AN ALTERNATIVE APPROACH TO MODELING TURBULENT PREMIXED COMBUSTION

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Abstract
We develop an alternative approach to the turbulent premixed combustion theory that permits to eliminate well known challenge of modelling of predominantly counter-gradient scalar flux and the stress tensor, which must describe, in particular, observed in experiments abnormal increasing in the premixed flame of the velocity fluctuations. We analyse two combustion mechanisms: instantaneous combustion takes place in wrinkled laminar or microturbulent flame. The approach is based on derived in the paper conditionally averaged momentum equations instead of traditionally used for modelling Favere averaged one. We state not only a system of the unclosed equations where requiring modelling unknowns are the conditional turbulent stresses in the unburned and burned gases $(\overline{u_i'u_j'})_u, (\overline{u_i'u_j'})_b$ and the mean chemical source $\overline{\rho W}$, but also develop model equations in the terms of these unknowns. Turbulence in model equations is characterized by conditional kinetic energies $\bar{k}_u, \bar{k}_b$ and dissipation rates $\bar{\varepsilon}_u, \bar{\varepsilon}_b$, the stresses are described $(\overline{u_i'u_j'})_u, (\overline{u_i'u_j'})_b$ in the standard gradient form using conditional turbulent viscosity coefficients $\nu_{t,u}, \nu_{t,b}$. We state the model $\overline{\rho W}$ using the theoretical expression for the turbulent flame speed, which we derive using Kolmogorov type assumptions of statistical equilibrium of the small-scale reaction structures and at the same time nonequilibrium large-scale ones. The scalar flux and stress tensor do not require special modelling as the former is described in terms of the conditional mean velocities $\bar{\vec{u}}_u$ and $\bar{\vec{u}}_b$, which are known from the conditionally averaged momentum equations, and the latter depends additionally on the conditional stresses $(\overline{u_i'u_j'})_u, (\overline{u_i'u_j'})_b$ that are described by the turbulence model. This approach was developed in the context of the agreement with Ansys with the aim to reformulate presented in Fluent and CFX codes TFC combustion model on a more theoretically justified basis, which yields additional potentialities of the model

Introduction

We analyze turbulent premixed combustion. The theoretical basis of turbulent premixed combustion modelling in the context of the current approach is well known system of the Favre averaged unclosed equations of combustion and hydrodynamics, which is as follows:

$$\begin{cases} \partial \overline{\rho}\widetilde{c}/\partial t + \nabla\cdot(\overline{\rho}\widetilde{\vec{u}}\widetilde{c}) + \nabla\cdot\overline{\rho\vec{u}''c''} = \overline{\rho}\widetilde{W}\ (a), \quad c = (\rho_u/\rho - 1)/(\rho_u/\rho_b - 1)\ (b), \\ \partial\overline{\rho}\widetilde{\vec{u}}/\partial t + \nabla\cdot(\overline{\rho}\widetilde{\vec{u}}\widetilde{\vec{u}}) + \nabla\cdot\overline{\rho\vec{u}''\vec{u}''} = -\nabla\overline{p}\ (c), \quad \partial\overline{\rho}/\partial t + \nabla\cdot\overline{\rho}\widetilde{\vec{u}} = 0,\ (d), \end{cases} \tag{1}$$

where Favre averaging (weighted by the density ensemble one) mean $\widetilde{a} = \overline{\rho a}/\overline{\rho}$ and instantaneous $a = \widetilde{a} + a''$, notation $\bar{a}$ identifies Reynolds (ensemble) averaging. Eq. $(1\,a)$ is the balance combustion equation where $\overline{\rho\vec{u}''c''}$ and $\overline{\rho}\widetilde{W}$ are the mean scalar flux and

chemical source. Eq. $(1\,b)$ expresses the instantaneous progress variable c in terms of the instantaneous density ρ and the densities ρ_u and ρ_b of unburned and burned gases. Eq. $(1\,c)$ is the momentum equation where $\overline{\rho\vec{u}''\vec{u}''}$ is the mean stress tensor with the components $\overline{\rho u_i'' u_j''}$ in the Cartesian coordinates. Eq. $(1\,d)$ is the mass equations. Eqs. $(1\,a,b)$ and Eqs. $(1\,c,d)$ describe correspondingly the combustion and attendant hydrodynamic sub-problems, which are coupled due to common density $\overline{\rho}$ and velocity $\widetilde{\vec{u}}$. Requiring modelling unknowns are $\overline{\rho\vec{u}''c''}$ and $\overline{\rho}\widetilde{W}$ in the combustion sub-problem, and $\overline{\rho\vec{u}''\vec{u}''}$ in the hydrodynamic one.

Our analysis refers to the case of the BML concept [1] where instantaneous combustion takes place is strongly wrinkled thin sheet travelling in reactants with the speed of the laminar flame S_L. In this case modelling of the transfer terms is a challenging problem as the scalar flux $\overline{\rho\vec{u}''c''}$ is predominantly counter-gradient and cannot be approximated by the standard gradient expression $\overline{\rho\vec{u}''c''} = -D_t\nabla\widetilde{c}$ (D_t is the turbulent diffusion coefficient), as well as the components of the stress tensor $\overline{\rho u_i'' u_j''}$ cannot be expressed accurately in terms of the turbulent viscosity coefficient ν_t. Advanced modelling of the scalar flux and stresses in the context of traditional approach is based on the turbulent type approximations of the unknown terms in the unclosed $\overline{\rho u_i''c''} -$ and $\overline{\rho u_i'' u_j''} -$ equations [2]. The fundamental limitation of such method is connected with the fact that the scalar flux and stresses are controlled not only by turbulence, but also by gasdynamics (different pressure-driven acceleration of relatively heavy reactants and light products), while turbulent type approximations mean the scalar flux and stresses are treated as pure turbulent parameters. It shows in frequently used terminology such as “countergradient turbulent diffusion of the progress variable” and “turbulent generation” in the premixed flame ([2], p. 558), while the nature of the countergradient scalar flux and strong increasing of the velocity fluctuations in the flame has predominantly gas dynamic nature. Using for modelling of the scalar flux in the impingent flame the turbulent type approximations in the unclosed $\overline{\rho u_i''c''} -$ equation results in [2] that simulations for the cases of a flame close to the wall with slightly increasing pressure across the flame and a free-standing with strong decreasing pressure give quite similar countergradient scalar fluxes, Fig. 5 and 6 in [2]. It means that turbulent type approximations do not describe properly the gasdynamic effect, which negligible in the close and strong in the free-standing flames. In the papers [3-5] we present the scalar flux as a sum of contributions of the gradient turbulent diffusion and the countergradient gasdynamic effect. Application of this model to the impingent flame results that in the closely set flame the scalar flux is gradient, while in the free-standing one the gasdynamic effect prevails in the most part of the flame and the scalar flux is counter-gradient except the vicinity of the front edge of the flame, Figs. 3 in [5], p. 85. The statement of this work is that developed here alternative approach makes unnecessary any special theories or models (including our “turbulent-gasdynamic” one [3]) for prediction of the scalar flux and stress tensor as in the context of the conditionally averaged equations they do not require modelling. The reason is that in the case of thin instantaneous flame the scalar flux and components of the stress tensor are described by the known expressions

