Kolmogorov methodology as a practical way to answer to the challenge of turbulent combustion

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Turbulent Premixed and Partially Premixed Combustion

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Kolmogorov methodology as a practical way to answer to the challenge of turbulent combustion

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Abstract

This paper analyses possible practical answer to so-called challenge of turbulent combustion (i. e. inability of combustion models predict accurately at real Reynolds and Damköhler numbers combustion rates) using Kolmogorov idea of equilibrium small-scale states. As this challenge is connected with inability to resolve at combustion modeling small space and time scales where takes place coupling between chemistry and turbulence, controlling the rates, our propose is based on assumption some equilibrium small-scale structures of reaction zones at flamelet combustion mechanism, whose properties could be expressed in terms of large-scale parameters. In other words the combustion rates enter in the combustion equation through a physical model similar to the molecular dissipation in the Kolmogorov "$k-\omega$ turbulence model.

The concrete analyzed premixed combustion problem refers to the case of strong turbulence and flames with increasing brush width (this combustion regime is preceded to the traditional stationary flames). Two main equilibrium states are assumed for quantitative description of this coupling: equilibrium fine-scale turbulence, which controls thickened flamelet parameters and equilibrium small-scale structure of strongly wrinkled flamelet sheet that controls the flamelet area. We examined integral turbulent flame speed U_t and the local combustion rates across the flame $\overline{\rho W}$. It has been shown that at the same U_t, the possibility of accurate prediction of the $\overline{\rho W}$ distribution is closely connected with the possibility to describe the counter-gradient transport phenomenon.

Finally we generalize the premixed combustion model equation in terms of the progress variable to the general case of partially premixed combustion. These more general equations are in terms of PDF of a passive concentration and a conditional progress variable, the transport terms are controlled only by physical gradient diffusion, equations contain only the dissipation of the passive concentration. At equilibrium products (fast chemistry) the coupling between chemistry and turbulence is described similar to the premixed case by a model source term.

all coupling effects contains only in the equation in the terms of the conditional progress variable and enter in the source term through the physical model.

1 Introduction

The term "challenge" has been used last years in scientific papers [1]-[2] to emphasize that application of actual turbulent combustion simulations to practical problems has very limited ability to predict the turbulent combustion process. Bray explains the reason of it in [2]: "As we shall see, the accurate prediction of mean reaction rates, which can be influenced strongly by molecular diffusion caused by small-scale turbulent mixing, represents the central problem and challenge of turbulent combustion". This challenge means that turbulent combustion models cannot describe experimental data on U_t dependences on fuel type, the air excess coefficient, initial temperature of a mixture, the pressure. In other words models cannot predict accurately dependence of U_t (and much less $\overline{\rho W}$) on the chemical kinetics and the molecular transfer coefficients. The main difficulty to answer this challenge is connected if fact with flamelet combustion mechanism at real Reynolds Re and Damköhler Da numbers.

For a 1-D case, the averaged picture of premixed combustion consists in a combustion front (a turbulent flame), so prediction of mean reaction rates means prediction of the local distribution of the averaged combustion rate across the flame $\overline{\rho W(x)} = \rho_u U_f \overline{\Sigma}(x)$ or only prediction of the combustion speed that is: $U_t = U_f \overline{(S/S_0)} = (1/\rho_u) \int \overline{\rho W(x)}\, dx$. Here U_f is the flamelet velocity (at theoretical estimations U_f often assumed to be the laminar combustion velocity U_l), $\overline{\Sigma}$ is the flamelet surface density, $\overline{(S/S_0)}$ is the dimensionless flamelet surface area, ρ_u is the density of unburned mixture.

At first glance, this problem seems intractable: we cannot resolve in the frames of combustion model equations space and time scales that are necessary for a correct description of chemical kinetics, molecular transfer processes and their coupling. If it were so it would mean that to design physically reasonable combustion model containing the key combustion mechanisms (and between them one of the main is mentioned coupling) would be impossible. It would mean that every possible combustion model even if it reproduces some limited experiments (by tuning empirical constants) could not describe a large ensemble of experimental data and, in general, could not give correct trends.

The aim of this paper is to show that from the application-oriented point of view this problem does not look unresolved, and that there are ideas that could give positive applied results. We try to formulate a practicable line of inquiry to answer this challenge and analyze its practical application not only to simulation of premixed combustion for large Re and Da numbers but also to the more general case of partially premixed combustion.

The character of this challenge and the main idea of our answer in fact is not new. A similar challenge was in past that of practical turbulence modeling as existed methods could not predict accurately the turbulent dissipation rates, which was influenced strongly by small-scale vortexes. Kolmogorov gave a practical answer to this challenge and it was in fact the cornerstone of all turbulence models for large Re numbers. In both cases, turbulence and turbulent combustion, controlling processes take place in such small scales that could not be resolved by model equations.

