Gas Premixed Combustion at High Turbulence. Turbulent Flame Closure Combustion Model.

V.L. Zimont*
CRS4 Research Centre – Cagliari, Italy

*Senior Researcher, CRS4, 6 Strada Ovest, Z. I. Macchiareddu, 09010 Uta(CA), Italy. zimont@crs4.it

Abstract

This paper is devoted to analyze the special class of turbulent premixed flames that we call intermediate steady propagation (ISP) flames. These flames are common to industrial premixed combustion chambers which operate at intensive turbulence when velocity pulsations are significantly higher than the flamelet combustion velocity. They are characterized by a practically constant turbulent combustion velocity, controlled by turbulence, chemistry and molecular processes, and by an increasing flame width, controlled mainly by turbulent diffusion.

The main content of this work is a description of physical backgrounds and outcome of the original asymptotical (i.e., valid at high Re and Da numbers) premixed combustion model, that, from a methodological point of view, is close to Kolmogorov analysis of developed turbulence at high Re numbers. Our analysis starts from the thickened and strongly wrinkled flamelets combustion mechanism. Quantitative results for this model are based on the Kolmogorov assumption of the equilibrium fine-scale turbulence and on additional assumption of the universal small-scale structure of the wrinkled flamelet sheet. From this background it is possible to deduce formulas for the thickened flamelets parameters and the flamelet sheet area and hence the turbulent combustion velocity of the premixed flame.

These formulas are used for the closure of the combustion equation written in terms of a progress variable leading to the so called turbulent flame closure (TFC) model for the numerical simulation of ISP flames. Consistent to the ISP flames, in this work the concept of countergradient transport phenomenon in premixed combustion is analyzed.

Introduction

Quantitatively correct computer simulation of turbulent premixed combustion is a very difficult problem, that nowadays has not general solution. In industrial chambers combustion takes place in flows with large turbulent pulsations and large integral scales. The first results in this field of Damköhler and Shchelkin [1-2] showed that the velocity of the 1-D turbulent front (the turbulent combustion velocity U_t) must not depend on chemical kinetics, i.e., $U_t \approx u'$. Nevertheless experiments show dependence of U_t on chemistry even at very high turbulence. The reason is that 1-D stationary flame structure is practically unattainable in real combustion chambers where instead combustion takes place in flames with increasing width. The second significant point is that in real flows fine-scale turbulence can influence the reaction zone structure and hence affect integral combustion characteristics.

Fortunately combustion at high Reynolds, Re, and Damköhler, Da, numbers has peculiarities that are connected with large velocity pulsations and developed fine-scale turbulence. This simplifies the problem and makes it possible to work out a simple asymptotical premixed combustion model suitable for practical quantitative engineering simulations. The main physical ideas of such premixed combustion model was proposed in [3]. The kinematical equation of the flame with increasing brush width for the model case of constant density in terms of the product probability was proposed in[4]. The premixed combustion model equation in terms of the progress variable and the first results of combustion numerical simulations was presented in [5]. References [6]-[10] contain mainly results of this combustion model validation using different standard experimental data in spherical bombs with artificial turbulisation [5-8], in a channel at high velocity combustion [9] and in industrial burners [10].

In this work we present an extensive analysis of the physical background of this model highlighting potentialities, limitations and fields of applicability.

To do this we present in five points the peculiarities of industrial premixed combustion which is characterized by high turbulent Reynolds number $Re_t = u'L/\nu$ and developed fine scale turbulence.

1. Turbulent combustion has flamelets mechanism, i.e. combustion takes place in thin strongly wrinkled flamelet sheets that separate fresh mixture and products. This result is not trivial, as the developed turbulence is characterized by a energy spectrum that corresponds to a continuous and wide spectrum of vortex sizes from the largest comparable with the chamber dimensions up to the smallest which are smaller than laminar flame width. Damköhler [1] was the first who left room for the thickening of the flamelets width by turbulence but he analyzed only the hypothetical case of vortexes with sizes smaller than the laminar flame thickness only. Reference [3] is, in our opinion, the first where theoretically was shown that, in spite of continuous spectrum of vortex sizes, flamelet width growth due to successive entrainement of vortexes with increasing sizes has a natural limit. This paper gave formulas for the thickened flamelet parameters that showed that this width increasing is not dramatical (at real parameters several times in comparison with the laminar flame width), i. e. at large Reynolds numbers we have still a thin flamelets combustion mechanism. Only recently this physical picture: the thickened (but thin) and wrinkled flamelets combustion mechanism has been confirmed by direct

experimental measurements of the flamelets width [11].

We emphasize that even though flamelets combustion mechanism was observed in experiments at relatively low Reynolds already in the 50th's, many people did not agree with the deductions of the paper [3] and they believed that at developed turbulence successive flamelet width increasing has no limit yielding to a combustion mechanism similar to that occurring in well-stirred reactors. It should be particularly emphasized that the latter mechanism is infeasible: increase of turbulence results in thickened and wrinkled flamelets combustion extinction before switching the combustion mechanism (see below).

