A Second-Order Model for Turbulent Reactive Flows with Variable Equivalence Ratio

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1 A four-Dirac delta functions presumed PDF model

The numerical modeling of turbulent reactive flows in partially premixed situations needs at least two scalar variables to describe the local thermochemistry. Here, we use the LW-P model of partially premixed combustion already described by Robin et al. [1] and based on the simplified thermochemistry introduced by Libby and Williams [2]. The scalar variables of this model are the mixture fraction ξ and the fuel mass fraction Y. Closed mean balance equations for the first and second order moments of Y and ξ i.e. $\widetilde{\xi}$, $\widetilde{\xi''^2}$, $\widetilde{Y}$, $\widetilde{Y''^2}$, $\widetilde{\xi''Y''}$ are derived and these five quantities are used inter alia to determine the 12 parameters of the four-Dirac presumed PDF: α_p, ξ_p, Y_p $(p = 1, 4)$. The quantities (ξ_p, Y_p) are the positions of the Dirac delta peaks in the composition space and α_p their respective magnitudes. This model has been already successfully used by Robin et al [1] with a k-ϵ model to represent turbulent transports. However, such a model cannot predict flame generated turbulence and counter-gradient turbulent diffusion. In order to take these phenomena into account a second-order LW-P model involving equations for scalar turbulent transports and Reynolds stresses is now proposed. This new model, applicable to flows with variable stoichiometry, is based on a development of the analysis made by Domingo and Bray [3] for the pressure terms.

Balance equations for the turbulent scalar fluxes $\overline{\rho u_i''\xi''}$ and $\overline{\rho u_i''Y''}$ $(i = 1, 3)$ are closed by using a mass-weighted joint PDF of u_i, ξ and Y: Eq.(1). As density is constant at each Dirac delta peak position, we can write: $\widetilde{P}(u_i|Y_p, \xi_p) = P(u_i|Y_p, \xi_p)$. Accordingly the mean conditional velocities are given by Eq. (2).

$$\widetilde{P}(u_i, Y, \xi) = \sum_{p=1}^{4} \alpha_p \widetilde{P}(u_i|Y_p, \xi_p)\delta(\xi - \xi_p)\,\delta(Y - Y_p) \qquad (1) \qquad\qquad \overline{u_{ip}} = \int u_i P(u_i|Y_p, \xi_p) du_i \qquad (2)$$

It can be shown that these conditional velocities depend only on the turbulent scalar fluxes $\overline{\rho u_i''\xi''}$ and $\overline{\rho u_i''Y''}$ and on the mean velocities $\widetilde{u}_i$. The PDF defined by Eq. (1) is also used to close the different scalar equations for mean quantities and turbulent fluxes.

2 Closure of scalar transport equations

The set of partial differential equations to be solved is given by Eqs.(3)-(7). Equation (3) for the first moment of the passive scalar does not require further attention since no unclosed correlation appears. Equation (4) for the second order moment of the passive scalar exhibits only two unknown terms. These

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terms are the turbulent flux of variance $\overline{\rho u_k'' \xi''^2}$ and the scalar dissipation $\overline{\rho \epsilon_\xi}$.

$$\frac{\partial}{\partial t}\left(\overline{\rho}\widetilde{\xi}\right) + \frac{\partial}{\partial x_k}\left(\overline{\rho}\widetilde{u}_k\widetilde{\xi}\right) = \frac{\partial}{\partial x_k}\left(\overline{\rho D \frac{\partial \xi}{\partial x_k}} - \overline{\rho u_k'' \xi''}\right) \tag{3}$$

$$\frac{\partial}{\partial t}\left(\overline{\rho \xi''^2}\right) + \frac{\partial}{\partial x_k}\left(\widetilde{u}_k \overline{\rho \xi''^2}\right) = \frac{\partial}{\partial x_k}\left(\overline{\rho D \frac{\partial \xi''^2}{\partial x_k}} - \overline{\rho u_k'' \xi''^2}\right) - 2\overline{\rho D \frac{\partial \xi''}{\partial x_k}\frac{\partial \xi''}{\partial x_k}} - 2\overline{\rho u_k'' \xi''}\frac{\partial \widetilde{\xi}}{\partial x_k} \tag{4}$$