Kolmogorov answer[3] was based on the assumption of equilibrium fine-scale turbulence (where actual dissipation took place) due to the Richardson cascade mechanism. This assumption yields that the turbulent dissipation rate is controlled by large scale turbulence and at large Reynolds numbers the averaged dissipation rate $\bar{\varepsilon}$ does not depend on the molecular viscosity coefficient: $\bar{\varepsilon} = Cu'^3/L$, where $C \sim 1$. Next year Kolmogorov designed using these ideas the first two parametric turbulence model ("$k - \omega$")[4], where the dissipation rate was described not in terms of the molecular viscosity coefficient, but through this physical mechanism.

In this paper we extend this Kolmogorov methodology to model turbulent combustion at large Reynolds and Damköhler numbers. We used Kolmogorov ideas in past[5] and TFC model that has some application (in "Fluent 5", for example) is based on them. Here we formulate and analyze the feasibility of these ideas for combustion modeling using as an example TFC model[5-8].

2 Kinematics picture of premixed combustion flame

In the case under review combustion takes place in thin highly wrinkled flamelet sheets that separates the reactants from the products and propagates relative to the reactants with velocity U_f. In our model the flamelet is not the laminar flame with the combustion velocity U_l , but is thickened by small scale turbulence flamelet with the combustion velocity $U_f > U_l$.

As a preliminary we assume that gas density $\rho = const$, i. e. combustion does not change hydrodynamic flow and turbulence. Let denote P_u, P_b and P_f the probabilities of unburned mixture (reactants), burned mixture (products) and flamelet compositions in every point of the turbulent flame. For kinematics description of the flame mechanism we assume that $P_u + P_b = 1$ as $P_f << 1$ (the flamelet combustion on mechanism). We will use the combustion product probability $P_b(\vec{x}, t)$ or the averaged progress variable $\overline{c}(\vec{x}, t)$ (at $\rho = const$, $\overline{c} = P_b$) for description of turbulent flames.

At first we will analyze a 1-D non-stationary flame front in gas moving along the x-axis at $u' >> U_f$. Assume that at the initial time $t = 0$ for $x < 0$ $\overline{c} = 1$ and for $x > 0$ $\overline{c} = 0$. For $t > 0$ the plane boundary becomes wrinkled at $t > 0$ and its dimensional area $\overline{(S(t)/S_0)}$ grows. So at the beginning we have a combustion front with increasing turbulent combustion velocity $U_t(t)$ and increasing flame brush width $\delta_t(t)$.

Let $F(k, t)$ be a spectrum of the flamelet sheet thought as being a random surface $x = h(y, z, t)$, where k is the wave-number ($k = 2\pi/\Lambda$ and Λ is the wave length). The dispersion of the flamelet sheet is determined by the large waves of the random flamelet sheet (small k):

$\sigma^2(t) = \overline{(x-\overline{x})^2} = \int_0^\infty F(k,t)\,dk$, whereas the flamelet area is determined by the small waves (large k): $\overline{(S(t)/S(0))} = const \int_0^\infty k^2 F(k,t)\,dk$, where the $const$ is order unity (in the case of Gauss random surface it can be calculated exactly). Without combustion $\overline{(S(t)/S(0))}$ increases very fast (approximately exponentially), but in the case of combustion the flamelet progress suppresses this fast increase. So after some time, that probably is the order of so called Gibson time $\tau_G = L_G/U_f = \tau_t(U_f/u')^2$, where $\tau_t = L/u'$[9], we would have $U_t \approx const$ (more exactly very slow increasing of U_t).

For $\tau_G < t < \tau_*$, when suppression of large wrinkles of the sheet by moving flamelet is negligible, we have flame with increasing brush width δ_t that is growing in accordance with the turbulent diffusion law $\delta_t \sim (\sigma^2)^{1/2} = (2D_t t)^{1/2}$, where σ^2 is the dispersion of the flamelet sheet and D_t is the turbulent diffusion coefficient. We estimated the time $\tau_* \approx 2D_t/U_f^2 \approx 2\tau_t(u'/U_f)^2$ from the condition $(\sigma^2(\tau_*))^{1/2} \approx U_f\tau_*$, i. e. when transport due to turbulent diffusion and due to the flamelet progress are of the same order (obviously this is a lower estimation, since due to fluctuation of the flamelet angles, the averaged flamelet velocity in some direction less U_f.

