Algebraic Models for Turbulent Transports in Flames : Applications to Stagnating and 2D Premixed Flames

Vincent Robin, Arnaud Mura, Michel Champion
Institut Pprime - UPR 3346 - CNRS - ENSMA - Université de Poitiers
86961 Futuroscope, France

1 Introduction

For several decades many works have been devoted to the modeling of premixed turbulent combustion, leading to different analyses whose main objective is the evaluation of the mean chemical rate $\overline{\omega}_c$ appearing as a source term in the average transport equation for the progress variable c:

$$\frac{\partial \overline{\rho}\widetilde{c}}{\partial t} + \boldsymbol{\nabla} \cdot \overline{\rho}\widetilde{\boldsymbol{u}}\widetilde{c} = \boldsymbol{\nabla} \cdot \left(\overline{\boldsymbol{F_c}} - \overline{\rho \boldsymbol{u}'' c''} \right) + \overline{\omega}_c, \tag{1}$$

where ρ, $\boldsymbol{u}$ and $\boldsymbol{F_c}$ are respectively the density, the flow velocity and the diffusion flux of c. The Favre decomposition is used here because of the strong density variations that exist in this kind of reactive flows.

However, fewer works devoted to turbulent combustion modeling have focused on the closure of turbulent transport terms appearing in equation (1), i.e. $\overline{\rho \boldsymbol{u}'' c''}$ as well as those appearing in the following mean momentum equation, i.e. $\overline{\rho \boldsymbol{u}'' \boldsymbol{u}''}$:

$$\frac{\partial \overline{\rho}\widetilde{\boldsymbol{u}}}{\partial t} + \boldsymbol{\nabla} \cdot \overline{\rho}\widetilde{\boldsymbol{u}}\widetilde{\boldsymbol{u}} = \boldsymbol{\nabla} \cdot \left(\overline{\boldsymbol{T}}_{\boldsymbol{u}} - \overline{\rho \boldsymbol{u}'' \boldsymbol{u}''} \right) - \boldsymbol{\nabla} \overline{p}, \tag{2}$$

where $\boldsymbol{T_u}$ and p denote respectively the viscous stress tensor and the pressure. Nevertheless, thermal expansion and related density changes have a strong effect on these turbulent transport terms, as shown in the pionnering work of Bray et al. [1]. Still today, in many models of turbulent combustion, turbulent transports in reactive flows are considered identical or at least similar to those observed in non reactive flows. Doing so, classical turbulent models like k-ϵ or R_{ij}-ϵ are used in association with gradient laws to model the scalar turbulent transports. Here we call k the turbulent kinetic energy, R_{ij} the Reynolds stresses ($i, j \in [1, 3]$) and ϵ the dissipation of k. The same conclusion applies to Large Eddy Simulation where subgrid scale transport relies in most modeling strategies on the turbulent viscosity and turbulent diffusivity concept, an assumption that does not take into account the influence of unresolved thermal expansion phenomena [2]. However, it is now well established that turbulent transports in reactive flows can be non gradient or counter-gradient and that combustion generates turbulence, see for example [3]. Accordingly, the usual transport equations based on representations of turbulent transports similar to those used for non reactive flows, are no longer valid and must be adapted to take thermal expansion into account.

Correspondence to: vincent.robin@ensma.fr

In the present study a description of the velocity field as made of two contributions is conjectured [4, 5] and is used as a theoretical basis to investigate the interaction effects between turbulence and premixed flames. This analysis is then used to propose detailed and general closure expressions of the terms representing turbulent transport, i.e., scalar flux $\overline{\rho \boldsymbol{u}'' c''}$ and Reynolds stresses components $\overline{\rho \boldsymbol{u}'' \boldsymbol{u}''}$. The corresponding set of algebraic closures, easier to handle than second order equations, has been successfully validated thanks to DNS data [4, 5] and provides an interesting alternative to incorporate the counter-gradient turbulent diffusion and flame generated turbulence phenomena in numerical simulations of practical configurations. These closures are validated through their applications to two different premixed flame geometries, i.e. (i) a flame stabilized in a turbulent stagnating flow and (ii) a turbulent flame stabilized by the sudden expansion of a 2D channel [6]. Numerical results are satisfactorily compared with the corresponding experimental data.

