasks like boundary layer on a plate or mixing layer. An option here is to use parameters, varying in the field depending on the local flow type, like it is done in SST turbulence model by F.R.Menter [44]. But it's the question for the next studies.

3.3 Test 2: Burrows-Kurkov experiment modelling

In Burrows-Kurkov experiment [37] hydrogen was injected parallel to the vitiated air flow. Composition measurements were done at the exit plane of the test section. The scheme of the experiment and parameters of the fuel jet and air flow are given in fig. 8.



	Hydrogen jet	Air stream
Mach number, M	1.00	2.44
Temperature, T, K	254	1270
Velocity, U, m/s	1216	1764
Pressure, P, MPa	0.1	0.1
Mass fractions:		
C_{H2}	1.000	0
C_{O2}	0	0.258
C_{N2}	0	0.486
C_{H2O}	0	0.256

Fig. 8 The scheme and conditions of Burrows-Kurkov experiment

The results obtained in the mixing task are in good accordance with experiment and calculations [40] (fig. 9 a)). The influence of used hydrogen kinetics scheme on obtained results in test calculations was also studied. The regarded kinetic schemes include Moretti scheme [45] used in our calculations with 6 active components and 8 reactions; scheme [46] developed in CIAM with 8 active components and 20 reactions; and [47] used in ONERA with 6 active components and 7 reactions. The results are given in fig. 9 b). One can see that the influence of kinetic scheme is insignificant.

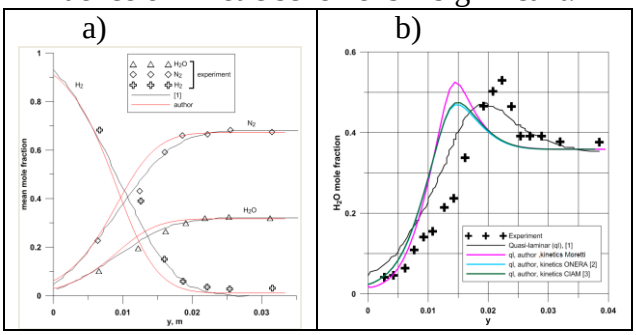


Fig. 9 H_2O mole fraction profiles in exit section x=0.356 m in Burrows-Kurkov experiment. Left: pure mixing case without combustion. Right: chemical kinetics scheme influence

On the contrary, the influence of the initial turbulent parameters at the entry is appreciably visible (fig. 10 a)). The best accordance with the experiment and work [40] was obtained with decreased turbulent parameter ω compared with [40] with keeping the same initial turbulent viscosity as in [40]. In fig. 10 a) the distributions obtained by the author and from [40] with the use of quasi-laminar approach and with simple PDF-flamelet model are compared. Again in this task it was possible to get some improvement by tuning flamelet library and its integration precalculation (clustering to z_{st} in z variable, dependence of definition domain and step in library in σ variable on z variable, larger amount of values in the library in scalar dissipation variable N) – see fig. 10 b).

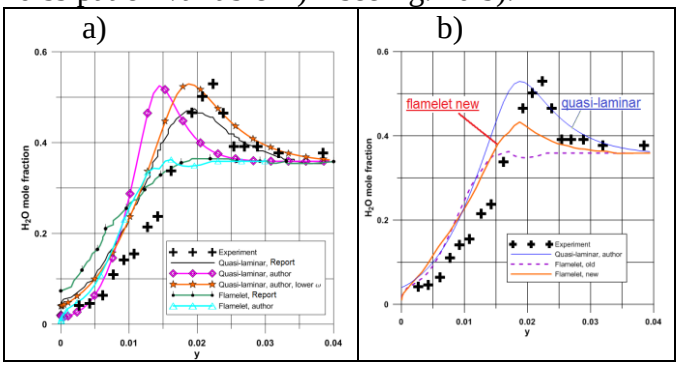


Fig. 10 H_2O mole fraction profiles in exit section x=0.356 m in Burrows-Kurkov experiment. Comparison of flamelet and quasi-laminar predictions with experimental data

4 Universal method development

After that the universal method was implemented into the code. Let us remind that in this case PDF approach together with some variant of flamelet model is used only for modeling source terms in equations for components of reacting gas, if the limit of diffusion combustion is locally realized ($\overline{SY}_i^{pdf}$). If the limit of premixed combustion arises, then the source terms are calculated using parameters of mean flow and usual Arrhenius-like formulas ($\overline{SY}_i^{lam}$). The final values of source terms are calculated as a linear combination of these two limiting cases:

$$\overline{SY_i} = c_{diff\_comb} \cdot \gamma \cdot \overline{SY}_i^{pdf}\left(\bar{z}, \overline{z'^2}, \bar{N}_t^s, \bar{p}\right) + \\ + \left(1 - c_{diff\_comb} \cdot \gamma\right) \cdot \overline{SY}_i^{lam}\left(\bar{T}, \tilde{\bar{Y}}, \bar{p}\right),$$

$$\overline{SY}_i^{pdf}\left(\bar{z}, \overline{z'^2}, \bar{N}_t^s, \bar{p}\right) = \\ = \int_0^1 \int_0^\infty \underbrace{SY_i\left(z, \bar{p}, \bar{N}_t^s\right)}_{\Uparrow \; SY_i\left(T, \tilde{Y}-flamelet\right)} \cdot \underbrace{P(z)P(N_s)}_{\tilde{P}(z,N_s)} \, dN_s dz$$