So for times $\tau_G < t < \tau_*$ we have a flame with increasing brush width and practically constant turbulent combustion velocity. We call these combustion fronts Intermediate Steady Propagation (ISP) flames and believe that they should be recognized as a special class of flames. They correspond to a combustion regime which is intermediate between the initial stage at $t < \tau_G$, when we have intensive forming of wrinkles on the flamelet sheet and fast increasing of $U_t(t)$ and the final stage corresponding to $t >> \tau_*$, when we have stationary turbulent combustion fronts with $U_t^{st} = const.$ and $\delta_t^{st} = const.$

Simple estimations show that for real industrial combustors, as a rule, the time τ_* is larger that the residence time (that could be $\sim 10\tau_t$), i. e. in real combustors a flame reaches a wall and combustion is completed long before forming a flame with constant brush width. As τ_G is much less than the residence time in many cases we can assume that ISP regime takes place at $t < \tau_*$. We will see below that properties of ISP and stationary flames and their controlling mechanisms are quite different.

The 3-D ISP flame kinematics equation for $\rho = const$ (as the special case of the model equation for the partially premixed combustion) was proposed in [6]:

$$\partial(P_b)/(\partial t) + \nabla \cdot (\overline{\mathbf{u}} P_b) = \nabla \cdot (D_t \nabla P_b) + U_t |\nabla P_b|, \tag{1}$$

where D_t is the turbulent diffusion coefficient.

The statement of this section: Premixed combustion at intensive turbulence $u' >> U_f$ and $\tau_t(U_f/u')^2 < t < \tau_t(u'/U_f)^2$ takes place in intermediate steady propagation (ISP) flames, i. e. in flames with $U_t \approx const$ (as approximate equilibrium between generation and dissipation of small-scales wrinkles of the flamelet sheet controlling its area is reached) and increasing by turbulent diffusion of the flame brush width (as at these times the regime is far from the equilibrium between formation of large-scale sheet wrinkles controlling this width and their consumption due to flamelet movement. Combustion models that based directly or indirectly on the only time τ_t in fact does not contain this regime.

3 Mean reaction rates and TFC combustion model

The main attention in this section would be devoted to the physical equilibrium mechanisms at developed turbulence which enable us to introduce into the TFC model equation the coupling between turbulence and chemistry. We will analyze the integral combustion rate U_t dependence on controlling parameters and the local combustion rate $\overline{\rho W}$ distribution across the premixed flame. It would be shown that in flames with known integral characteristics U_t and δ_t the distribution of $\overline{\rho W}$ and counter-gradient transport phenomenon are closely connected.

The main physico-chemical mechanism controlling U_t :

The main controlling mechanism responsible for much weaker U_t dependence on chemistry in comparison with the laminar flame velocity U_l (more exactly with the actual flamelet velocity U_f) is the smoothing of wrinkled flamelet sheet due to moving of their elements with the velocity U_l. It means, for example, that a more fast chemistry increases U_l, but at the same time implies a decrease of the flamelet sheet area $\overline{(S/S_0)}$ due to consumption by more fast flamelet of additional small-scale wrinkles and makes it more smooth. We have what we call hydrodynamic "flamelet combustion self-compensation mechanism".

For stationary flames at $u' >> U_l$ in accordance with Damköhler[10], Shchelkin[11] ideas U_t^{st} does not depends on chemistry ($U_t^{st} \sim u'$), i. e. complete compensation: $\overline{(S/S_0)} \sim 1/U_l$. This situation is similar to turbulent dissipation at large Re numbers [3], when the effect of the kinematic viscosity increase is completely compensated by a decrease of instantaneous velocity gradients.

We will see below that for ISP flame, that takes place at $t < \tau_t(u'/Uf)^2$, takes place a partial combustion velocity compensation: U_t depends on chemistry but much weaker than U_l or U_f and this flame takes place at $t < \tau_t(u'/Uf)^2$. At the same time the most part of combustion model equations give at $t > \tau_t$ the stationary flame (see, for example, result of simulation in [12]) and this 1-D flame dependence on chemistry in fact corresponds to laminar flames. It is worth noting that the model that contains the result as an limiting case $U_t^{st} \sim u'$ was developed recently by Peters[13].