2. For industrial combustion it is typical that the flamelets velocity is $U_f \ll u'$. This implies that the flame brush width δ_t (or the flamelets sheet dispersion σ^2) increases in accordance with the turbulent diffusion law as the averaged turbulent transport of the boundary between fresh mixture and products due to velocity pulsations (the turbulent diffusion) preponderate over the transport due to flamelets combustion movement. A consequence is that combustion completion in chambers takes place long time before flames with constant brush width (i. e. the flames with 1-D front structure) can be formed. In other words at real mixtures and turbulence the combustion chamber lengths are not enough for forming flames with constant brush width and proper structure and the combustion velocity. This makes possible to do not consider 1-D stationary fronts in practical simulation of flames and therefore simplify the combustion model equations.

3. The turbulent combustion velocity of the flame with increasing width is expressed by the same classical expression as in the case of 1-D stationary front $U_t = U_f\overline{(\delta S/\delta S_0)}$. At large Reynolds numbers U_f is controlled in parallel with combustion kinetics and molecular transport by the equilibrium fine scale Kolmogorov turbulence. The thickened flamelet sheet area S is controlled mainly by small scale turbulence (by contrast to the flamelets sheet dispersion that is controlled by large scale turbulent diffusion and flamelets structure that is controlled by fine scale turbulent transport). We assume in our combustion model the equilibrium small-scale sheet disturbance structure that results in the constant sheet area $\overline{(\delta S/\delta S_0)} = const$, i. e. for assigned mixture properties and turbulent conditions, a constant combustion velocity.

We call these flames with constant U_t and increasing δ_t Intermediate Steady Propagation (ISP) Flames.

4. It is well know from experiments that U_t dependence on chemistry (for example, by the fresh mixture temperature variation) is much weaker than the dependence shown by U_l for laminar combustion. The physical reason of it is the so called hydrodynamical compensation mechanism: an increase of U_f decreases $\overline{(\delta S/\delta S_0)}$ (as it smoothing a flamelet sheet mainly due to suppressing small scale perturbations) and vice versa. So in our example the temperature variations have strong effect on U_f but at the same time moderate effect on U_t and practically do not effect on the flame brush width. Our combustion model contains this mechanism and an analysis on ISP flames gave $\overline{(\delta S/\delta S_0)} \sim (u'/U_f)^{2/3}$ and $U_t \sim \tau_{ch}^{1/4}$ (for laminar flame $U_l \sim \tau_{ch}^{1/2}$), where τ_{ch} is the chemical times.

5. Existence the ISP flames (at $u' >> U_f$) is connected with large difference between two characteristic times at high turbulence combustion: the well known turbulence time $\tau_t = L/u'$ and new specific turbulent-combustion time when turbulent diffusion transport and flamelet combustion transport have the same order $((u'L\tau_*)^{1/2} \sim U_f\tau_*)$

$\tau_* \sim \tau_t(u'/U_f)^2$. Only at $t >> \tau_*$ the flame has a structure of the stationary 1-D turbulent combustion front. At $t < \tau_*$ (more strictly at $\tau_t < t < \tau_*$ we have ISP flame. As for large scale gasturbine combustors characteristic residence times are as a rule less than τ_* combustion takes place in ISP flames. Notice that the process of forming of ISP flames can be significant in spark ignition engines.

6. The nature and the physical mechanisms responsible for turbulent combustion velocities and widths of stationary 1-D turbulent combustion fronts and ISP flames are different. For 1-D stationary flames the turbulent combustion velocity and the velocity of the flame front edge are the same. This front edge is the plane boundary that goes through the most advanced portions of flamelets in fresh mixture, the so called "leading points". In accordance with Zel'dovich's leading point concept [12] the stationary turbulent flame combustion velocity U_t^{st} is controlled by the velocity of propagation of these leading points, that is for $u' >> U_f$ this velocity does not depend on chemistry. This concept is in agreement with the well known Damkohler[1] and Shchelkin[2] results that at strong turbulence $U_t^{st} \sim u'$. At the same time the stationary flame width δ_t^{st} obviously depends on U_f (the greater is U_f, the less is δ_t^{st} and vice versa) as the flame "adapts" its structure for "imposed" turbulent combustion velocity. So in our example increasing (or decreasing) the fresh mixture temperature practically does not change U_t^{st} but decreases (or increases) δ_t^{st}.

For ISP flames instead the leading points velocity does not control the turbulent combustion velocity U_t, this velocity is controlled directly by U_f and the physical processes that form the flamelets sheet. Therefore as we mentioned above U_t depends on turbulence, chemical kinetics and molecular transfer processes.

In conclusion it may be said that premixed combustion models are usually based on using only one turbulent characteristic time τ_t. This assumption leads to this model to reproduce only flames with constant width (i. e. at $t > \tau_t$ they have a structure close to it of 1-D stationary flames). At the same time for these flames the turbulent combustion velocity dependence on chemistry is close to laminar flames. It is unlikely that these model can be used fruitfully for quantitative modelling of industrial combustion at strong turbulence.

The objective of the present work is to describe a physical concept and a modelling equation, in terms of the progress variable, suitable for premixed combustion simulation at $Re >> 1$, $Da >> 1$, and $u' >> U_f$. This close equation is obtained by accounting for concepts of the turbulent combustion flame derived theoretically. Hereinafter it will be called Turbulent Flame Closure (TFC) combustion model equation.