$$\frac{\partial}{\partial t}\left(\overline{\rho}\widetilde{Y}\right) + \frac{\partial}{\partial x_k}\left(\overline{\rho}\widetilde{u}_k\widetilde{Y}\right) = \frac{\partial}{\partial x_k}\left(\overline{\rho D \frac{\partial Y}{\partial x_k}} - \overline{\rho u_k'' Y''}\right) + \overline{\omega} \tag{5}$$

$$\frac{\partial}{\partial t}\left(\overline{\rho}\widetilde{Y''^2}\right) + \frac{\partial}{\partial x_k}\left(\overline{\rho}\widetilde{u}_k\widetilde{Y''^2}\right) = \frac{\partial}{\partial x_k}\left(\overline{\rho D \frac{\partial Y''^2}{\partial x_k}} - \overline{\rho u_k'' Y''^2}\right) - 2\overline{\rho D \frac{\partial Y''}{\partial x_k}\frac{\partial Y''}{\partial x_k}} - 2\overline{\rho u_k'' Y''}\frac{\partial \widetilde{Y}}{\partial x_k} + 2\overline{Y''\omega} \tag{6}$$

$$\begin{aligned}\frac{\partial}{\partial t}\left(\overline{\rho Y''\xi''}\right) + \frac{\partial}{\partial x_k}\left(\widetilde{u}_k\overline{\rho Y''\xi''}\right) &= \frac{\partial}{\partial x_k}\left(\overline{\rho D \frac{\partial Y''\xi''}{\partial x_k}} - \overline{\rho u_k'' Y''\xi''}\right) - 2\overline{\rho D \frac{\partial Y''}{\partial x_k}\frac{\partial \xi''}{\partial x_k}} \\ &\quad - \overline{\rho u_k'' Y''}\frac{\partial \widetilde{\xi}}{\partial x_k} - \overline{\rho u_k'' \xi''}\frac{\partial \widetilde{Y}}{\partial x_k} + \overline{\xi''\omega}\end{aligned} \tag{7}$$

The first one is obtained through Eq.(8), and the second is closed by using a linear relaxation model for the fluctuation decay rate, Eq.(9). Similar terms appear in Eq.(6) for the reactive scalar and in Eq.(7) for the cross-correlation. The turbulent fluxes $\overline{\rho u_k'' Y''^2}$ and $\overline{\rho u_k'' Y''\xi''}$ are closed using the PDF as for the term $\overline{\rho u_k'' \xi''^2}$.

$$\overline{\rho u_i'' \xi''^2} = \overline{\rho}\sum_{p=1}^{4}\alpha_p\left(\xi_p - \widetilde{\xi}\right)^2\left(\overline{u}_{ip} - \widetilde{u}_i\right) \tag{8}$$

$$\overline{\rho\epsilon_\xi} = \overline{\rho D \frac{\partial \xi''}{\partial x_k}\frac{\partial \xi''}{\partial x_k}} = \frac{\overline{\rho \xi''^2}}{R_\xi \tau_T} \tag{9}$$

Closures for the dissipation terms $\overline{\rho\epsilon_Y} = \overline{\rho D \frac{\partial Y''}{\partial x_k}\frac{\partial Y''}{\partial x_k}}$ and $\overline{\rho\epsilon_{\xi Y}} = \overline{\rho D \frac{\partial Y''}{\partial x_k}\frac{\partial \xi''}{\partial x_k}}$ are the most critical points because these terms together with the chemical contribution drive the evolution of the PDF shape in the composition space. Here, these dissipation functions are closed using the recent proposal of Mura et al. [4].

Additional terms related to the chemical reaction, i.e. $\overline{\omega}$, $\overline{Y''\omega}$ and $\overline{\xi''\omega}$ appear in this last three equations. These terms are closed by using the PDF and assuming a single step global chemistry with an instantaneous rate of fuel consumption written as follows:

$$\omega = \rho\Omega = \rho(\xi, Y)B(\xi)\left(Y - Y_{min}(\xi)\right)\exp\left(-T_a/T(\xi, Y)\right) \tag{10}$$

where T_a is the activation temperature, B the pre-exponential factor and Y_{min} the minimum value of Y.