The parameters of thickened flamelet and its area, U_t dependence:

a. In accordance with [5] transfer process inside the thickened flamelet depend on vortices from equilibrium inertial interval and the value of the relevant transfer coefficient follows directly from dimensional analysis $\chi_f \approx \varepsilon^{1/3}\delta_f^{4/3}$, which is in fact the well-known Richardson law of the turbulent diffusion for scales inside the inertial interval (δ_f is the flamelet width). U_f and δ_f are function of χ_f and of the characteristic chemical time τ_{ch}, and by using dimensional analysis considerations (for laminar flames $U_l \approx (\chi/\tau_{ch})^{1/2}$, $\delta_l \approx (\chi\tau_{ch})^{1/2}$), we obtain:

$$U_f \approx (\chi_f/\tau_{ch})^{1/2} \approx u'(Da)^{-1/2}, \quad \delta_f \approx (\chi_f\tau_{ch})^{1/2} \approx L(Da)^{-3/2}, \chi_f \approx D_t(Da)^{-2}. \tag{2}$$

This formulas can be derived straightforward using the inertial interval spectrum $E(k) = Ck^{-5/3}$[5]. The relationships (2) are equivalent to the fact that, in a coordinate system where the thickened flamelet is fixed, the heat fluxes in the front due to heat transfer and convection are of the same order of magnitude of the heat release due to chemical reactions [5]. Notice that chemical dependence of U_f in (2) is identical to that of the laminar flame.

b. For the estimation of $\overline{(S/S_0)} >> 1$ dimensional analysis is not sufficient and it is necessary to use also some general property of random surfaces $x = h(y, z, t)$. Our estimation is as follows:

$$\overline{(S/S_0)} = \overline{(1 + |grad\, h|^2)^{1/2}} \approx \overline{|grad\, h|} \approx \overline{(|grad\, h|^2)^{1/2}} \approx \int k^2 F(k)\, dk \approx \sigma/\lambda, \tag{3}$$

where $\sigma^2 = \overline{(x - \overline{x})^2} = \int F(k)\, dk = 2D_t\, t$ is the dispersion, λ is the micro-scale of the length of the random surface and $F(k)$ is the spectrum of the flamelet surface disturbances. We see, that σ^2 is defined by large scale and $\overline{(S/S_0)}$ by small scale disturbances of the flamelet surface. In ISP flames the spectrum $F(k, t))$ a small wave number k part is non-steady (increasing of large wrinkles by turbulence) and at the same time a large wave number part is steady (equilibrium between generation and consumption of small wrinkles).

The micro-scale λ, due to the assumed equilibrium, is a function of large scale turbulence characteristics L, u', flamelet parameters δ_f, U_f and time, t. Applying then the Π-theorem of a dimensional analysis yields $\lambda/\delta_f = f_1(u't/\delta_f, u'/U_f, L/\delta_f)$. Taking into account expressions (2) and using the condition of $\overline{(S/S_0)}$ stationary, we obtain that $\lambda/\delta_f = (u't/\delta_f)^{1/2} f_2(Da) \approx$

$(u't/\delta_f)^{1/2} f_2(\infty) \approx (u't/\delta_f)^{1/2}$. Hence using (3), the expression for the averaged flamelet sheet area reads:

$$\overline{(S/S_0)} \approx (Da)^{3/4} \approx (u'/U_f)^{3/2} \approx (L/\delta_f)^{1/2} >> 1. \tag{4}$$

We see that assumption of physical equilibriums made possible to express parameters of U_f, δ_f and $\overline{(S/S_0)}$, controlled mainly by small-scale turbulence, in terms of large-scale turbulent characteristics, as shown by formulas (2) and (4).

c. Expressions (2) and (4) and well known formula for the chemical time $\tau_{ch} = \chi/U_l^2$ give finally the expression of the turbulent combustion velocity for the ISP flames:

$$U_t = U_f\overline{(S/S_0)} = Au'(Da)^{1/4} = Au'^{3/4} U_l^{1/2} \chi^{-1/4} L^{1/4}, \tag{5}$$

where $A \sim 1$ is an empirical parameter. It is worth emphasizing that all powers have been derived from the physical model and they don't contain any quantitative empirical information.

The chemistry dependence of U_t that is given by (5) ($U_t \sim \tau_{ch}^{-1/4}$) is much weaker than for laminar combustion ($U_l \sim \tau_{ch}^{-1/2}$). The reason is mentioned above partial flamelet combustion self-compensation mechanism: increasing of U_f decreasing in accordance with (4) $\overline{(S/S_0)}$ and vice-versa. Comparison of this prediction with empirical correlations for U_t and the range of applicability of (5) are presented in [8]. We have to mention that, for the hypothetical case of thickened but not wrinkled flame at $L << \delta_l$ proposed by Damköhler [10] the turbulent flame speed is $U_t \sim (D_t/\tau_{ch}$. This flame has laminar flame chemistry dependence, i. e. more strong than ISP flame. This regime is contained as a limiting case in the new Peters model [13].

It should be particularly emphasized that the thickened flamelet in our model have no quasi-laminar structure: in accordance with analysis of temperature pulsation balance presented in [5] the temperature pulsations inside the thickened flamelet are high, i. e. instantaneous reaction sheet strongly wrinkled inside the flamelet. It seems that this model closely correspond to the thin reaction zone regime[13]. In our analysis we ignore the temperature pulsation inside a flamelet. From a methodological point of view it is similar to ignore the dissipation rate pulsations in the Kolmogorov theory of the fine-scale turbulence[3].