$$\overline{\rho\vec{u}''c''} = \overline{\rho}\widetilde{c}(1-\widetilde{c})(\vec{\overline{u}}_b - \vec{\overline{u}}_u), \tag{3}$$

$$\overline{\rho u_i'' u_j''} = \overline{\rho}(1-\widetilde{c})(\overline{u_i'u_j'})_u + \overline{\rho}\widetilde{c}(\overline{u_i'u_j'})_b + \overline{\rho}\widetilde{c}(\overline{u}_{i,b} - \overline{u}_{i,u})(\overline{u}_{j,b} - \overline{u}_{j,u}), \tag{4}$$

where $\vec{\overline{u}}_u, \vec{\overline{u}}_b$ and $(\overline{u_i'u_j'})_u, (\overline{u_i'u_j'})_b$ are conditional averaged velocities and Reynolds stresses in the unburned and burns gases. We state below the unclosed conditionally averaged

equations of mass and momentum where requiring modelling are only the conditional mean stresses $(\overline{u_i'u_j'})_u, (\overline{u_i'u_j'})_b$ and chemical source $\overline{\rho W} = \overline{\rho}\widetilde{W}$. For application we state model conditionally averaged equations of the "$\kappa - \varepsilon$" turbulence model for approximation of the conditional mean stresses. We also present a Kolmogorov's type analysis, which is based on an assumption of the statistical equilibrium small-scale structures of wrinkled by turbulence instantaneous flame, that yields a theoretical expression for the chemical source $\overline{\rho}\widetilde{W}$. The crucial point that permitted to state proposed alternative approach is deduced below conditionally averaged momentum equations, which in contrast to known from the literature ones [6-8] do not contain requiring modelling surface averaged velocities and pressure terms.

The conditionally averaged mass equations

In the premixed flame takes place instantaneous transformation due to combustion of the conditional mean parameter $\rho_u, \overline{p}_u, \overline{\vec{u}}_u \Rightarrow \rho_b, \overline{p}_u, \overline{\vec{u}}_b$. The intensity of this transformation, the chemical source, is equal to the mass flow rate of the unburned gas through the instantaneous flame is equal to $\overline{\rho}\widetilde{W} = \rho_u S_L \overline{\Sigma}$, where the flame surface density $\overline{\Sigma}$ equal to the mean flame area per unit volume. To avoid invoking the tool of the generalized function (at first glance inevitable due to assumption of zero width of instantaneous flame) we directly split up each of these Favre averaged equations into two conditionally averaged ones using obvious identity

$$\overline{\rho a} = \rho_u \overline{a}_u P_u + \rho_b \overline{a}_b P_b = \rho_u \overline{a}_u (1-\overline{c}) + \rho_b \overline{a}_b \overline{c}\,, \tag{5}$$

To deduce the conditionally averaged continuity equations we transform Eq. (1d) using Eq. (5). We put in it $a = 1$ and $a = \vec{u}$. It results the following equation:

$$\left\{\partial[\rho_u(1-\overline{c})]/\partial t + \nabla\cdot[\rho_u(1-\overline{c})\overline{\vec{u}}_u]\right\}_u + \left\{\partial(\rho_b\overline{c})/\partial t + \nabla\cdot(\rho_b\overline{c}\overline{\vec{u}}_b)\right\}_b = 0\,, \tag{6}$$

where the expressions in the braces $\{\}_u$ and $\{\}_b$ refer to reactants and products. We can easy to check that the expression in the second braces are equal to $\{\}_b = \overline{\rho}\widetilde{W}$. (For this we must eliminate $\widetilde{\vec{u}}$ from Eq. (1a) using Eq. (3) and the obvious expressions:

$$\overline{\rho}\widetilde{c} = \overline{\rho c} = \rho_b \overline{c}\ (a), \quad \widetilde{\vec{u}} = \overline{\vec{u}}_u(1-\widetilde{c}) + \overline{\vec{u}}_b\widetilde{c}\ \ (b). \tag{7}$$

Then using Eq. (6) gives $\{\}_u = -\overline{\rho}\widetilde{W}$, i.e. the conditional mass equations are as follows:

$$\partial[\rho_u(1-\overline{c})]/\partial t + \nabla\cdot[\rho_u(1-\overline{c})\overline{\vec{u}}_u] = -\overline{\rho}\widetilde{W}\ \ (a),\ \ \partial(\rho_b\overline{c})/\partial t + \nabla\cdot(\rho_b\overline{c}\overline{\vec{u}}_b) = \overline{\rho}\widetilde{W}\ \ (b). \tag{8}$$

The conditionally averaged mass equations

For deriving the conditional averaged momentum equations we transform similar Eq. (1c) and present it as a sum of two groups of the terms, which contain conditional averaged parameters referring only to reactants or products. For this we insert in Eq. (1c) the expressions yielded by Eq. (5) with $a = \vec{u}$ and $a = \vec{u}\vec{u}$. It results the following equation

$$\begin{aligned}&\left\{\partial[\rho_u(1-\overline{c})\overline{\vec{u}}_u]/\partial t + \nabla\cdot[\rho_u(1-\overline{c})\overline{\vec{u}}_u\overline{\vec{u}}_u)] + \nabla\cdot[\rho_u(1-\overline{c})(\overline{\vec{u}'\vec{u}'})_u]\right\}_u \\ &+ \left\{\partial(\rho_b\overline{c}\overline{u}_{i,b})/\partial t + \nabla\cdot(\rho_b\overline{c}\overline{\vec{u}}_b\overline{\vec{u}}_b) + \nabla\cdot(\rho_b\overline{c}(\overline{\vec{u}'\vec{u}'})_b)\right\}_b = -\nabla[(1-\overline{c})\overline{p}_u] - \nabla(\overline{cp}_b),\end{aligned} \tag{9}$$

where $(\overline{\vec{u}'\vec{u}'})_u$, $(\overline{\vec{u}'\vec{u}'})_b$ and $\overline{p}_u$, $\overline{p}_b$ are conditionally averaged turbulent stresses and pressures. Splitting of Eq. (9) yields the following conditional momentum equations:

$$\begin{cases} \partial[\rho_u(1-\overline{c})\overline{\vec{u}}_u]/\partial t + \nabla\cdot[\rho_u(1-\overline{c})\overline{\vec{u}}_u\overline{\vec{u}}_u)] + \nabla\cdot[\rho_u(1-\overline{c})(\overline{\vec{u}'\vec{u}'})_u] = -\nabla[(1-\overline{c})\overline{p}_u] + \overline{\vec{F}}_u \ (a), \\ \partial[\rho_b\overline{c}\overline{\vec{u}}_b]/\partial t + \nabla\cdot[\rho_b\overline{c}\overline{\vec{u}}_b\overline{\vec{u}}_b)] + \nabla\cdot[\rho_b\overline{c}(\overline{\vec{u}'\vec{u}'})_b] = -\nabla(\overline{c}\overline{p}_b) + \overline{\vec{F}}_b \ (b), \end{cases} \quad (10)$$