This approach was proposed in fact twenty years ago in [3, 4] but only recently has been elaborated and tested on a certain number of premixed combustion test cases [5-10].

Intermediate Steady Propagation (ISP) Flames

We call ISP flames turbulent combustion fronts with practically constant U_t and flame brush width increasing in time (for 1-D nonstationary problem) or in space (for 2-D or 3-D stationary problem). Here we bring forward arguments and theoretical estimations in favour of actual combustion in such flames in high intensive large scale industrial burners (but not in flames that has the structure like to 1-D stationary flames).

In the case under review combustion takes place in thin (in comparison with the integral turbulent scale) and strongly wrinkled flamelet sheets that separates the reactants from the products and propagates at $\rho = const$ with a speed U_f, Fig. 1. Denote the probabilities of unburned mixture (the reactants), burned mixture (the products) and flamelet compositions in every point of the turbulent flame by P_u, P_b and P_f. For kinematic description we assume that $P_u + P_b = 1$, i.e. $P_f << 1$. We will use $P_b(\vec{x}, t)$ or average temperature $\overline{T}(\vec{x}, t)$ for description of turbulent flames, $\overline{T} = T_u + (T_b - T_u)P_b$, where T_u and T_b are unburned and burned gas temperatures.

1-D case. Propagation of a plane turbulent flame:

Let u', L and $\tau_t = L/u'$ refer to uniform, homogeneous and stationary turbulence in a motionless gas ($\overline{u} = 0$). Assume that at initial time $t = 0$ for $x < 0$ $T = T_b$, i.e. $P_b = 1$ and $P_u = 0$; for $x > 0$, $T = T_u$, i.e. $P_b = 0$ and $P_u = 1$. The plane flame boundary at $t > 0$ becomes wrinkled and its area $F(t)$ grows. Symbolically the turbulent combustion velocity can be written as $U_t(t) = U_f\overline{(F(t)/F(0))}$. If we approximate the PDF of flamelet elements $p(x, t)$ in terms of the Gaussian distribution $p_G(x, t) = (1/\sqrt{2\pi\sigma^2(t)})e^{-(x-a(t))^2/2\sigma^2(t)}$, where $\sigma^2(t) = \overline{(X - a(t))^2}$ is the flamelets dispersion, X is the random coordinate of flamelet element $a(t) = \overline{X}$ is the statistical boundary between unburned and burn gases, so $U_t(t) = da(t)/dt$ and a characteristic width of the combustion flame δ_t is proportional to $\sigma(t) = (\sigma^2(t))^{1/2}$. It furnishes the result, that $P_b(x, t) = (1/\sqrt{2\pi\sigma_f^2(t)}) \int_{\infty}^{x} e^{-(x-a(t))^2/2\sigma_f^2(t)}\, dt = 1 - \Phi((x - a)/\sigma_f)$, $\Phi(X)$ is the probability integral. It follows that $P_b(x, t)$ (and $\overline{T}(x, t)$) obeys to the equation ($D_t(t) = 1/2(d\sigma^2(t)/dt)$):

$$\frac{\partial P_b}{\partial t} = D_t \frac{\partial^2 P_b}{\partial x^2} + U_t(t) \left| \frac{\partial P_b}{\partial x} \right|. \tag{1}$$

At $U_t = 0$ Eq.1 describes a mixing layer evolution and we can assume that $D_t \approx u'L = u'^2\tau_t$

At $u' >> U_f$ for an appreciable length of time $\sigma(t)$ with and without combustion is practically the same and we can estimate this time. Taking the time τ_{st} it takes for forming steady flame width from condition that turbulent diffusion transfer $\sigma(\tau_{st}) = (2D_t\tau_{st})^{1/2}$ and flamelet combustion transfer $U_f\tau_{st}$ are of the the same order. It results $\tau_{st} \sim 2 \sim (u'/U_f)^2$ and we can assume that as $0 < t < \tau_t(u'/U_f)^2$, $\sigma(t)$ with and without combustion is practically the same: in the case $U_f = 0$ we have a motionless ($a = 0$) turbulent mixing layer, whereas in the case $U_f > 0$ we have a moving mixing layer ($da/dt = U_t$) with the same width.

Without combustion the dimensionless flamelet sheet area $\overline{(S(t)/S(0)}$ increases in time very fast (in accordance with known G. K. Batchelor estimation approximately exponentially), but in the case of combustion the flamelets progress suppresses this fast increase. For some time, that we estimate be of order τ_t $\overline{(S(t)/S(0)}$ and U_t increase and after this in the ISP flame there is an equilibrium situation being $\overline{(S(t)/S(0)}$ increased by turbulence and simultaneously decreased by flamelet movement. So at $\tau_t < t < \tau_t(u'/U_f)^2$ (formally more exactly at $0 << t << 2\tau_t(u'/U_f)^2$) we have ISP flames with actual positive $D_t \approx u'L$ in Eq.1 and $\sigma(t) \approx (2D_t t)^{1/2}$, i.e the characteristic flame width $\delta_t(t) \approx (2-4)\sigma(t)$ does not depend directly on combustion. At the same time a practically constant U_t is defined by both the turbulence and the physico-chemical parameters of the mixture.