Turbulent flame closure (TFC) combustion model:

TFC combustion model is based on the kinematics equation (1) modified of $\rho \neq const$[7]. This equation is as follows (the conventional and Favre averaging are symbolized $\overline{a}$ and $\tilde{a} = \overline{\rho a}/\overline{\rho}$,):

$$\partial(\overline{\rho}\tilde{c})/(\partial t) + \nabla \cdot (\overline{\rho}\tilde{\mathbf{u}}\tilde{c}) = \nabla \cdot (\overline{\rho} D_t \nabla \tilde{c}) + (\rho_u U_t)|\nabla \tilde{c}|. \quad (6)$$

Eq. (6) describes only ISP flames and does not contain limiting case of 1-D stationary flames, it strongly simplifies the combustion model and the same time does not impose a limitation on its practical applications for simulation combustion at strong turbulence.

In TFC model the theoretical expression (5) for U_t as a function of the physico-chemical properties of the combustible mixture and turbulent parameters is substituted in the Eq. (6). In other words we introduce directly in the model equation the properties of the ISP flames (their combustion velocity and width dependences) that why we name it the turbulent flame closure (TFC) equation. TFC model equation simulated together with fluid dynamics Reynolds equations and "$k - \varepsilon$" turbulence (at simulations it was assumed $\chi = \chi_u$ and local u' and L expressed in terms of k and ε). This set of equations simulated only large-scale processes but in accordance with the foregoing it describes the small-scale coupling between turbulence, molecular transport and chemistry. It is interaction between turbulence and molecular viscosity (dissipation rate), between turbulence and instantaneous reaction zone (flamelet parameters), between turbulence and flamelet sheet (its area). To describe experimental bending for U_t at regimes close to a blow-out boundary (Lipatnicov proposal) Bray model[14] was used of the stretch effect in terms of flamelet critical velocity gradient based in fact on the assumption of universal equilibrium PDF for instantaneous dissipation (i. e. for instantaneous characteristic velocity gradients in small scales controlling flamelet extinction). It was in fact the forth equilibrium mechanism used in our combustion simulations.

Good agreement with a great body of Karpov experimental data in spherical bombs with artificial turbulence for different fuels, air excess coefficients and turbulence[15] (i. e. at large variation of kinematics, molecular transport and turbulent properties of mixtures) is good indirect evidence that their coupling using idea of physical equilibrium is fruitful. The comparison with Moreau data on high velocity combustion in a channel[16] confirm existence of ISP flames with increasing brush width.

$\overline{\rho W}$ and the counter-gradient transport in the TFC model:

In the equation (6) the transport and the source terms are not real transport and source terms of the unclosed equation, i. e. $\nabla \cdot (\overline{\rho} D_t \nabla \tilde{c}) \neq -\nabla \cdot (\overline{\rho \mathbf{u}" c"})$, and $(\rho_u U_t)|\nabla \tilde{c}| \neq \overline{\rho W}$. In TFC model equation transport term has gradient nature, while the transport term $\nabla \cdot (\overline{\rho \mathbf{u}" c"})$ has in many turbulent premixed flames counter-gradient nature. It means that in the model equation transport term we include only the gradient physical diffusion part (to describe flames with increasing flame brush width) whereas the counter-gradient part was included in the model source term $(\rho_u U_t)|\nabla \tilde{c}|$. So though TFC model equation describe physical distributions of $\tilde{c}$ and connected with it $\overline{\rho}$, $\overline{T}$ and concentration of species, for extraction of the physical source term $\overline{\rho W} = \rho_u U_f \overline{\Sigma}$ from the model source term it is necessary, as it would seen below, to have additionally some hydrodynamic model for the progress variable transport term. We illustrate it by the example of 1-D stationary combustion front. The kinematic equation and the exact unclosed equation are as follows:

$$\frac{d}{dx}(\overline{\rho}\tilde{u}\tilde{c}) = \rho_u U_t^{st} \frac{d\tilde{c}}{dx}, \quad \frac{d}{dx}(\overline{\rho}\tilde{u}\tilde{c}) + \frac{d}{dx}(\overline{\rho u'' c''}) = \overline{\rho}\widetilde{W} = \rho_u U_f \Sigma, \tag{7}$$