where $\overline{\vec{F}}_u$ and $\overline{\vec{F}}_b$ are equal opposite forces due to impulse exchange between reactants and products caused by combustion.. These volume forces do not appear in the Eq. (1c) as $\overline{\vec{F}}_u + \overline{\vec{F}}_b = 0$. It is obvious that Eq. (1c) is a sum of Eqs. (10a) and (10b).
To find $\vec{F}_u$ .and $\vec{F}_b$ we attract the equation of the momentum conservation on the boundary that divides the unburned gas with $\vec{u}_u, \overline{p}_u$ and $\vec{u}_b, \overline{p}_b$, which is as follows:

$$\overline{\rho}\widetilde{W}(\overline{\vec{u}}_b - \overline{\vec{u}}_u) = -(\nabla\overline{\mathrm{p}})_c \quad [-\nabla[(1-\overline{c})\overline{p}_{cu}] - \nabla(\overline{c}\cdot\overline{p}_{cb})] \quad (11)$$

where $\nabla\overline{\mathrm{p}}_c$ is the pressure gradient generated by combustion, which yields transformation $\vec{u}_u \Rightarrow \vec{u}_b$. We represent RHS of Eq. (1c) as follows:

$$-\nabla\overline{p} = -\nabla\overline{p} + \{\nabla\overline{p}_c + (\overline{\vec{u}}_b - \overline{\vec{u}}_u)\overline{\rho}\widetilde{W}\} = -\nabla\overline{p}^{\circ} + \overline{\vec{u}}_b\overline{\rho}\widetilde{W} - \overline{\vec{u}}_u\overline{\rho}W \quad (12)$$

where the expressions in the braces is equal zero in accordance with Eq. (11) and $\overline{p}^{\circ} = \overline{p} - \overline{p}_c$. and splitting Eq. (12) we have as follows:

$$\begin{cases} = -\nabla[(1-\overline{c})\overline{p}_u] + \nabla[(1-\overline{c})\overline{p}_{c,u}] - \overline{\vec{u}}_u\overline{\rho}\widetilde{W} = -\nabla[(1-\overline{c})\overline{p}_u^{\circ}] - \overline{\vec{u}}_u\overline{\rho}\widetilde{W} \ (a), \\ = -\nabla[(1-\overline{c})\overline{p}_b] + \nabla[(1-\overline{c})\overline{p}_{c,b}] - \overline{\vec{u}}_b\overline{\rho}\widetilde{W} = -\nabla(\overline{c}\cdot\overline{p}_b^{\circ}) + \overline{\vec{u}}_b\overline{\rho}\widetilde{W} \quad (b) \\ \overline{\vec{F}}_u = -\nabla[(1-\overline{c})\overline{p}_{c,u}] - \overline{\vec{u}}_u\overline{\rho}\widetilde{W} \ (c), \quad \overline{\vec{F}}_b = -\nabla[(1-\overline{c})\overline{p}_{c,b}] - \overline{\vec{u}}_b\overline{\rho}\widetilde{W} \ (d), \end{cases} \quad (13)$$

where $\overline{p}_u^{\circ} = \overline{p}_u - \overline{p}_{c,u}$ and . $\overline{p}_{b^{\circ}} = \overline{p}_b - \overline{p}_{c,b}$. Rqs. (13a) and (13b) present correspondingly the RHSs of Eqs. (10a), and (10b), Eqs. (13c) are expression for $\overline{\vec{F}}_u$ and $\overline{\vec{F}}_b$ in Eqs. (10). So Eqs. (10) and (13) yields directly the following conditional averaged momentum equations:

$$\begin{cases} \partial[\rho_u(1-\overline{c})\overline{\vec{u}}_u]/\partial t + \nabla\cdot[\rho_u(1-\overline{c})\overline{\vec{u}}_u\overline{\vec{u}}_u)] + \nabla\cdot[\rho_u(1-\overline{c})(\overline{\vec{u}'\vec{u}'})_u = -\nabla[(1-\overline{c})\overline{p}_u^{\circ}] - \overline{\vec{u}}_u\overline{\rho}\widetilde{W} \ (a), \\ \partial[\rho_u\overline{c}\overline{\vec{u}}_b]/\partial t + \nabla\cdot[\overline{\rho c}\overline{\vec{u}}_b\overline{\vec{u}}_b)] + \nabla\cdot[\rho_u\overline{c}(\overline{\vec{u}'\vec{u}'})_b] = -\nabla(\overline{c}\cdot\overline{p}_b^{\circ}) + \overline{\vec{u}}_b\overline{\rho}\widetilde{W} \ (b). \end{cases} \quad (14)$$

In Eqs. (14) $\overline{p}_u^{\circ}$ and $\overline{p}_b^{\circ}$ are the conditional mean pressures in the unburned and burned gasses in the case of combustion. We omit the index"$^{\circ}$" below.

The system of the unclosed equation of turbulent premixed combustion

The system of the unclosed equations in terms of the conditionally averaged $\overline{\vec{u}}_u, \overline{p}_u$, $\overline{\vec{u}}_b, \overline{p}_b$. and Reynolds averaged $\overline{c}$ includes two scalar continuity equations Eqs. (8), two vector momentum equations Eqs. (14) (i.e. 6 scalar equations) and one scalar equation Eq. (15):

$$\overline{p}_u - \overline{p}_b = \rho_u S_L \, | \overline{\vec{u}}_u - \overline{\vec{u}}_b \, | \tag{15}$$

Eq. (15) is the condition of the momentum conservation on the boundary that divides gases with conditional mean parameters $\overline{\vec{u}}_u, \overline{p}_u$ and $\overline{\vec{u}}_b, \overline{p}_b$. Known from the literature analogous equation connects the surface averaged velocities $\overline{\vec{u}}_{su}$ and $\overline{\vec{u}}_{sb}$, Eq. (13) in [7], is as follows:

$$\overline{\vec{u}}_{su} \overline{\rho} \widetilde{W} - (\overline{p\vec{n}})_{su} \overline{\Sigma} = \overline{\vec{u}}_{sb} \overline{\rho} \widetilde{W} - (\overline{p\vec{n}})_{sb} \overline{\Sigma}. \tag{16}$$