2 Splitting of the velocity field

We consider here the flamelet regime of turbulent combustion, see for instance [7, 8], where a turbulent flame, whose propagating velocity and thickness are denoted respectively S_T and δ_T, is thought as a collection of local reactive interfaces that retain their identifiable laminar flame structure, i.e., the laminar propagating velocity S_L and the laminar flame thickness δ_L [7]. Moreover, using the progress variable c, and considering a low Mach number description of the flow, leads to the well known equation of state $\rho_r = \rho(\ 1 + \tau c\ )$, where $\tau = \rho_r/\rho_p - 1$ is the expansion factor, ρ_r and ρ_p denote the density of fresh reactants and combustion products respectively. Then, according to the continuity equation, the total increase of velocity associated with thermal expansion through this turbulent flame is τS_T and results from (i) the heat release that takes place through the local laminar flame, namely τS_L, which is called here the *direct thermal expansion effect*, and from (ii) the turbulent motion that increases the flame surface and can be associated with an *indirect thermal expansion effect* [5]. Accordingly, we consider that these two contributions of the thermal expansion can be treated separately in the velocity field so that the total velocity vector $\boldsymbol{u}$ is split as follows [4, 5]:

$$\boldsymbol{u} = \boldsymbol{v} + \boldsymbol{w}, \tag{3}$$

where $\boldsymbol{w}$ is the velocity field resulting from the acceleration induced by a local flame front (*direct effect*) and $\boldsymbol{v}$ represents the turbulent motion and its consequences on the flame surface (*indirect effect*). In Eq.(3) the contribution $\boldsymbol{w}$ is subjected to the constraint that its norm corresponds to the acceleration that takes place through a local laminar flame. Thus, we have $\parallel \boldsymbol{w} \parallel = \tau S_L c$. By introducing now the unit vector $\boldsymbol{m}$ that characterizes the orientation of the acceleration field induced by thermal expansion through the local laminar flames, we obtain the following definition for $\boldsymbol{w}$:

$$\boldsymbol{w} = \boldsymbol{m} \parallel \boldsymbol{w} \parallel = \boldsymbol{m} \tau S_L c. \tag{4}$$

The norm $\parallel \boldsymbol{w} \parallel$ grows only through a local flame and is constant elsewhere whereas the unit vector $\boldsymbol{m}$ is affected by both the flame surface orientation and turbulent motion.

Superimposing the two velocity fields as proposed by Eq.(3) leads to the following form of the momentum equation:

$$\frac{\partial \rho \boldsymbol{v}}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u} \boldsymbol{v}) + \frac{\partial \rho \boldsymbol{w}}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u} \boldsymbol{w}) = \boldsymbol{\nabla} \cdot \boldsymbol{T_v} + \boldsymbol{\nabla} \cdot \boldsymbol{T_w} - \boldsymbol{\nabla} p. \tag{5}$$

In this equation $\boldsymbol{T_a}$ is defined as: $\boldsymbol{T_a} = \rho\nu \left(\boldsymbol{\nabla a} + (\boldsymbol{\nabla a})^T \right) - \frac{2}{3} \rho\nu \boldsymbol{I}\ \boldsymbol{\nabla} \cdot \boldsymbol{a}$, where $\boldsymbol{I}$ is the identity tensor. A set of two similar transport equations can now be introduced for each velocity contribution $\boldsymbol{v}$

and $\boldsymbol{w}$:

$$\frac{\partial \rho \boldsymbol{v}}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}\boldsymbol{v}) = \boldsymbol{\nabla} \cdot \boldsymbol{T_v} - \boldsymbol{\nabla} p_{\boldsymbol{v}}, \tag{6}$$

$$\frac{\partial \rho \boldsymbol{w}}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}\boldsymbol{w}) = \boldsymbol{\nabla} \cdot \boldsymbol{T_w} - \boldsymbol{\nabla} p_{\boldsymbol{w}}, \tag{7}$$