The coefficient c_{diff_comb} is obtained from the comparison of characteristic times of the proceeding processes: $c_{diff\_comb} = f(t_{chem}, t_\eta, t_l)$, where t_{chem} - characteristic chemical time, t_η - Kolmogorov time scale and t_l - macroturbulent scale. The limiting cases include purely diffusion regime $c_{diff\_comb} = 1$ if $t_{chem} << t_\eta$ and purely premixed combustion if $t_{chem} > t_l$. t_{chem} is estimated as the maximum between inverse value of laminar source term for reaction product ($\sim \frac{1}{\overline{SY}_{product}^{lam}}$) and inverse critical value of scalar dissipation rate (at which flame quenching occurs) $\sim \frac{1}{N^{cr}}$.

4.1 Stationary flamelet approach failure

The first results of Burrows-Kurkov experiment [37] modelling showed that the flame was blown out. The reason for that is too small value of H_2O (which is combustion product here) production source term in the region where ignition occurs (fig. 11), section A-A). It could be immediately seen from the comparison of the laminar H_2O source calculated through the mean flow parameters values with no TCI ($\overline{SY}_{H_2O}^{lam}$) with the source term, calculated with the PDF - $\overline{SY}_{H_2O}^{pdf}$ (fig. 12) (see def. above). One can see that in the section A-A in fig. 11 a) where combustion is initiated the *laminar* source has very large values in the region where combustion appears. On the contrary *pdf* source term has much lower values than laminar and there's no rapid source term growth in the region of ignition. Thus it leads to the flame blown down and hence the method turned out to be inapplicable in its initial formulation.

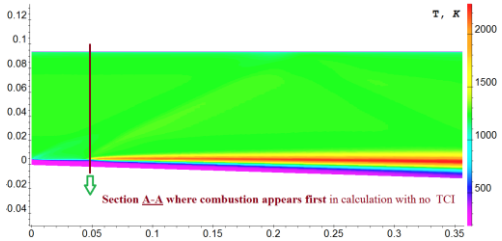


Fig. 11 Temperature field with no TCI in Burrows-Kurkov experiment (section of ignition A-A)

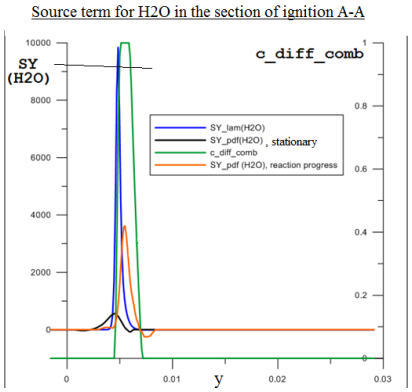


Fig. 12 H_2O laminar, *pdf* stationary and *pdf* transient source terms in the section of ignition A-A

To understand the reason let us remind that we use stationary flamelet formulation. If we have a look at the transient development process during flamelet library calculation for one parameters set we can understand the reason of this small source term. In fig. 13 development of H_2O production rate value in time is depicted for some fixed *z*. What we use in the stationary flamelet library is final source values taken at the end of the process when there're no more changes and thus the source is small. But doing this the enormous values arising at the moment of ignition are not taken into account.

4.2 Transient flamelet approach attempt

So to make the method applicable to flows in which ignition is essential it's necessary to add the transient phenomena into the model. For this purpose the reaction progress variable was introduced.

Different models for accounting transient flamelet phenomena exist. Among them the Transient Laminar Flamelet Model (TLFM) developed by Ferreira [48] and recited in [32]. In this model, usual parameters of the flamelet libraries are supplemented with two new parameters: the reaction progress variable (c) and the turbulent residence time (τ_R). In [32] another transient approach is also developed called the "Flame Age Model (FAM)" – it includes only one additional parameter - flame age (τ_F) - added to usual parameters of the flamelet libraries.