To gain a better insight into our consideration we first transform known Eq. (16). We present the pressure terms as follows:

$$(\overline{p\vec{n}})_{su} = \overline{p}_{su} \overline{\vec{n}} + \overline{p'_{su} \vec{n}'} \ (a), \quad (\overline{p\vec{n}})_{sb} = \overline{p}_{sb} \overline{\vec{n}} + \overline{p'_{sb} \vec{n}'} \ (b), \tag{17}$$

where the correlations $\overline{p'_{su} \vec{n}'}$ and $\overline{p'_{sb} \vec{n}'}$ are in general case nonzero as the pressures and unit vector $\vec{n}$ are defined at the same adjacent surfaces. But if to ignore these correlations Eq. (16) reduces to the Eq. (18a) and then remembering that $\overline{\rho} \widetilde{W} = \rho_u S_L \overline{\Sigma}$ to Eq. (18b):

$$\overline{\rho} \widetilde{W} \cdot \overline{\vec{u}}_{su} - \overline{p}_{su} \overline{\vec{n}} \overline{\Sigma} = \overline{\rho} \widetilde{W} \cdot \overline{\vec{u}}_{sb} - \overline{p}_{sb} \overline{\vec{n}} \overline{\Sigma} \ (a), \ \ \rho_u S_L \overline{\Sigma} \cdot \overline{\vec{u}}_{su} - \overline{p}_{su} \overline{\vec{n}} \overline{\Sigma} = \rho_u S_L \overline{\Sigma} \cdot \overline{\vec{u}}_{sb} - \overline{p}_{sb} \overline{\vec{n}} \overline{\Sigma} \ (b). \tag{18}$$

It is evident from Eqs. (14) that $\overline{\vec{n}} \sim \overline{\vec{u}}_u - \overline{\vec{u}}_b$ and $\overline{\vec{n}} = (\overline{\vec{u}}_u - \overline{\vec{u}}_b) / | \overline{\vec{u}}_u - \overline{\vec{u}}_b |$. Installing the latter in Eq. (14b) we have the following impulse conservation law :

$$\overline{p}_{su} - \overline{p}_{sb} = \rho_u S_L \, | \overline{\vec{u}}_{su} - \overline{\vec{u}}_{sb} \, |). \tag{19}$$

In our case there is no correlation between $\vec{n}$ and p_u, p_b as the vector $\vec{n}$ is defined on the surface, while the pressures p_u, p_b are defined in the unburned and burned gases. Hence

$$\overline{\rho} \widetilde{W} \cdot \overline{\vec{u}}_u - \overline{p}_u \overline{\vec{n}} \overline{\Sigma} = \overline{\rho} \widetilde{W} \cdot \overline{\vec{u}}_b - \overline{p}_b \overline{\vec{n}} \overline{\Sigma}, \tag{20}$$

which after similar presented above manipulations reduces to Eq. (15).

The unknown terms in the system Eqs. (8), (14) and (15), which require modelling, are the conditional Reynolds stresses $(\overline{u'_i u'_j})_u, (\overline{u'_i u'_j})_u$ and the chemical source $\overline{\rho} \widetilde{W}$. Others 3 scalar ($\overline{c}, \overline{p}_u, \overline{p}_b$ and two vectors ($(\overline{\vec{u}}_u, \overline{\vec{u}}_b)$ unknowns are described by 3 scalar (Eqs. (8) and (15) and 2 vector (Eqs. (14) equations of the system. All others Reynolds and Favre averaged variables of the problem can be expressed in terms of defined by the system variables $\overline{c}, \overline{p}_u, \overline{p}_b, \overline{\vec{u}}_u, \overline{\vec{u}}_b$. But we think that more convenient for practical applications (especially keeping in mind an opportunity of implementation in the commercial code) to state a system that described all conditionally, Reynolds and Favre averaged variables of the problem directly, i.e. avoiding their post-processor simulations.

This system is as follows:

$$\mathrm{A}:\begin{cases}\partial\overline{\rho}\widetilde{c}/\partial t+\nabla\cdot\overline{\rho}\widetilde{\vec{u}}\widetilde{c}=-\nabla\cdot\overline{\rho\vec{u}''c''}+\overline{\rho}\widetilde{W}\ (a),\\ \overline{\rho}=(1-\overline{c})\rho_u+\overline{c}\rho_b=\rho_u/[1+\widetilde{c}(\rho_u/\rho_b-1)]\ (b),\\ \overline{c}=\rho_u\widetilde{c}/[\rho_b+\widetilde{c}[\rho_b+\widetilde{c}(\rho_u-\rho_b)]\ (c),\ \ \overline{\rho\vec{u}''c''}=\overline{\rho}\widetilde{c}(1-\widetilde{c})(\vec{\overline{u}}_b-\vec{\overline{u}}_u)\ (d).\end{cases}$$

(21)

$$\mathrm{B}:\begin{cases}\partial\overline{\rho}/\partial t+\nabla\cdot\overline{\rho}\widetilde{c}\widetilde{\vec{u}}=0\ (e),\quad \widetilde{\vec{u}}=\overline{\vec{u}}_u(1-\widetilde{c})+\overline{\vec{u}}_b\widetilde{c}\ (f),\\ \partial(\overline{\rho}\widetilde{c}\overline{\vec{u}}_b)/\partial t+\nabla\cdot(\overline{\rho}\widetilde{c}\overline{\vec{u}}_b\overline{\vec{u}}_b)=-\nabla\cdot(\overline{\rho}\widetilde{c}(\overline{\vec{u}'\vec{u}'})_b-\nabla(\overline{c}\cdot\overline{p}_b)+\overline{\vec{u}}_b(\overline{\rho}\widetilde{W})\ (g),\\ \partial[\overline{\rho}(1-\widetilde{c})\overline{\vec{u}}_u]/\partial t+\nabla\cdot[\overline{\rho}(1-\widetilde{c})\overline{\vec{u}}_u\overline{\vec{u}}_u=-\nabla\cdot[\overline{\rho}(1-\widetilde{c})(\overline{\vec{u}'\vec{u}'})_u]\\ -\nabla[(1-\overline{c})\overline{p}_u]-\overline{\vec{u}}_u(\overline{\rho}\widetilde{W})\ (h),\qquad \overline{p}_u-\overline{p}_b=\rho_u S_L|\overline{\vec{u}}_u-\overline{\vec{u}}_b|\ \ (i),\\ \partial\overline{\rho}\widetilde{\vec{u}}/\partial t+\nabla\cdot(\overline{\rho}\widetilde{\vec{u}}\widetilde{\vec{u}})+\nabla\cdot\overline{\rho\vec{u}''\vec{u}''}=-\nabla\overline{p}\ \ (j),\\ \overline{\rho u_i''u_j''}=\overline{\rho}(1-\widetilde{c})(\overline{u_i'u_j'})_u+\overline{\rho}\widetilde{c}(\overline{u_i'u_j'})_b+\overline{\rho}\widetilde{c}(\overline{u}_{i,b}-\overline{u}_{i,u})(\overline{u}_{j,b}-\overline{u}_{j,u})\ (k).\end{cases}$$