where $\boldsymbol{\nabla} p_{\boldsymbol{v}}$ and $\boldsymbol{\nabla} p_{\boldsymbol{w}}$ are the pressure gradient contributions introduced to characterize the velocity fields $\boldsymbol{v}$ and $\boldsymbol{w}$. Consistency with the momentum equation (5) yields the following relationship between the two pressure gradients: $\boldsymbol{\nabla} p = \boldsymbol{\nabla} p_{\boldsymbol{v}} + \boldsymbol{\nabla} p_{\boldsymbol{w}}$. Within the present framework the contribution $\boldsymbol{\nabla} p_{\boldsymbol{v}}$ is thought as the part of the pressure gradient induced by the turbulent motion and its *indirect thermal expansion effect* on the flame surface, though the contribution $\boldsymbol{\nabla} p_{\boldsymbol{w}}$ is associated with the local heat release and corresponds to the local flamelet crossing effect or *direct effect* [4, 5].

Averaging or filtering processes can now be applied to the new momentum equation (6) and are eventually used to write a transport equation for the turbulent kinetic energy, $\overline{\rho k}_{\boldsymbol{v}} = \frac{1}{2}\overline{\rho \boldsymbol{v}'' \cdot \boldsymbol{v}''}$:

$$\frac{\partial}{\partial t}\left(\overline{\rho k}_{\boldsymbol{v}}\right) + \boldsymbol{\nabla} \cdot \left(\widetilde{\boldsymbol{u}}\overline{\rho k}_{\boldsymbol{v}}\right) = \tfrac{1}{2}\left(\overline{D_{\boldsymbol{v}}} + \overline{P_{\boldsymbol{v}}} - \overline{\rho\epsilon_{\boldsymbol{v}}} + \overline{H_{\boldsymbol{v}}}\right), \tag{8}$$

where $\overline{D_{\boldsymbol{v}}}$, $\overline{P_{\boldsymbol{v}}}$, $\overline{\rho\epsilon_{\boldsymbol{v}}}$, and $\overline{H_{\boldsymbol{v}}}$ are diffusion, production, dissipation and pressure terms. More details concerning these terms can be found in [4, 5].

The interesting point in this new transport equation is that pressure terms as well as dissipation terms do not explicitely depend on the local heat release (*direct effect*) but depend only on the turbulent motion and its *indirect thermal expansion effect*. Put in other words the turbulent phenomena described by these terms (related to the $\boldsymbol{v}$-velocity) are similar to those observed in non-reactive flows. Then, the use of classical closures, developed for non-reactive flows, to model in reactive flows the corresponding pressure and dissipation terms is indeed more relevant to describe the $\boldsymbol{v}$-velocity field, as provided by Eq.(8), than the $\boldsymbol{u}$-velocity field. Consequently, these closures lead to the introduction of a new turbulent viscosity $\nu_T = c_\mu \overline{\rho k}_{\boldsymbol{v}}^{\,2} / \overline{\rho\epsilon}_{\boldsymbol{v}}$ that is independent of the thermal expansion through the local flame (*direct effect*) and is much closer to the turbulent viscosity concept originally proposed for non-reactive and incompressible flows.

3 Algebraic closures for turbulent reactive flows

Relation (3) leads also to the following expression for the scalar turbulent fluxes [4]:

$$\overline{\rho \boldsymbol{u}'' c''} = \overline{\rho \boldsymbol{v}'' c''} + \overline{\rho \boldsymbol{w}'' c''}, \tag{9}$$

where the terms of the right hand side are respectively contributions related to (i) turbulence and (ii) thermal expansion through local flames (*direct effect*). The first contribution must take into account the turbulent mixing and the *indirect thermal expansion effect* that may lead to counter gradient diffusion [5]. Nevertheless, for the sake of simplicity, we choose here to close the first contribution, i.e. related to turbulence, by using a classical gradient law: $\overline{\rho \boldsymbol{v}'' c''} = -\overline{\rho}(\nu_T/\sigma_T)\boldsymbol{\nabla}\widetilde{c}$, where σ_T is a turbulent Schmidt number and ν_T the turbulent viscosity introduced in previous section. The main difference between the present closure and the classical one that relates $\overline{\rho \boldsymbol{u}'' c''}$ to a turbulent viscosity approximation, is that the turbulent viscosity in the proposed gradient law describes the $\boldsymbol{v}$ velocity field induced by turbulence instead of the total $\boldsymbol{u}$ velocity field that includes local or *direct thermal expansion effect*.