Turbulent Flame Closure (TFC) Combustion Model

TFC combustion model is in fact an asymptotical model valid at $Re_t >> 1$, $Da >> 1$, and $u' >> U_f$. It is based on the concept of ISP flames and general Kolmogorov methodology: assumptions of existence of equilibrium fine scale turbulence (controlling flamelets structure) and equilibrium small scale structure of the random flamelet sheet. Our fundamental idea is that at high Re_t and Da numbers, the effects of combustion chemistry, molecular transfer processes and other small scale and fast processes can be introduced in the averaged governing equations in terms of physical closures. In the following this idea will be explained in details.

The basic equation of the TFC combustion model:

It is known that at $\rho \neq const$ more fruitful to use the averaged progress variable $\tilde{c} = (\rho_b/\overline{\rho})P_b)$ instead of the probability P_b, where $\overline{\rho} = \rho_u P_u + \rho_b P_b$ is the averaged density (ρ_u and ρ_b is the densities of unburned and burned gas). So the ISP flame equation ($\overline{a}$ and $\tilde{a}$ indicate conventional and Favre averaging):

$$\frac{\partial}{\partial t}(\overline{\rho}\tilde{c}) + \frac{\partial}{\partial x_k}(\overline{\rho}\tilde{u_k}\tilde{c}) = \frac{\partial}{\partial x_k}(\overline{\rho} D_t \frac{\partial \tilde{c}}{\partial x_k}) + (\rho_u U_t)|grad\,\tilde{c}|. \quad (2)$$

In order to discuss the theoretical foundation of Eq. 2, consider it and the equation of continuity for a 1-D case. Changing the coordinate system to one moving with velocity $U_t = const$ and integrating these equations between $x = -\infty$ ($\tilde{c} = 1$) and $x = +\infty$ ($\tilde{c} = 0$) we obtain $\rho_u U_t = \rho_b(U_t + u_b)$, where $u_b = \tilde{u}(x = -\infty)$; i.e. $\rho_u U_t$ represents the mass burning velocity. Replacing $\tilde{c}$ in Eq.2 with P_b violates this results. The application of the gradient form of the source term is connected with the necessity to obtain an invariant form of 3-D equation.

To close Eq.2 we must express U_t as a function of the physico-chemical properties of combustible mixture and turbulence parameters. In the 1-D case U_t is the turbulent combustion velocity $U_t = U_f\overline{(\delta S/\delta S_0)}$, where U_f and $\overline{(\delta S/\delta S_0)}$ are the flamelet velocity and dimensionless flamelet area. These two quantities must be defined accounting for fast chemistry ($\tau_{ch} << \tau_t = L/u'$), micro-turbulence and molecular transfer processes. The approach can be simplified if we assume the equilibrium of fine scale vortices and of small scale wrinkled flamelet sheet, the controlling parameters of the combustion model would be molecular transfer coefficient χ, chemical time $\tau_{ch} = \chi/U_l^2$ and integral turbulent characteristics $u' = \sqrt{\overline{u'^2}}$ and L.

The parameters of thickened flamelet and its area:

In accordance with [3] transfer process inside the thickened flamelet depend on vortices from the 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 turbulent diffusion (δ_f is the flamelet width). U_f and δ_f are function of χ_f and of the characteristic chemical time τ_{ch}, by using dimensional analysis we obtain (notice that for laminar flames it is: $U_l \approx (\chi/\tau_{ch})^{1/2}$, $\delta_l \approx (\chi\tau_{ch})^{1/2}$):

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

The relationships 3 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 [3].

For the model the following inequality must be valid (where η is the Kolmogorov microscale, $\varepsilon \sim u'^3/L$, $Re_t = u'L/\nu >> 1$): $\delta_f >> \eta = \nu^{3/4}\varepsilon^{-3/4} \approx L Re_t^{-3/4}$, whence using expressions (6) we have $U_f^{3/2} >> U_l^{3/2}$, $\delta_f^{3/2} >> \delta_l^{3/2}$, $\chi_f^{3/4} >> \chi^{3/4}$.

For the estimation of $\overline{(\delta S/\delta S_0)} >> 1$ dimensional analysis is not sufficient and it is necessary to use also some general property of random surfaces. Let us consider that the surface of flamelets is $x = h(y, z, t)$. Then,

$$\overline{(\delta S/\delta S_0)} = \overline{(1 + |grad\, h|^2)^{1/2}} \approx \overline{|grad\, h|} \approx \overline{(|grad\, h|^2)^{1/2}} \approx \int k^2 E(k)\, dk \approx \sigma/\lambda, \qquad (4)$$

where $\sigma^2 = \overline{(x - \overline{x})^2} = \int E(k)\, dk = 2D_t t$ is the dispersion and λ is the microscale of the length of the random surface and $E(k)$ is the spectrum of the flamelet surface disturbances. We see, that σ^2 is defined by large scale and $\overline{(\delta S/\delta S_0)}$ by small scale disturbances of the flamelet surface. In ISP flames $E(k)$ has nonstationary increasing small wave number k part and equilibrium (stationary for the constant turbulence) large wave number part.