We split the system into two coupled subsystems A and B , which describe correspondingly the combustion and hydrodynamic sub-problems. Eq. (21a) is the traditional balance combustion equation; Eq. (21b) expresses $\overline{\rho}$ in terms of $\overline{c}$ and $\widetilde{c}$; Eq. (21c) expresses $\overline{c}$ in terms of $\widetilde{c}$; Rq. (21d) express the scalar flux in terms of described by the system conditional mean velocities, i.e. $\overline{\rho\vec{u}''c''}$ does not need modelling. Eq. (21e) is the global continuity equation, Eq. (21f) expresses the Favere averaged velocity in terms of conditional mean ones; Eqs. (21g) and (21h) are correspondingly conditionally averaged momentum equations for the burned and unburned gases, Eq. (21i) express the impulse conservation on the boundary that divides the unburned and burned gases; Eq. (21j) is the global impulse equation, Eq. (21k) describes the components of the stress tensor that appear in Eq. (21j), i.e. the stress tensor, similar to the scalar flux, do not require modeling. The LHSs in Eqs. (21g) and (21h) are modified in comparison with Eqs. (14a) and (14b) using obvious relations $\rho_b\overline{c}=\overline{\rho}\widetilde{c}$ and $\rho_u(1-\overline{c})=\overline{\rho}(1-\widetilde{c})$. In the system Eqs. (21) we keep traditional in the premixed combustion theory Favre averaged combustion equation in terms of $\widetilde{c}$, and the global continuity and momentum equations. The only unknowns in the system that require modelling are conditional averaged turbulent stresses $(\overline{\vec{u}'\vec{u}'})_u,(\overline{\vec{u}'\vec{u}'})_b$ and mean chemical source $\overline{\rho W}=\overline{\rho}\widetilde{W}$, while $\overline{c},\widetilde{c},\overline{\rho},\widetilde{\vec{u}},\overline{u}_u,\overline{u}_b,\overline{p}_u,\overline{p}_b,\overline{\rho\vec{u}''c''},\overline{\rho u_i''u_j''}$ are known as they described by Eqs. (21).

Modelling of the conditional Reynolds stresses

We start from the Favre averaged equations of the standard "$\widetilde{k}-\widetilde{\varepsilon}$" turbulence model:

$$\begin{cases}\left.\begin{aligned}&\partial(\overline{\rho}\widetilde{k})/\partial t+\partial(\overline{\rho}\widetilde{u}_\alpha\widetilde{k})/\partial x_\alpha=-\overline{\rho u_i''u_j''}\partial\widetilde{u}_j/\partial x_i\\ &+\partial\left[\overline{\rho}(\nu_t/\sigma_k)\partial\widetilde{k}/\partial x_i\right]/\partial x_i-\overline{\rho}\widetilde{\varepsilon}\end{aligned}\right]\ (a),\\ \left.\begin{aligned}&\partial(\overline{\rho}\widetilde{\varepsilon})/\partial t+\partial(\overline{\rho}\widetilde{u}_i\widetilde{\varepsilon})/\partial x_i=-C_{\varepsilon1}\overline{\rho u_i''u_j''}(\widetilde{\varepsilon}/\widetilde{k})\partial\overline{u}_j/\partial x_i\\ &-C_{\varepsilon2}\overline{\rho}(\widetilde{\varepsilon}^2/\widetilde{k})+\partial\left[\overline{\rho}(\nu_t/\sigma_\varepsilon)\partial\widetilde{\varepsilon}/\partial x_i\right]\partial x_i\ \ (b),\end{aligned}\right]\end{cases}\quad (b),$$

(22)

where $C_{\varepsilon 1}=1.44,\ C_{\varepsilon 2}=1.92,\ \sigma_k=1.3,\ \sigma_\varepsilon=1.0$. The equations in terms of the conditional mean kinetic energy $\bar{k}_u$ and dissipation rate $\bar{\varepsilon}_u$ (splitting Eqs. (22)) are as follows:

$$\begin{cases} \partial[\bar{\rho}(1-\tilde{c})\bar{k}_u]/\partial t+\partial[\bar{\rho}(1-\tilde{c})\bar{u}_{\alpha,u}\bar{k}_u]/\partial x_\alpha=-\bar{\rho}(1-\tilde{c})(\overline{u_i'u_j'})_u\partial\bar{u}_{i,u}/\partial x_j-\bar{\rho}(1-\tilde{c})\bar{\varepsilon}_u \\ +\partial\left[\bar{\rho}(1-\tilde{c})(\nu_{t,u}/\sigma_k)\partial\bar{k}_u/\partial x_i\right]/\partial x_i-\underline{\underline{(1-\bar{c})(\overline{u_i'\cdot\partial p/\partial x_i})_u}}-\underline{\bar{k}_u\bar{\rho}\tilde{W}}\ \ (a), \\ \partial[\bar{\rho}(1-\tilde{c})\bar{\varepsilon}_u]/\partial t+\partial[\bar{\rho}(1-\tilde{c})\bar{u}_{i,u}\bar{\varepsilon}_u]/\partial x_i=-C_{\varepsilon 1}\bar{\rho}(1-\tilde{c})(\bar{\varepsilon}_u/\bar{k}_u)(\overline{u_i'u_j'})_u\partial\bar{u}_{i,u}/\partial x_j \\ -C_{\varepsilon 2}\bar{\rho}(1-\tilde{c})(\bar{\varepsilon}_u^2/\bar{k}_u)+\partial\left[\bar{\rho}(1-\tilde{c})(\nu_{t,u}/\sigma_k)\partial\bar{k}_u/\partial x_\alpha\right]/\partial x_\alpha-\underline{\underline{(1-\bar{c})(?)_u}}-\underline{\bar{\varepsilon}_u\bar{\rho}\tilde{W}}\ \ (c). \end{cases} \tag{24}$$

Two new physical mechanisms appear in Eqs. (24) in comparison with Eqs. (22). They the single underlined sink terms caused by transformation of reactants into products with the intensity $\bar{\rho}\tilde{W}$, and double underlined terms connected with the pressure field. The later terms describe mainly effect of the instantaneous reaction zone on turbulence of the unburned gas. This effect is not significant in contrast to an effect of similar terms in conditional averaged equations in terms of the turbulent energy $\bar{k}_b$ and dissipation rate $\bar{\varepsilon}_b$ in the burned gas. The point is that transformation of reactants into products in strongly wrinkled instantaneous flame is accompanied by significant turbulization of products, which is difficult for quantitative modeling. To avoid the problem we exclude from analysis the conditional averaged $\bar{k}_b-$ and $\bar{\varepsilon}_b-$equations.

We propose to use for turbulence modelling the system of differential equations that include and the conditional averaged equations in the unburned gas Eqs. (24) with omitted double underlined terms and (instead of conditional averaged $\bar{k}_b-$ and $\bar{\varepsilon}_b-$equations) the Favre averaged Eqs. (22) together with the exact expressions for the components of the stress tensor, Eq. (4).