From Eqs. (7) it readily follows that

$$\overline{\rho}\widetilde{W} = \frac{d}{dx}(\rho_u U_t^{st}\tilde{c} + \overline{\rho u''c''}), \tag{8}$$

i. e. to extract the physical source term it is also necessary to know the transport term. The latter can be reported in terms of conditional averaged velocities of the cold (unburned) and hot (burned) volumes $\overline{u}_u$ and $\overline{u}_b$, namely $-\overline{\rho u"c"} = \overline{\rho}(\overline{u}_u - \overline{u}_b)\tilde{c}(1-\tilde{c})$. A qualitative analysis where we put $\overline{u}_u(x) = U_t^{st}$ and $\overline{u}_b(x) = (\rho_u/\rho_b)U_t^{st}$ (the upper estimation of the progress variable transport), yields

$$\frac{\overline{\rho u''c''}}{\rho_u U_t} = (1 - \frac{\rho_b}{\overline{\rho}})P_b = (\frac{\overline{\rho}}{\rho_b} - 1)\tilde{c} = P_b - \tilde{c} > 0, \quad (\frac{d\tilde{c}}{dx} > 0, \quad 0 < \tilde{c} < 1). \tag{9}$$

As obviously $\rho_u > \overline{\rho} > \rho_b$, Eq. (9) corresponds to the counter-gradient diffusion as the signs of $\overline{\rho u''c''}$ and of $d\tilde{c}/dx$ are the same. This and more accurate gasdynamic estimation of conditional averaged velocities testifies that the function $\overline{\rho u''c''}(\tilde{c})$ practically does not depends on turbulence and combustion rates but mainly controlled by ρ_u/ρ_b. At the same time the front width δ_t^{st} and the distributions $P_b(x)$ and $\tilde{c}(x)$ are controlled by flamelet properties and turbulence, i. e. by the coupling between chemistry, molecular transport and turbulence. It means that $\overline{\rho u''c''}(x)$ is controlled by gasdynamics, turbulence and combustion.

From Eqs. (8) and (9) it follows that the "physical" source term (for this simplified hydrodynamic model) is $\overline{\rho W} = \overline{\rho}\tilde{W} = \rho_u U_t^{st} dP_b/dx$. It is clear that in spite of $U_t^{st} \approx u'$ the local combustion rate $\overline{\rho W}(x)$ is controlled by the flamelet and turbulence properties, i. e. coupling between chemistry, molecular transport and turbulence.

For ISP flames the physical source term is $\overline{\rho}\widetilde{W} = d(\rho_u U_t^{st}\tilde{c} + \overline{\rho u''c''} + D_t d\tilde{c}/dx)$, assuming used above estimation $\overline{u}_u(x) = U_t$ and $\overline{u}_u(x) = (\rho_u/\rho_b)U_t$ (i. e. ignoring at large ρ_u/ρ_b flame width increasing on the gasdynamics) we have

$$\overline{\rho}\widetilde{W} = \rho_u U_t \frac{dP_b}{dx} + \frac{d}{dx}(D_t \frac{d\tilde{c}}{dx}) \tag{10}$$

For ISP flames the bush width $\delta_t(t)$ and the distributions $P_b(x,t)$ and $\tilde{c}(x,t)$ are controlled by turbulent diffusion and coupling between chemistry, molecular transport and turbulence appears in (10) through expression for U_t (5). The paper [16] contains some results of combustion simulation in a channel, taking into account the counter-gradient transport and presents the calculation results for the model and the physical source terms.

The statement: We believe that TFC model is an combustion analogue of "$k-\omega$" *or* "$k-\varepsilon$" *turbulence models, i. e. it is a first approximation combustion model, that nevertheless contains the main large-scale and small-scale mechanisms including coupling between turbulence, chemistry and molecular transport.*

4 Partially Premixed Turbulent Combustion Modeling

Partially premixed combustion is the most complicated case for modeling as it contains elements both of premixed and non-premixed combustion. Luckily in the case of developed turbulence and fast combustion kinetics practical combustion simulation can be more simple as assumptions of equilibrium of turbulence and reaction sheet structures are physically justified and useful also here. In the premixed case presented above we installed combustion in equations through a physical model, the same idea is the basis for designing of the equations for partially premixed combustion modeling.

Reaction zone structure at partially premixed combustion.

We generalized to the case of partially premixed combustion the model of a reaction zone structure at non-premixed combustion that in fact very closely corresponds to the Bilger concept of QEDR quasi-equilibrium distributed reaction (QEDR) flames[17]. For combustion regimes far from the blow-out boundary, the instantaneous reaction zone at non-premixed combustion consists of a layer of quasi-equilibrium products in the neighborhood of the instantaneous stoichiometric surface, and a rich and a lean flamelet-like sheet, a non-equilibrium chemical reactions zone inside of them that separate the equilibrium products and frozen mixture. The heat release intensity in quasi-equilibrium layer is controlled by molecular mixing (dissipation) as $\tau_{ch} << \tau_{mix}$, in rich and lean flamelet-like sheets where $\tau_{ch} \sim \tau_{mix}$ chemical reactions are in non-equilibrium and in the frozen mixture where $\tau_{ch} >> \tau_{mix}$ heat release is negligible. The instantaneous reaction zone at the beginning looks like a single flamelet, but then rich and lean flamelet breaks down into two independent non-equilibrium combustion zones with a broad area of equilibrium reactions between them.