Microscale λ is a function of L, u', δ_f, U_f and t. 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 3 and using the condition of $\overline{\delta S/\delta S_0)}$ 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 it follows using (7) the expression for the averaged flamelet sheet area

$$\overline{(\delta S/\delta S_0)} \approx (Da)^{3/4} \approx (u'/U_f)^{3/2} \approx (L/\delta_f)^{1/2} >> 1. \qquad (5)$$

Expressions (6) and well known formula for the chemical time $\tau_{ch} = \chi/U_l^2$ give the final result, the formula for the turbulent combustion velocity of the ISP flames:

$$U_t = U_f \overline{(\delta S/\delta S_0)} = Au'(Da)^{1/4} = Au'^{3/4} U_l^{1/2} \chi^{-1/4} L^{1/4}, \qquad (6)$$

where A is an empirical parameters of O(1). (It is worth emphasizing that all powers have been derived from the physical model and the don't contain any quantitative empirical information)

The chemistry dependence of the U_t that is given by (9) ($U_t \sim \tau_{ch}^{-1/4}$) is much weaker than for laminar combustion ($U_l \sim \tau_{ch}^{-1/2}$). The reason is mentioned in the paragraph 2 nonlinear compensation mechanism: increasing of U_f decreasing in accordance with (8) $\overline{(\delta S/\delta S_0)}$ (due to smoothing of the flamelet sheet) and contrary. It is interesting to note that in accordance with (6) and (8) more fast chemistry results smaller U_f and larger $\overline{(\delta S/\delta S_0)}$ of the thickened flamelets. At laminar flamelet combustion mechanism the result obviously would be opposite (larger $U_f = U_l$ and smaller $\overline{(\delta S/\delta S_0)}$. But in both cases the integral effect would be similar.

It should be particularly emphasized that the thickened flamelets have no quasi-laminar structure: in accordance with analysis presented in [3] the temperature pulsations inside the thickened flamelets are high (so the model assumption of same chemical times for thickened and laminar flamelets is strong). The thickened flamelets are in some degree result of small-scale averaging of real instantaneous reaction zone and this concept gives an opportunity to deduce several analytical dependences of the turbulent combustion. From a methodological point of view this situation is similar to Kolmogorov's theory of the fine-scale turbulence: only the assumption that there are no pulsations of the turbulent energy dissipation gives an opportunity to deduce the "5/3" law and other analytical dependences of the fine-scale turbulence at $Re >> 1$.

To validate (9) experimental data at reasonable Re numbers are needed. During the '50s and '60s a considerable body of such experiments for premixed combustion was performed in Russia. Recently, correlation of many experimental data was suggested by Bradley et al in [13]. This correlation can be rewritten for the case of molecular transfer coefficients identical for all species as $U_t \approx u'(Da)^{0.3} Re_t^{-0.15}$.

Comparison of the results given in Table 1 (the Russian papers cited there are referenced in [3]). shows that theoretical and experimental exponents are very similar. It should be particularly emphasized that the correlation by Bradley et al[13] also predicts a negative exponent for the molecular transfer coefficient χ. A lower exponent for u' in comparison with (9), most probably is from having included in the Bradley correlation data with significant flame-stretch that reduce dependence U_t on u'.

For the Eq.2 closure we use the expression (9), i.e. we directly integrate theoretical properties of the ISP flames into the model equation (Turbulent Flame Closure). Empirical parameter A of the combustion model was practically the same $A = 0.5$ for all tested hydrocarbon fuels (CH_4, C_2H_6, C_3H_8) and all conditions (combustion in the bombs, in the high velocity channel flow and in the industrial burner), and only an analysis of H_2 combustion in the bomb results $A \approx 0.6$. In our simulations [5-8] we took into account the stretch effect (to describe bending in the dependence $U_t(u')$ and estimate blow off boundary) the preferential effect (to describe without model tuning combustion of light and heavy fuels). We used as a multiplier in the formula (9) the expression for the probability $P(\varepsilon < \varepsilon_{cr})$ that the instantaneous dissipation $\varepsilon < \varepsilon_{cr}$ in accordance with Bray[14] analysis and modified the excess air coefficient in the formula (9) in accordance with Kuznetsov theoretical result[15] for critical conditions in leading points. Here $\varepsilon_{cr} = 15\nu g_{cr}^2$, g_{cr} is the critical velocity gradient, which can be estimated as $g_{cr} \sim U_l^2/\chi_u$ or using numerous theories.

The field of combustion model application:

As $\overline{\delta S/\delta S_0)} >> 1$ and $U_t \sim u'$, we deduce $U_f << u'$. From this and $\delta_f >> \eta \approx L Re_t^{-3/4}$ inequalities, using expressions (6) it follows (in terms of the Damkohler Da and turbulent Reynolds Re_t numbers):

$$Da^{1/2} >> 1 \ (a) \qquad\qquad 1 >> Da^{3/2} Re_t^{-3/4} \ (b), \tag{7}$$

or (in terms of u'/U_l and L/δ_l):

$$(u'/U_l)^{1/2} << (L/\delta_l)^{1/2} \qquad (i.e.\ u'/U_l <<< L/\delta_l) \tag{8}$$

$$(u'/U_l)^{9/4} >> (L/\delta_l)^{9/4} \qquad (i.e.\ u'/U_l > L/\delta_l), \tag{9}$$

that are the conditions of the existence of a strongly wrinkled and thickened flamelet properly.