In this case $\bar{k}_b$ and $\bar{\varepsilon}_b$, which are necessary for modelling of the turbulent stresses $(\overline{u_i'u_j'})_b$, are described by following algebraic expressions:

$$\bar{k}_b=[\tilde{k}-\bar{k}_u(1-\tilde{c})]/\tilde{c}\ \ (a),\quad \bar{\varepsilon}_b=[\tilde{\varepsilon}-\bar{\varepsilon}_u(1-\tilde{c})]/\tilde{c}\ \ (b). \tag{25}$$

The viscosity coefficient, turbulent stresses and strain-rate in reactants, $\nu_{t,u}$, $(\overline{u_i'u_j'})_u$, $S_{ij,u}$, and in products, $\nu_{t,b}$, $(\overline{u_i'u_j'})_b$, $S_{ij,b}$, are described by the following expressions:

$$\begin{aligned} &\nu_{t,u}=C_\mu\bar{k}_u^2/\bar{\varepsilon}_u\ \ (a),\qquad (\overline{u_i'u_j'})_u=-2(\nu_{t,u}/\rho_u)S_{ij,u}+(2/3)\bar{k}_u\delta_{ij}\ \ (b), \\ &S_{ij,u}=(1/2)(\partial\bar{u}_{i,u}/\partial x_j+\partial\bar{u}_{j,u}/\partial x_i)\ \ (c). \\ &\nu_{t,b}=C_\mu\bar{k}_b^2/\bar{\varepsilon}_b\ \ (d),\qquad (\overline{u_i'u_j'})_b=-2(\nu_{t,b}/\rho_u)S_{ij,b}+(2/3)\bar{k}_b\delta_{ij}\ \ (e), \\ &S_{ij,b}=(1/2)(\partial\bar{u}_{i,b}/\partial x_j+\partial\bar{u}_{j,b}/\partial x_i)\ \ (f), \end{aligned} \tag{26}$$

where $C_\mu=0.09$ is an empirical coefficient.

Obviously, this compromise approach, which is aimed at modelling of turbulence in the unburned and burned gases, needs validation: it is not clear in advance how accurately the

Favre averaged Eqs. (22), which is widely used in simulations of nonisothermic turbulent flows, describe actual global turbulization in the premixed flame.

Modelling of the chemical source

A problem of theoretically justified modeling of the mean chemical source $\overline{\rho W} = \overline{\rho}\widetilde{W}$ is called the challenge of turbulent premixed combustion. The point is that actual instantaneous combustion takes place in very small-scale zones that cannot be resolved by the model moment combustion equations, so we cannot express the mean chemical source using directly the equations of chemical kinetics. Conceptually similar situation takes place in turbulence where the dissipation of the turbulent kinetic energy takes place small eddies with the sizes of the Kolmogorov micro-scale $\eta = L\,\mathrm{Re}_t^{-3/4}$. So the mean dissipation rate ε cannot be expresses in terms of the molecular viscosity coefficient ν. Kolmogorov resolve this fundamental difficulty assuming the statistical equilibrium of small-scale eddies that permits his to express the dissipation rate in terms of the large-scale turbulent parameters $\varepsilon \approx u'^3 / L$. We resolved in the context of the Kolomorov ideas similar difficulty in modelling the chemical source for more complicated than analyse here case when instantaneous flame is not laminar, but miscroturbulent one. Below we present analogous analysis for the case of the laminar instantaneous flame with zero width. This mathematical model corresponds to the limiting case when in the known expressions for the speed and width of the laminar flame

$$S_L \approx (\chi / \tau_{ch})^{1/2}\ (a), \quad \delta_L \approx (\chi \cdot \tau_{ch})^{1/2}\ (b), \tag{27}$$

the molecular transfer coefficient χ and chemical time τ_{ch} tend to zero, $\chi \to 0$, $\tau_{ch} \to 0$, but their ratio tends to constant $(\chi / \tau_{ch}) \to const$. In terms of the turbulent Reynolds $\mathrm{Re}_t = u'L/\nu$ (the kinematical viscosity coefficient $\nu \approx \chi$) and the Damköhler $Da = \tau_t / \tau_{ch}$ ($\tau_t = L/u'$ is the turbulent time) these conditions are as follows:

$$\lim_{Da\to\infty,\mathrm{Re}_t\to\infty}(Da/\mathrm{Re}_t) = const\ (a), \quad \lim_{Da\to\infty,\mathrm{Re}_t\to\infty}(\delta_L/\eta) = 0\ (b), \tag{28}$$

In this case the progress variable is bimodal: $p(c) = \alpha\delta(c) + \beta p(1-c)$, where $\alpha = (1-\bar{c})$ and $\beta = \bar{c}$ are the probabilities of the unburned and burned gases $p(c) = \alpha\delta(c) + \beta p(1-c)$.

The speed and width of the turbulent flame in the case of the bimodal PDF

We assume that the one-dimensional flame travels along the $x-$axis and the flamelet surface is described by the random function $x = h(y,z,t)$ with the spectrum $F(k)$. In the initial moment $t = 0$ the flamelet is the surface with $x = 0$. Our theoretical estimation of the mean area $(\overline{A}/A_0)$ refers to the case of strongly wrinkled surface when $(\overline{A}/A_0) >> 1$, i.e. the mean area of the flamelet is many times larger than the area of the plane flamelet. Our estimation is as follows:

$$(\overline{A}/A_0) \underset{1}{=} \overline{(1+|\nabla h|^2)^{1/2}} \underset{2}{\approx} \overline{|\nabla h|} \underset{3}{\approx} \left(\overline{|\nabla h|^2}\right)^{1/2} \underset{4}{=} \left(\int_0^\infty k^2 F(k)dk\right)^{1/2} \tag{29}$$

The equality 1 is an exact expression for the area of the random surface described by the equation $x = h(y,z,t)$; the transition 2 is valid as $|\nabla h|^2 >> 1$ due to assumption

$(\overline{A}/A_0) >> 1$; the transition 3 is estimation (averaging of the absolute magnitude of a random function with zero mathematical expectation is approximately equal to the square root of its dispersion; the equality 4 is exact expression of this root in terms of the spectrum of the random surface. Hence the final estimation for the area of the flame surface is as follows:

$$(\overline{A}/A_0) \approx (\int_0^\infty k^2 F(k)dk)^{1/2}. \qquad (30)$$

Eq. (5) shows that the small-scale wrinkles with large values of the wave number k give the main contribution in the mean area of the flame surface gives (quite similar to well known result in the turbulence theory where the main contribution in the mean dissipation rate gives small-scale vortexes $\bar{\varepsilon} = 2\nu\int_0^\infty k^2 E(k)dk$, $E(k)$ is the spectrum of turbulence). At the same time the main contribution in the flame width $\delta_t \sim (\sigma_t^2)^{1/2} = \sigma_t$ give the large scale wrinkled as the dispersion of the flame surface σ_t^2 is described by Eq. (31 a):

$$\sigma_t^2(t) = \overline{(x - \bar{x}(t))^2} = \int_0^\infty F(k,t)dk \ (a), \quad \sigma_t^2(t) = 2D_t t \ (D_t \approx u'L) \ (b). \qquad (31)$$