The structure of the wrapping rich and lean sheets are close to thickened premixed flamelet and the progress variable changes from zero (frozen mixture) to one (quasi-equilibrium mixture) and as the probability of intermediate $\tilde{c}$ is small we have in frame of this model a bimodal distribution $p(\tilde{c})$. We assume these flamelet-like sheets as premixed combustion flamelet. The instantaneous position of these flamelet for non-premixed combustion is controlled by the instantaneous dissipation ($\tau_{ch} \sim \tau_{mix}$), but in the case of partially premixed combustion (turbulent mixing of "lean" and "reach" combustible jets) these flamelet travel through lean and rich frozen mixtures like ordinary premixed flamelet.

Governing equations

Let C_f, C_o and C_p be concentrations of fuel, oxygen and products. For identical molecular transfer coefficient $C_f(Z,T)$, $C_o(Z,T)$, $C_p(Z,T)$ and $\rho(Z,T)$, where $Z = C_f + C_p/(1+L_0)$ is the passive concentration and L_0 is the mass stoichiometric coefficient. The general problem reduces to determining the join probability function $p = p(Z,T)$.

Unclosed equation for $p(Z,T)$ is as follows [18]:

$$\frac{\partial \rho p}{\partial t} + \frac{\partial \rho (\overline{u}_k)_{ZT} p}{\partial x_k} - \frac{\partial}{\partial x_k}(\overline{\rho} D \frac{\partial p}{\partial x_k}) + \frac{\partial^2 \rho p \overline{N}_T}{\partial T^2} + 2\frac{\partial^2 \rho p \overline{N}_{ZT}}{\partial T \partial Z} + \frac{\partial^2 \rho p \overline{N}_Z}{\partial Z^2} + \frac{q}{c_p}\frac{\partial W p}{\partial T} = 0, \quad (11)$$

where $\rho = \rho(Z,T)$ is the density, $W = W(Z,T)$ is the heat release intensity, $(u_k)_{ZT}$ is the conditional average velocity, and $\overline{N}_T = (\overline{D(\partial T/\partial x_k)^2})_T$, $\overline{N}_Z = (\overline{D \partial Z/\partial x_k)^2})_Z$, $\overline{N}_{ZT} = (\overline{D\partial Z/\partial x_k \partial Z/\partial x_k})_{ZT}$ are the conditional average dissipation rates. The last term is the source term that has a closed form, i. e. this term can be expressed exactly using chemical kinetics equations. (Equation in this form at $\rho = const$ was derived using characteristic function technology by A. Sabelnikov in 1977, but was not published.)

At large Re numbers (developed turbulence) there are two limit cases:

1. $Da = \tau_t/\tau_{ch} << 1$ (slow chemistry in comparison with characteristic large scale turbulent time). In this case the instantaneous picture of the reaction field has a distributed character and all dissipative terms can be treated as turbulent terms that do not depend on chemistry, i. e. the equation contains chemistry in closed form.

2. $Da = \tau_t/\tau_{ch} >> 1$ (fast combustion chemistry). In this case we have flamelet combustion mechanisms, the "dissipative" terms $\overline{N}_T$ and $\overline{N}_{ZT}$ depend on not only turbulence mixing but also on actual combustion kinetics. It means that chemistry cannot be introduced in physically correct model equation in closed form.

The flamelet mechanism simplify the problem as in every point exist conditional probabilities of unburned and burned volumes $P_u(Z)$, $P_b(Z)$ $(P_u(Z) + P_b(Z) = 1)$, the conditional averaged density $\overline{\rho}_Z = \rho_u(z)P_u(Z) + \rho_b(Z)P_b(Z)$, the conditional progress variable $\tilde{c}_Z = (\rho_b(Z)/\overline{\rho}_Z)P_b(Z)$. The general model equations for the partially premixed combustion (when flamelet travel through volumes of lean and rich frozen mixture) for the ISP flames regime in terms of PDF of the passive concentration $p(Z, \vec{x}, t)$ and conditional progress variable $\tilde{c}_Z(\vec{x}, t)$ are as follows $(\overline{\rho} = \int \rho(Z)p(Z)dZ$ is the averaged density and and $\overline{N}_Z$ is the conditional turbulent dissipation of the passive concentration that does not depend directly on chemistry):