On Fig. 2 the straight line A and the curve B correspond to the equations $u'/U_l = L/\delta_l$ and $u'/U_l = (L/\delta_l)^{1/3}$. On line A $Da = 1$ while on the curve B, as it easy to check, $U_f = U_l$, $\delta_f = \eta$; i.e. A and B correspond to the Borghi diagram[16]. The parameters which correspond to Eqs. (10) and (11) are situated between them and considering the character of the inequalities ($<<<$ and $>$), much closer to the curve B. It should be emphasized that the concept of thickened flamelets as a fruitful working hypothesis for theoretical estimations proposed in [3] and analytical expressions for the boundaries of different regimes derived in it was used Borghi at elaborating his diagram. (The paper [16] contains correct citing of the paper [3].) There is an additional extinction boundary, which narrows the area of real combustion. It is connected with flamelets quenching by stretching. This mechanism is absent directly in the model. We assume for the estimation that on the boundary $\varepsilon = \varepsilon_{cr}$ or (at high Re_t) $0.5u'^3/L = 15\nu g_{cr}^2$, where ε_{cr} and g_{cr} are the critical dissipation and velocity gradient quenching flamelets. Hence, the equation for the extinction boundary (the curve C) follows $u'/U_l = Q(L/\delta_l)^{1/3}$, $Q = (30\nu^2 g_{cr}^2/U_l^4)^{1/3}$. As $g_{cr} \sim U_l^2/\chi(\chi \approx \nu)$ it follows $Q \sim 3$. It is easy to show that on the curve C $U_f/U_l = \delta_f/\delta_l = Q^{3/2} \sim 5$. As at the curve B $U_f/U_l = \delta_f/\delta_l = 1$ we have between A and B $1 < U_f/U_l \approx \delta_f/\delta_l < 5$. The curve D (that correspond to $Re_t = 100$) is the limitation $Re_t >> 1$. There is also analyzed above the restriction $\tau_t < t < \tau_t(u'/U_f)^2 \approx \tau_t Da$.

TFC model and the countergradient transport in flames

The countergradient transport of the progress variable $\tilde{c}$ in many turbulent premixed flames at flamelets combustion mechanism is well-known and puzzling phenomena [19-21].

The countergradient or gradient transport in one-dimensional premixed turbulent combustion flames depends on identical or opposite in sign are the transport $\overline{\rho u''c''}$ and gradient $\partial\tilde{c}/\partial x$ terms in the equation

$$\frac{\partial}{\partial t}(\overline{\rho}\tilde{s}) + \frac{\partial}{\partial x}(\overline{\rho}\tilde{u}\tilde{s}) = -\frac{\partial}{\partial x}(\overline{\rho u''c''}) + \overline{\rho}\widetilde{W}. \tag{10}$$

It the case of the countergradient transport $\overline{\rho u''c''}$ and the space derivative of the progress variable $\partial\tilde{c}/\partial x$ have the same sign. If we assume this transport as "the turbulent diffusion flux" (this term sometimes is used loosely in the literature) the corresponding effective "turbulent diffusion coefficient" would be negative $D_{ef} = -\overline{\rho u''c''}/(\overline{\rho}\partial\tilde{c}/\partial x) < 0$. It means in fact that the "turbulent flux" of combustion products takes place in the direction from fresh mixture to burn gas and at the same time "turbulent diffusion flux" of unburned mixture takes place in direction from combustion products to fresh mixture.

If we compare exact unclosed Eq. 10 with the TFC model equation at 1-D case we would see in TFC combustion model the transport term contains only the physical gradient turbulent diffusion part of the transport $\overline{\rho u''c''}$ that controls the flame brush width of ISP flames and another part of this term (that usually has the countergradient character) is in fact included in the model source term $\rho_u U_t|\partial\tilde{c}/\partial x|$ (it is necessary to stress that in accordance with previous analysis increasing of the flame brush width is not in contradiction with the countergradient character of the transport term $\overline{\rho u''c''}$).

$$\rho_u U_t \left| \frac{\partial \tilde{c}}{\partial x} \right| = \overline{\rho}\widetilde{W} - \frac{\partial}{\partial x}\left(\overline{\rho u''c''} + D_t \frac{\partial \tilde{c}}{\partial x}\right) \tag{11}$$

So the TFC model is intended for description of gasdynamical parameters and for the progress variable and connected with it species concentrations, temperature, probabilities of the fresh mixture and products of the bimodal mechanism, but it gives only models (not physical) source term. To extract real physical source term it would be necessary to invoke some hydrodynamical model of the countergradient transport, that is strongly connected with nonuniform pressure distribution.