The second contribution of Eq.(9) is obtained by using Eq.(4) and by neglecting the cross correlations between c and $\boldsymbol{m}$:

$$\overline{\rho \boldsymbol{w}'' c''} = \tau S_L \widetilde{\boldsymbol{m}} \overline{\rho c''^2}. \tag{10}$$

Equation (3) also leads to the following expression for the turbulent kinetic energy:

$$\overline{\rho k} = \overline{\rho k}_{\boldsymbol{v}} + \overline{\rho k}_{\boldsymbol{w}} + 2\overline{\rho k}_{\boldsymbol{vw}}, \tag{11}$$

where we can identify contributions related to (i) turbulence ($\overline{\rho k}_{\boldsymbol{v}}$), (ii) local heat release ($\overline{\rho k}_{\boldsymbol{w}} = \frac{1}{2}\overline{\rho \boldsymbol{w}'' \cdot \boldsymbol{w}''}$), and (iii) heat release-turbulence interactions ($\overline{\rho k}_{\boldsymbol{vw}} = \frac{1}{2}\overline{\rho \boldsymbol{v}'' \cdot \boldsymbol{w}''}$). As a first approximation, we choose to neglect the cross correlations $\overline{\rho k}_{\boldsymbol{vw}}$. The contribution due to thermal expansion through local flames $\overline{\rho k}_{\boldsymbol{w}}$ is obtained by using Eq.(4) and by neglecting the cross correlations between c and $\boldsymbol{m}$:

$$\overline{\rho k}_{\boldsymbol{w}} = \tfrac{1}{2}(\tau S_L)^2 \left[\overline{\rho c''^2} + \overline{\rho}\widetilde{c}^2(1 - \widetilde{\boldsymbol{m}} \cdot \widetilde{\boldsymbol{m}})\right]. \tag{12}$$

The only remaining unknown quantity in the above description is the mean unit vector $\widetilde{\boldsymbol{m}}$ which is aproximated by the following expression: $\widetilde{\boldsymbol{m}} = \lambda \boldsymbol{m}_{\widetilde{c}}$, where $\lambda = \| \widetilde{\boldsymbol{m}} \|$ is a scalar parameter that characterizes the fluctuations of orientation. In absence of fluctuations $\lambda = 1$ and if $\boldsymbol{m}$ fluctuates isotropicaly in all space directions λ vanishes ($\| \widetilde{\boldsymbol{m}} \| = 0$). For the sake of conciseness, the algebraic closure for λ is not detailed here and can be found in [5]. The unit vector $\boldsymbol{m}_{\widetilde{c}}$ which gives the orientation of the mean scalar flux can be estimated from $\boldsymbol{\nabla}\widetilde{c}/\|\boldsymbol{\nabla}\widetilde{c}\|$.

Eventually, the strategy proposed here consists in solving the mean scalar and mean momentum equations, Eqs.(1-2), associated with a classical non reactive k-ϵ model but related to the $\boldsymbol{v}$-velocity field instead of the $\boldsymbol{u}$-velocity field. Then, the only additional transport equations used are those for $\overline{\rho k}_{\boldsymbol{v}}$ and $\overline{\rho \epsilon}_{\boldsymbol{v}}$. Classical non reactive models are used to close these additional transport equations.

The scalar turbulent fluxes in Eq.(1) are closed according to relations (9-10), which leads to:

$$\overline{\rho \boldsymbol{u}'' c''} = -\overline{\rho}\frac{\nu_T}{\sigma_T}\boldsymbol{\nabla}\widetilde{c} + \tau S_L \lambda \overline{\rho c''^2}\boldsymbol{m}_{\widetilde{c}}. \tag{13}$$

The Reynolds stresses in Eq.(2) are closed in a usual way as:

$$\overline{\rho \boldsymbol{u}'' \boldsymbol{u}''} = -\rho\nu_T\left(\boldsymbol{\nabla}\widetilde{\boldsymbol{u}} + (\boldsymbol{\nabla}\widetilde{\boldsymbol{u}})^T\right) + \tfrac{2}{3}\boldsymbol{I}\left(\rho\nu_T\, \boldsymbol{\nabla}\cdot\widetilde{\boldsymbol{u}} + \overline{\rho k}\right), \tag{14}$$