$$\frac{\partial(\overline{\rho}_Z p)}{\partial t}+\frac{\partial(\overline{\rho}_Z \tilde{u_k} p)}{\partial x_k}=\frac{\partial}{\partial x_k}(\overline{\rho} D_t \frac{\partial p}{\partial x_k})-\frac{\partial^2(\overline{\rho}_Z \overline{N}_Z p)}{\partial Z^2}, \tag{12}$$

$$\frac{\partial \overline{\rho}_Z \tilde{c}_Z p}{\partial t}+\frac{\partial \overline{\rho}_Z \tilde{u_k} \tilde{c}_Z p}{\partial x_k}=\frac{\partial}{\partial x_k}(\overline{\rho} D_t \frac{\partial \tilde{c}_Z p}{\partial x_k})-\frac{\partial^2 \overline{\rho}_Z \overline{N}_Z \tilde{c}_Z p}{\partial Z^2}+\rho_u(Z) U_t(Z) p |grad(\tilde{c}_Z)|, \tag{13}$$

In these equations the second terms in the right-hand side (convection) and the first terms in the left-hand side (physical turbulent diffusion) is the part of the second term in the right-hand side of Eq. (11) and they correspond to the ISP flames regime (flames with controlling by turbulent diffusion increasing brush width). In the model equations only the last term in Eq. (13) (the model source term) depends directly on chemistry. But this term, described by the formula (5) depends also on turbulence, molecular mixing and it contains hydrodynamic peculiarities including possible the counter-gradient transport. At $p(Z)=\delta(Z-Z_o)$ (premixed system) Eq.(13) transforms to Eq. (6), i. e. the premixed combustion model is a degenerate case of this more general combustion model.

For combustion simulation at equilibrium products (i.e. passive concentration dissipation rate not too high) we must put $\tilde{c}_Z=1$ as $Z=Z_s$ (the stoichiometric composition). For $0<U_t(Z)<\infty$ and proper initial conditions (e. g., a reach combustible jet and ambient air) we have premixed flame in the jet and diffusion combustion in the mixing area.

Eqs. (12)-(13) correspond to the case of "dispersed" combustion, when the combustion zone is the superposition of independent "conditional" premixed flames (i. e. corresponding to different Z) moving with different combustion velocities $U_t(Z)$. In the paper [18] we simulated partially premixed combustion using another limit case: strong interaction between "conditional" flames. In this case $\tilde{c}$ in every point does not depend on Z. In this paper was applied a more simple procedure: instead of the equation for $p(Z)$ was used equations for $\overline{Z}$ and $\overline{Z'^2}$ for modeling $p(Z)$. This work contains the computational results of a premixed H_2-air jet with different air excess coefficients ($0 \leq \alpha \leq 1$) issuing in an environment of air. In our numerical simulations we had for $\alpha = 0$ non-premixed, for $\alpha = 1$ premixed and for $0 < \alpha < 1$ partially premixed combustion.

The statement: Though PDF equation in the terms $p(Z, T)$ *is the most adequate line to describe partial premixed combustion, PDF methods does not give an opportunity to introduce chemistry in physically reasonable equations in closed form so using a physical model to induce combustion in equations is inevitable. Ideas developed in sections 2 and 3 for premixed combustion were generalized here for this case yielding to general equations in terms of passive concentration PDF* $p(Z, \vec{x}, t)$ *and conditional progress variable* $\tilde{c}(\vec{x}, t)$.

5 Conclusions

Without answer the turbulent combustion challenge is how to describe interaction between turbulence and chemistry, coupling between reaction and diffusive processes on the small turbulent scales that cannot be resolved by accessible methods impossible to develop physically correct combustion models that could describe a great body of experimental data and predict correct trends. It is especially important for premixed case where the combustion rates are completely controlled by this coupling. For non-premixed case the most part of the combustion processes is connected with dissipation rate of a passive concentration, that is physically reasonable described by turbulence models so improper coupling in a model is not so noticeable in simulations.

We see the answer to this challenge in using and developing for turbulent combustion at developed turbulence and fast chemistry Kolmogorov ideas of existing of equilibrium small-scale hydrodynamic structures at combustion modeling. Of course the equilibrium process used must exist in reality, but we believe that such is in the case of real industrial full-scale large velocities combustors. The experience of using TFC model suggested that this approach could be useful for real applications.

In summary we can say that if a turbulent combustion model expresses combustion rates at $Da >> 1$ and $Re_t >> 1$ in terms of chemical kinetic equations, this model is physically incorrect just as incorrect is a turbulence model that expresses at $Re_t >> 1$ the dissipation rate in terms of the molecular viscosity coefficient.

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