If we compare the kinematical and unclosed equation for 1-D stationary flame:

$$\frac{d}{dx}(\overline{\rho}\tilde{u}\tilde{c}) = \rho_u U_t^{st} \left| \frac{d\tilde{c}}{dx} \right|, \quad \frac{d}{dx}(\overline{\rho}\tilde{u}\tilde{c}) = -\frac{d}{dx}(\overline{\rho u''c''}) + \overline{\rho}\widetilde{W}. \tag{12}$$

we would see that the model source term is controlled by the real source term and the transport term. As combustion reduces the pressure across the flame, i. e. the conditional averaged velocities of burned gas $\overline{u}_b$ are higher than they of the unburn mixture $\overline{u}_u$ the transport term $-\overline{\rho u''c''} = \overline{\rho}(\overline{u}_u - \overline{u}_b)\tilde{c}(1-\tilde{c})$ gives the countergradient flux and as it easy to show the real source term in Eq.12 is shifted to the forward part of flame in comparison with the model source. Some results of numerical simulations of the counter gradient transport and comparisons of the modelled and "physical" source term can be found in [22].

Conclusions

We analyzed turbulent combustion at large Re and Da numbers. This case is the most difficult for rigorous modelling at statistical approaches including PDF methods. Combustion chemistry control here not only the source terms of the equations, that are intended for real combustion description, but other terms as well. (Wide spread statement that PDF equations contain chemistry in the closed form is valid in fact only at $Re >> 1$ and $Da << 1$. Only in this case molecular dissipative terms practically does not depend on chemistry.)

At the same time this case presents with a new possibility connected with applying and developing Kolmogorov principle of existence of equilibrium hydrodynamical structures at large Re and Da numbers.

The main results of this analysis are:

1. At $\tau_t < t < \tau_t Da$ combustion takes place in the intermediate steady propagation (ISP) flames, i.e. in the flames with increasing width, that is defined mainly by turbulent diffusion;

2. The process of widening and acceleration of flamelets due to the entrainement in the combustion zone of more and more large vortexes has a natural limit in spite of the fact that at large Reynolds number turbulence contains continuous spectrum of vortexes sizes. The equilibrium flamelets thickness and combustion velocity (formulas (3)) corresponds to the condition, that in a coordinate system where the flamelet is fixed, the heat fluxes

in the front because of heat conduction and convection, and heat liberation because of combustion have the same order of magnitude.

3. Increasing of turbulence does not transform thickened and strongly wrinkled flamelet combustion mechanism into a distributed flame mechanism because, in accordance with theoretical estimations, combustion extinction takes place long before forming the volume combustion mechanism.

4. The flamelet combustion velocity influences the flamelet sheet area. The theoretical formula (5) for this phenomenon explains quantitatively the relatively low influence of chemical kinetics on the turbulent combustion velocity.

5. The theoretical formula for the turbulent combustion velocity of ISP flames (6) contains only one empirical parameter A ($A = 0.5$ for CH_4, C_2H_6, C_3H_8 and H_2 for air excess $\alpha = 0.6 - 1.6$; $A = 0.6 - 0.7$ for H_2 at $\alpha = 0.17 - 0.2$ and $\alpha = 2.5 - 2.7$ [7]).

6. Well known countergradient transport phenomenon at premixed combustion is not in contradiction with the concept of ISP flames with increasing flame brush width.

Acknowledgment

The author thanks Prof. K. Bray who looked through the draft and made several significant remarks and Dr. F. Biagioli, eng. M. Barbato and Dr. A. N. Lipatnikov for many useful discussions. The role of the last in bringing life and development of this model is difficult to overestimate. Among another things he found the weak point of the model namely the absence of the flamelet stretch mechanism and proposed to use the Bray model[14]. He also proposed an original idea to account for the effect of real Le numbers in the model.

The financial contribution of Sardinian Regional Government is gratefully acknowledged.

References

[1]. Damkohler, G., *NACA Tech. Memo.* 1112 (1947).

[2]. Shchelkin, K.I., *NACA Tech. Memo.* 1110 (1947).

[3]. Zimont, V.L., *Combust. Expl. and Shock Waves* 15: 305-311, (1979).

[4]. Zimont, V.L., In: *Combustion of heterogeneous and gas systems*, USSR Academy of Science, Chernogolovka, 1977, pp 76-80 (in Russian).

[5]. Zimont, V.L., and Lipatnikov, A.N. *Proceedings of the Academy of Sciences (Doklady Physical Chemistry)*, New York, 1994, pp 440- 443.

[6]. Karpov, V.P., Lipatnikov, A.N. and Zimont V.L., *Archivum Combustionis* 4(3-4): 125-141 (1994).

[7]. Zimont, V.L., and Lipatnikov, A.N., *Chem. Phys. Reports* 14(7): 993-1025 (1995).

[8]. Karpov, V. P., Lipatnikov, A. N., and Zimont V. L., *Twenty-Sixth Symposium (Int.) on Combustion,* The Combustion Institute, Pittsburg, PA, 1996, p 249.

[9]. Maciocco, L., and Zimont, V. L., In: *20-th Annual Meeting of the Italian Section of the Combustion Institute "Frantic '97"*, 1997, pp X-2.1 - 2.4.

[10]. Zimont, V., Polifke, W., Bettelini, M., and Weisenstein, W., *Journal of Engineering for Gas Turbines and Power (Transactions of the ASME)* 120: 526-532 (1998).

[11]. Chen, Y., and Mansour, M.S., *Twenty-Seventh Symposium (Int.) on Combustion,* The Combustion Institute, Pittsburg, PA, 1998.