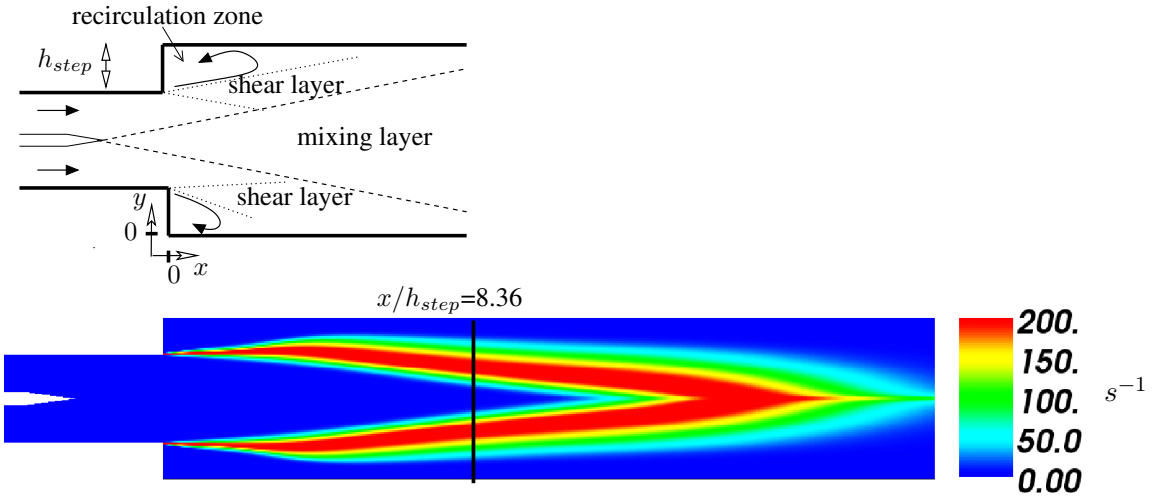

Figure 1: Mean flow structure in the ORACLES test rig (top) and mean chemical term $\overline{\omega}_c/\overline{\rho}$ obtained by numerical simulation (bottom)