In current work another approach is used that is based on the work [50]. While creating usual stationary flamelet library the stationary solution of equation (1) is used - $f(z, p, N^s, t \to \infty)$. For accounting non-stationary effects the library based on full non-stationary solution of the same equation is used - $f(z, p, N^s, t)$. Linear distribution f based on the hypothesis of "black-white mixing" is used as initial conditions for this solution: $f(z, p, N^s, 0) = z \cdot f^F + (1-z) \cdot f^O$. Instead of the formula (2) the following expression is used:

$$\bar{f}_i = \gamma \int_0^1 \int_0^1 f_i^{flamelet}\left(z, \bar{p}, \bar{N}_t^s, t(c)\right) \mathrm{pdf}(z,c)\,dz\,dc + (1-\gamma)\left((1-\bar{z}) \cdot (f_i)_O + \bar{z}(f_i)_F\right) \quad (3)$$

Here $t(c)$ - time moment when in non-stationary solution of equation (1) the prescribed value of reaction progress variable c is reached. In [50] the values z and c are supposed to be statistically independent: $\mathrm{pdf}(z,c) = \mathrm{pdf}(z) \cdot \mathrm{pdf}(c)$. In [50] beta-function is taken for $\mathrm{pdf}(c)$, based on given values of $\bar{c}$ and $\overline{c'^2}$. Additional partial differential equations are solved in order to find these values. However in [50] no differential equations for averaged in time components mass fractions ($\bar{Y}_i$) are solved. On the contrary in current work such equations are solved; and in addition the water mass fraction Y_{H_2O} characterizes reasonably well the reaction progress (in particular it is monotonely increased from its minimum to maximum value together with reaction proceeding). In current work for simplicity $\mathrm{pdf}(c) = \delta(c - \bar{Y}_{H_2O})$. Thus in (3) time moment $t(c)$ is chosen in such a way that the formula gives $\bar{Y}_{H_2O}$ coinciding with the local solution of partial differential equation for $\bar{Y}_{H_2O}$. On creating the flamelet library the integrals $\int_0^1 \int_0^1 f_i^{flamelet}\left(z, \bar{p}, \bar{N}_t^s, t(c)\right) \mathrm{pdf}(z,c)\,dz\,dc$ are written into computer memory for every set of values $\bar{p}$, $\bar{N}_t^s$, $\bar{Y}_{H_2O}$, $\bar{z}$ and $\sigma = \overline{z'^2}$.

The transient model leads to the increase of H_2O *pdf* source term in the region of ignition (obtained in laminar calculation) so that the flame isn't blown down. In fig. 12 one can compare the values of H_2O laminar, *pdf* stationary and *pdf* transient source terms in the section of ignition A-A.

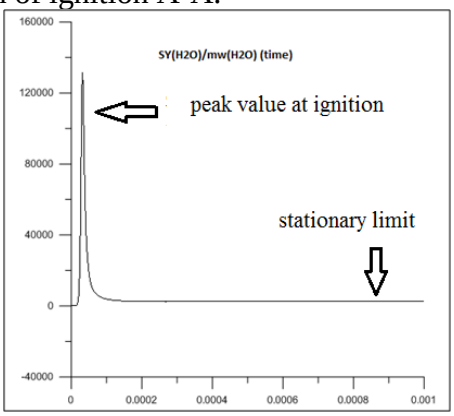


Fig. 13 H2O production rate development in time for some fixed z during flamelet library calculation

The new model application lead to slight changes in the regarded test tasks. Parametric calculations were held and some their results are presented in fig. 14-15. We should remind that the switch from one regime to another is done by comparison of characteristic times. In order to see the influence of implemented *pdf* source the regime was artificially set as "diffusion" ($c_{diff\_comb} \equiv 1$) so that the final source term is

equal to *pdf* source ($\overline{SY_i} \equiv \overline{SY}_i^{pdf}\left(\bar{z}, \overline{z'^2}, \bar{N}_t^s, \bar{p}\right)$). In fig. 14 one can see some most recent results of the new model application to Beach et al. experiment and in fig. 15 to Burrows & Kurkov task. Some influence of model empirical coefficients (Sc_T^z, Pr_T^Ψ and C_Ψ) is presented. But this influence is to be studied deeper and once more we'll remind about possible implementing variable coefficients. Besides one more remaining question is the kind of dependence $c_{diff\_comb} = f(t_{chem}, t_\eta, t_l)$.

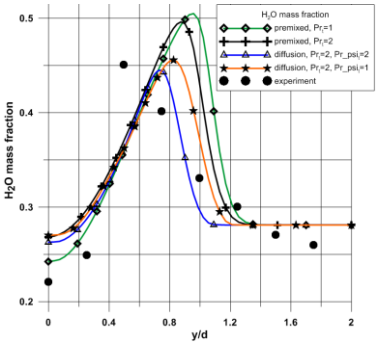


Fig. 14 Recent results of the new model application to Beach et al. experiment

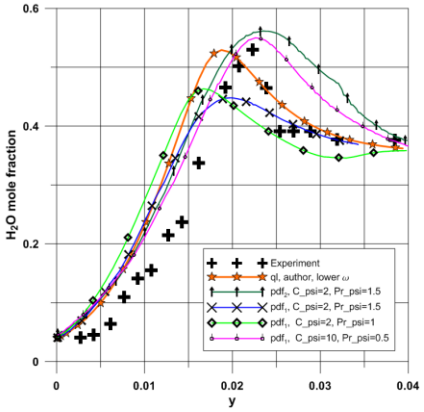


Fig. 15 Recent results of the new model application to Burrows and Kurkov experiment

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