[12]. Zel'dovich, Ya.B., Barenblatt, G.I., Librovich, V.B., and Makhviladze, G.M., *The Mathematical Theory of Combustion and Explosions*, Plenum Publishing Corporation, New York, 1985.
[13]. Bradley, D., Lau, A. K. C., and Lawes, M.: Phil. Trans. Royal Soc. London A 338, pp. 359-387, 1994.
[14]. Bray, K.N.C., (1987), In: *Complex chemical reaction systems, Mathematical Modelling and Simulation*, Springer Verlag, Heidelberg, 1987, p356.
[15]. Kuznetsov, V.R., and Sabel'nikov, V.A., *Turbulence and Combustion*, Hemisphere Publishing Corporation, New York, 1990.
[16]. Borghi, *R. Recent Advances in Aerospace Sciences*, Pergamon, 1985, pp 117-138.
[17]. Whol, K., and Shor, I., *Ind. Eng. Chem* 47: 828-834 (1955).
[18]. Khramtsov, V.A.(1959), *Seventh Symposium (Int.) on Combustion,* The Combustion Institute, Pittsburg, PA, 1959, pp 609-614.
[19]. Bray, K. N. C., Libby, P. A., Masuya, G., and Moss, J. B., *Combust. Sci. Technol.* 25:127-140 (1981).
[20]. Pope, S. B., *Twenty-Third Symposium (International) on Combustion*, The Combustion Institute, Pittsburg, pp. 1207-1214 (1994).
[21]. Li, S. C., Libby, P. A., Williams, F. A., *Twenty-Fifth Symposium (International) on Combustion*, The Combustion Institute, Pittsburg, pp. 591- 612 (1990).
[22]. Zimont, V. L., Biagioli, F., Syed, K., *Journal of Computer Application and Technology*, special issue *Computational Reactive Flow Dynamics: Modelling, Software, Tools and applications* (accepted for publication).

TABLE I
The influence of different parameters (exponents) on combustion velocity ($U_t \sim$).

Our theoretical result (6)	$\sim (u')^{0.75}$	$\sim L^{0.25}$	$\sim \chi^{-0.25}$	$\sim T^{0.5\star)}$	$\sim p^{(0.10\div 0.15)\star\star)}$
Correlation of Bradley et al [13]	$\sim (u')^{0.55}$	$\sim (L)^{0.15}$	$\sim \chi^{-0.15}$		
Other empirical Data	$\sim (u')^{0.7\div 0.8}$ Several Russian works	$\sim L^{0.18}$ Talantov 1969	$\sim L^{0.3}$ Whol, Shor 1955 [17]	$\sim T_u^{0.4}$ Doroshenko 1956	$\sim p^{0.12}$ Hramtsov 1959 [18]

$\star$) For $u_n \sim T_u^2$, $\chi \sim T_u^2$; $\star\star$) For $\chi \sim p^{-1}$, $u_n \sim p^{-(0.2\div 0.3)}$ (propane).

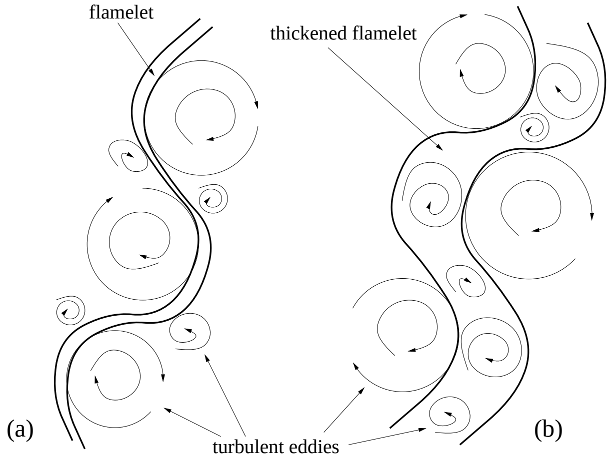

Figure 1: Pictorial representation of wrinkled (a) and thickened-wrinkled (b) flamelets.

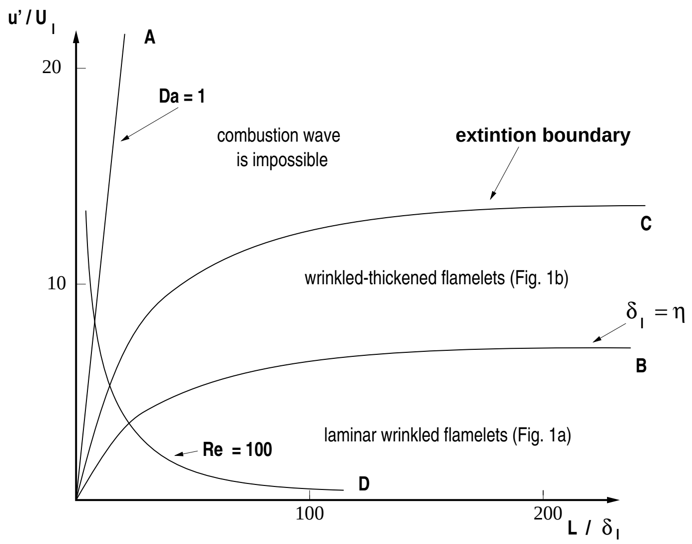

Figure 2: Diagram (region) of validity for the TFC premixed combustion model.