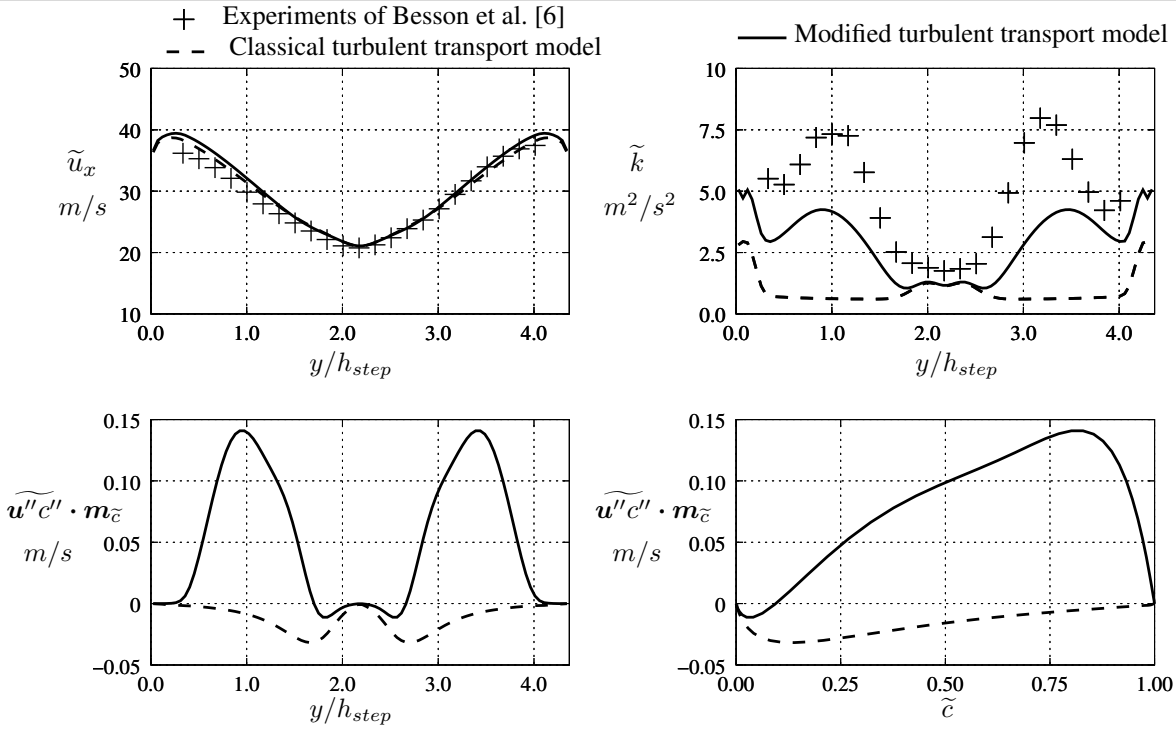

Figure 2: Profiles of mean velocity (top left), turbulent kinetic energy (top right), and scalar turbulent flux (bottom left) versus the tranverse direction in the combustion chamber at x/h_{step}=8.36. Profile of scalar turbulent flux is also presented versus the mean progress variable (bottom right).

where the turbulent kinetic energy $\overline{\rho k}$ is obtained from Eqs.(11-12) by using the following algebraic closure:

$$\overline{\rho k} = \overline{\rho k}_{\boldsymbol{v}} + \tfrac{1}{2}(\tau S_L)^2 \left[\overline{\rho c''^2} + \overline{\rho}\widetilde{c}^2(1-\lambda^2)\right]. \tag{15}$$

Finally, we chose to express the mean chemical rate in Eq.(1) by using the model proposed in a recent work of Bray et al. [9]: $\overline{\omega}_c = \overline{\rho}\widetilde{c}(1-\widetilde{c})(1-S)I_\omega/(I_1-I_2)$, where $S = \overline{\rho c''^2}/(\overline{\rho}\widetilde{c}(1-\widetilde{c}))$ is the segregation factor and I_ω, I_1, I_2 are integral quantities that can be calculated from flamelets properties.

4 Application to a flame stabilized by the sudden expansion of a 2-D channel

In this abstract, we focus on the simulation of 2D turbulent flame stabilized by backward facing steps (ORACLES experiment ; Besson et al. [6]). In this experiment two superimposed fully developped turbulent channel flows of fully premixed reactants of propane and air are exposed to a sudden expansion, see Fig.(1). In the case investigated here the equivalence ratio of the mixture in both channels is set to 0.8. The algebraic model described in the previous sections has been incorporated in the CFD code developed by EDF, *Code_Saturne*. The mesh retained for the numerical simulations is made of 50000 hexahedral cells. The inlet boundary conditions applied to the computational domain have been optimized thanks to preliminary calculations, see Robin et al. [10]. The field of the mean chemical rate obtained from simulation is presented in Fig.(1).

Two numerical simulations were performed, (i) one that uses the new model for the turbulent transport terms described in the previous sections and (ii) another one that relies on classical models for these turbulent transport terms, i.e. gradient law and $k-\epsilon$ model. A very good agreement between calculations

and experimental data is obtained for the mean velocity fields using both types of closure, see Fig.(2). However, only the use of the new model for the turbulent transport terms provides (i) an increase of turbulent kinetic energy of the same order of magnitude as the experimental one, although a slight underestimation of the maximum is observed and (ii) a reversal of the sign of the turbulent scalar flux so that it becomes counter gradient almost everywhere in the flame brush. As expected, only a small area in front of the flame brush (fresh gas side) is found to be of the same sign as the gradient law. This gradient-like diffusion zone is required for the flame brush to be stabilized. Moreover, it is remarkable that the use of such an algebraic model provide better results than those obtained previously with the most recent second order closures [11].

The algebraic model for the turbulent transport terms proposed here is simple to incorporate in CFD codes and gives rise to a very good behavior when compared to experiments. In view of the discrepancies still observed in Fig.(2) of the present work, concerning the profile of turbulent kinetic energy, it must be recalled that in the calculations reported here the *indirect thermal expansion effects* have not been taken into account yet. Addition of this contribution is the purpose of ongoing work.

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