In the case the passive boundary between gases with $c = 0$ and $c = 1$ (there is no combustion) the dispersion of the instantaneous surface is controlled by the turbulent diffusion coefficient D_t, Eq. (31 b). At the same time the mean area of the passive surface increases exponentially [9]. The physical reason of such fast increasing of the area is generation of the small-scale wrinkles of the material surface in the field of developed turbulence. In the case of combustion this exponential increasing of the flame area $(\overline{A}/A_0)$ is suppresses by movement of the flame. The reason is that the movement even with the relatively low speed $S_L << u'$ smoothes controlling the area small-scale wrinkles, which are caused by small-scale eddies with relatively small characteristic velocity fluctuations. In fact there are two processes: turbulence generates and combustion consumes the small-scale wrinkles, which result some statistically, equilibrium small-scale structure of the flamelet surface. We estimate the characteristic time t_1 when this equilibrium is reached, invoking the value of the velocity fluctuation u_e' of the small-scale eddy that depends on its size δ_e. For the "5/3" turbulent spectrum, Eq. (32 a), dependence of u_e' on δ_e is describe by Eq. (32 b):

$$E(k) = C\bar{\varepsilon}^{2/3}k^{-5/3} \ (a), \quad u_e'^2 \approx \int_{1/\delta_e}^\infty E(k)dk \approx \bar{\varepsilon}^{2/3}\delta_e^{2/3} \ (b), \quad t_1 \approx (S_L/u')^2\tau_t \ (c). \qquad (32)$$

The order of the magnitude of t_1 is equal to the time that is necessary for the flamelet to cross such eddy, which has the velocity fluctuation equal to the speed of the flamelet, $u_e' \approx S_L$. The following estimation is presented by Eq. (32 c), where $\tau_t = L/u'$ is the turbulent time. At the same the relatively slow movement of the instantaneous does not influence on the large scale wrinkles during some period of time $t < t_2$ and the dispersion of the flamelet surface is described by Eq. (31 b) similar to the turbulent mixture layer. For estimation of t_2 we assume that significant influence of S_L on the dispersion σ_t^2 takes place when the linear displacement of the flame is caused by the self-moving $S_L t_2$ and the transfer due to turbulent diffusion $\sigma_t(t_2)$ have the same order of the magnitude, Eq. (33 a), and it gives the estimation of the time presented by Eq.(33 b):

$$S_L t_2 \approx [\sigma_t^2(t_2)]^{1/2} \approx (u'Lt_2)^{1/2} \ (a) \qquad t_2 \approx (u'/S_L)^2 \tau_t \ (b).\,, \tag{33}$$

Finally, Eqs. (32c) and (33b) show the time interval, Eq. (34a), when the small-scale structures of the reaction zone are already statistically equilibrium, while the large-scale ones are not yet. The latter results increasing width of the flame, Eq. (34b). An assumption that the equilibrium structures are controlled by large-scale turbulence and the speed S_L, which is in fact the only physicochemical characteristic of the mixture, results that the flame speed U_t is constant. Eq. (34c) gives an expression for this constant speed that we derive below ($A_1 \sim 1$ is an empirical coefficient). At the same time the flame width increases similar to the turbulent mixing layer, Eq. (34c).

$$\begin{aligned} &(S_L/u')^2 \tau_t < t < (u'/S_L)^2 \tau_t \ (a), \quad \delta_t \approx \sigma_t \approx (u'Lt)^{1/2} \ (b), \\ &U_t = S_L(\overline{\mathrm{A}}/\mathrm{A}_0) = A_1(u'S_L)^{1/2} \ (c), \end{aligned} \tag{34}$$

For deriving Eq. (34c) we present the mean area using Eqs. (5) and (6) as follows:

$$(\overline{\mathrm{A}}/\mathrm{A}_0) \approx \sigma_t/\lambda \ \ (a), \quad \lambda^2 \approx \int_0^\infty F(k)dk \Big/ \int_0^\infty k^2 F(k)dk \ \ (b), \tag{35}$$

where λ is the Taylor microscale of the random flame surface in accordance with general definition (with precision of a multiplier) of this microscale [10]. The Taylor microscale can be presented as follows:

$$\lambda = f(u', L, S_L, t) \underset{1}{\Rightarrow} \frac{\lambda}{L} = f_1\left(\frac{S_L t}{L}, \frac{S_L}{u'}\right) \underset{2}{\Rightarrow} \frac{\lambda}{L} = \sqrt{\frac{S_L t}{L}} f_3\left(\frac{u'}{S_L}\right) \underset{3}{\Rightarrow} \frac{\lambda}{L} \approx \sqrt{\frac{S_L t}{L}}. \tag{36}$$

The arrow 1 in Eq. (11) denotes transition from general presentation to the formula that follows using the Buckingham $\Pi-$theorem of the dimension theory [11]. For transition 2 we put that $(\overline{\mathrm{A}}/\mathrm{A}_0) = const$ and $\sigma_t \sim \sqrt{t}$, hence $\lambda \sim \sqrt{t}$. For the transition 3 we take into account that at strong turbulence $(u'/S_L) >> 1$, so we put $f_3(u'/S_L) \approx f_3(\infty) \sim 1$. Using Eq. (34$b$), (35$a$) and the last expression in Eq. (36) results the formula $(\overline{\mathrm{A}}/\mathrm{A}_0) \approx (u'/S_L)^{1/2}$, which yields the desired expression for the speed of the flame: We notice that Eq. (34c) shows weaker chemistry dependence of the flame speed ($U_t \sim \sqrt{S_L}$) than of the laminar flamelet. The reason is that increasing of S_L smoothes the small-scale wrinkles that results decreasing of the area $(\overline{\mathrm{A}}/\mathrm{A}_0)$ and vice-versa.

The mean chemical source in the cases laminar and microturbulent instantaneous flame

The stated theoretical (in the context of the Kolmogorv's ideas) expression for the turbulent flame speed , Eq. (x), results the expression for the source presented by Eq. (36a):

$$\overline{\rho}\widetilde{W} = \mathrm{A}_1 \sqrt{\overline{k}_u^{1/2} S_L} \, |\nabla \widetilde{c}| \ \ (a), \quad Da_u^{1/2} >> \mathrm{Re}_{t,u}^{1/4} \ \ (b), \tag{37}$$

were $Da_u = L_u / u_u' / \tau_{ch}$ and $\mathrm{Re}_{t,u} = u_u' L_u / \nu_u$. Eq. (36a) also valid with good accuracy in the case of actual laminar flame as its width is small, $\delta_L \sim (0.1-1)mm$. Eq. (36b) is the condition of it that follows from the inequality $\delta_L << \eta_u = L_u \mathrm{Re}_{t,u}^{-3/4}$ and Eq. (27b). Appearing in Eq. (37) of the parameters of the unburned gas is connected with the fact that the instantaneous flame propagate through reactants and namely they control the chemical source .

In [4] we state similar expression for the chemical source and corresponding conditions in the case of the microturbulent instantaneous flame that in our case as follows:

$$\begin{aligned} &\overline{\rho}\widetilde{W} = \mathrm{A}_2 u_u' Da_u^{1/4} \,|\nabla\widetilde{c}\,| = \mathrm{A}_2 u_u'^{3/4} S_L^{1/2} \chi_u^{1/4} L_u^{1/4} \;\; (\mathrm{A}_2 \approx 0.52) \quad (a), \\ &Da_u^{3/4} >> 1 >> Da_u^{3/2} \,\mathrm{Re}_{t,u}^{-3/4} \quad (b). \end{aligned} \tag{38}$$

Eq. (37) are valid for the laboratory low velocity flame, while Eq. (38) refer to the cases of high speed gas turbine combustion.

The alternative approach and the TFC combustion model

We developed proposed alternative approach trying to overcome the challenge of theoretically justified modelling the scalar flux (predominantly counter-gradient) and the stress tensor (describing, in particular, abnormal increasing in the premixed flame of velocity fluctuations. These effects are a gasdynamic nature: they are coursed by different pressure-driven acceleration of the heavy unburned and light burned gases by the pressure gradient generated by the flame, which acts in parallel with the turbulent diffusion. In fact in the context of the alternative approach we reformulated the TFC model on the more theoretically justified basis which both gasdynamic and turbulent mechanisms and their interaction are contained in the conditionally averaged equations.

For comparison we remind how this problem was treated in the standard version of the TFC model implemented in the Ansys Fluect and CFX codes. We presented the scalar flux as a sum of the turbulent gradient $(\overline{\rho\vec{u}''c''})_t$ and gasdymic countergradient $(\overline{\rho\vec{u}''c''})_g$.For closure of Eq. (39) we included the gasdynamic component of the flux in the model chemical source and approximate remaining turbulent components in terms of the turbulent diffusion coefficient D_t as follows:

$$\partial(\overline{\rho}\widetilde{c})/\partial t + \nabla\cdot(\overline{\rho}\widetilde{\vec{u}}\widetilde{c}) = -\nabla\cdot(\overline{\rho\vec{u}''c''}) + \overline{\rho}\widetilde{W} \tag{39}$$

$$(\overline{\rho\vec{u}''c''})_t + (\overline{\rho\vec{u}''c''})_g$$

$$\partial(\overline{\rho}\widetilde{c})/\partial t + \nabla\cdot(\overline{\rho}\widetilde{\vec{u}}\widetilde{c}) = \nabla\cdot(\overline{\rho}D_t\nabla\widetilde{c}) + \rho_u U_t\left|\nabla\widetilde{c}\right| \tag{40}$$

We developed in [3] a gasdynamic model which yields to derive for the one-dimensional algebraic expression for the gasdynamic component $(\overline{\rho\vec{u}''c''})_g$. This model, which does not contain any empirical constants permitted to estimate at post-processor stage actual scalar flux $\overline{\rho\vec{u}''c''}$ and source $\overline{\rho}\widetilde{W}$. These predictions was validated against known experimental data in the Bunsen and impinging flames. But our attempt to generalise this gasdynamic model for the three-dimensional case met some difficulties. Furthermore, the post-processor simulations are not appropriate in commercial codes. Developed alternative approach permits to simulate all actual parameters directly.

Conclusions

1. We show that known challenge of modelling of the scalar flux and stress tensor is not an inherent in the theory of turbulent premixed combustion, but it appears due to inappropriate Favre averaging and conditional averaging of the moment equation eliminates this difficulty.
2. We present the alternative system of the unclosed equations, which describes all Reynolds and Favre averaged paramagnets of the premixed combustion problem formulated for the BML combustion mechanism, where requiring modelling unknowns are the conditional mean stresses in the unburned $(\overline{u_i'u_j'})_u$ and burned $(\overline{u_i'u_j'})_b$ gases, and mean chemical source $\overline{\rho W}$. The components of the scalar flux $\overline{\rho u_i'' c''}$ and stress tensor $\overline{\rho u_i'' u_j''}$ do not require modelling.
3. We state the models for turbulence and source. $(\overline{u_i'u_j'})_u$, $(\overline{u_i'u_j'})_b$ and $\overline{\rho W}$. The former is reformulated in terms of the conditional mean $\bar{k}_u, \bar{\varepsilon}_u$ and $\bar{k}_b, \bar{\varepsilon}_b$ standard "$k-\varepsilon$" model. The latter is based on the theoretical expression for the flame speed U_t deduced in the context of the Kolmogorov methodology. The results for BML mechanism is original, for completeness we present also the expression for the case of wrinkled microturbulent instantaneous flame.
4. Presented equations are comprehensive for implementation in a code and simulations.

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References

[1] Bray, K.N.C., Libby, P.A., Moss, J.B., "Unified modeling approach for premixed turbulent combustion--Part I: General formulation". *Combust. Flame,* 61:87-102 (1985).
[2] Bray, K.N.C., Champion, M., and Libby, P.A., "Premixed Flames in Stagnating Turbulence Part IV: A New Theory for the Reynolds Stresses and Reynolds Fluxes Applied to Impinging Flows", *Combustion and Flame,* 120:1–18 (2000).
[3] Zimont, V.L., Biagioli, F., "Gradient, counter-gradient transport and their transition in turbulent premixed flames"*Combust. Theory Modelling* 6**,** 79–101 (2002).
[4] Biagioli, F., Zimont, V.L., "Gasdynamics modeling of cauntergradient transport in open and impinging turbulent premixed flame", *Proc. Comb. Inst.* 29: 2087–2095 (2002).
[5] Zimont, V.L., "Kolmogorov's legacy and turbulent premixed combustion modelling"/ Chapter 1 in a book: *New Developments in Combustion Research*. Nova Science Publishers, Inc, New York. Editor: William J. Carey, pp. 1-93, 2006.
[6] Im, Y.H. et al., "Zone conditional assessment of flame-generated turbulence with DNS database of a turbulent premixed flame". *Combust. Flame*137: 478-488-224 (2004).
[7] Lee, E., Huh, K.Y., "Zone conditional modeling of premixed turbulent flames at a high Damköhler number", *Combust. Flame* 138: 211-224 (2004).
[8] Lipatnikov, A.N., "Conditionally averaged balance equations for modeling premixed turbulent combustion in flamelet regime", *Combust. Flame* 152: 529-547 (2008).
[9] Batchelor, G.K., "The effect of homogeneous turbulence on material lines and surfaces", *Proc. Roy. Soc.*, A213**:** 349-366 (1952).
[10] Monin, A.S., Yaglom, A.M., *Statistitical Fluid Mechanics: Mechanics of turbulence,* Volume II. The MIT Press, 1987, p. 55.
[11] Barenblatt, G.I., *Similarity, Self-similarity, and Intermediate Asymptotics,* Consultants Bureau, New York, 1979.