3 Closure of turbulent flux transport equations

Six additional transport equations for the turbulent passive and reactive scalar fluxes $\overline{\rho u_i'' \xi''}$ and $\overline{\rho u_i'' Y''}$ are necessary to obtain a full second-order closure. Attention is focused on the transport equations for the turbulent reactive scalar fluxes $\overline{\rho u_i'' Y''}$ (11). Equations for $\overline{\rho u_i'' \xi''}$ are similar but without the chemical terms ψ_i^Y.

$$\frac{\partial}{\partial t}\left(\overline{\rho u_i'' Y''}\right) + \frac{\partial}{\partial x_k}\left(\widetilde{u}_k\overline{\rho u_i'' Y''}\right) = D_i^Y + P_i^Y - \overline{\rho\epsilon_i^Y} + H_i^Y + \psi_i^Y \tag{11}$$

$$D_i^Y = -\frac{\partial}{\partial x_k}\left(\overline{\rho u_k'' u_i'' Y''} - \overline{u_i''\rho D\frac{\partial Y''}{\partial x_k}} - \overline{Y''\tau_{ik}}\right) \qquad P_i^Y = -\overline{\rho u_k'' u_i''}\frac{\partial \widetilde{Y}}{\partial x_k} - \overline{\rho u_k'' Y''}\frac{\partial \widetilde{u}_i}{\partial x_k}$$

$$\overline{\rho\epsilon_i^Y} = \overline{\tau_{ik}\frac{\partial Y''}{\partial x_k}} + \overline{\rho D\frac{\partial Y''}{\partial x_k}\frac{\partial u_i''}{\partial x_k}} \qquad H_i^Y = -\overline{Y''\frac{\partial P}{\partial x_i}} \qquad \psi_i^Y = \overline{u_i''\omega}$$

If we except the terms P_i^Y, all terms of the RHS of Eq (11) must be closed. First, the diffusion terms D_i^Y are modeled with the classical generalized diffusion approximation, Eq.(12). Using the PDF defined by Eq. (1) chemical terms ψ_i^Y are closed by Eq.(13).

$$D_i^Y = \frac{\partial}{\partial x_k}\left(C_Y \frac{k}{\epsilon}\overline{\rho u_k'' u_j''}\frac{\partial}{\partial x_j}\left(\frac{\overline{\rho u_i'' Y''}}{\overline{\rho}}\right)\right) \qquad (12)$$

$$\psi_i^Y = \overline{\rho}\sum_{p=1}^{4}\alpha_p \Omega_p\left(\overline{u}_{ip} - \widetilde{u}_i\right) \qquad (13)$$

Now, considering that $\tau_{ik} \approx \rho\nu\frac{\partial u_i}{\partial x_k}$, a Lewis number equal to unity and high Reynolds number, we can rewrite the dissipation terms $\overline{\rho\epsilon_i^Y}$, Eq.(14). For a perfectly premixed system, we consider that $\partial u_i/\partial Y$ is constant accross the local flamelets. This leads to $\partial u_i/\partial Y = \overline{\rho u_i'' Y''}/\overline{\rho Y''^2}$. In a first approximation, this assumption is assumed to be valid for a partially premixed system, so that dissipation terms are closed by Eq.(15).

$$\overline{\rho\epsilon_i^Y} = 2\overline{\rho D\frac{\partial Y}{\partial x_k}\frac{\partial u_i}{\partial x_k}} = 2\overline{\rho D\frac{\partial Y}{\partial x_k}\frac{\partial Y}{\partial x_k}\frac{\partial u_i}{\partial Y}} \qquad (14)$$

$$\overline{\rho\epsilon_i^Y} = 2\overline{\rho\epsilon^Y}\frac{\overline{\rho u_i'' Y''}}{\overline{\rho Y''^2}} \qquad (15)$$

The last term that requires special attention is H_i^Y. This term is known to be responsible for the counter gradient diffusion effects. The corresponding term in the R_{ij} equations i.e. $\overline{u_j''\frac{\partial P}{\partial x_i}}$ induces the flame generated turbulence phenomena. To close this term, the gradients of mean conditional pressures are introduced [3] so that H_i^Y can be expressed as:

$$\overline{Y''\frac{\partial P}{\partial x_i}} = \widetilde{TY''\frac{\partial P}{\partial x_i}}/\widetilde{T} \;=\; \sum_{p=1}^{4}\alpha_p\frac{T_p}{\widetilde{T}}(Y_p - \widetilde{Y})\frac{\partial\overline{P}_p}{\partial x_i} \qquad (16)$$

$$\text{and}\quad \overline{u_j''\frac{\partial P}{\partial x_i}} \;=\; \sum_{p=1}^{4}\alpha_p\frac{T_p}{\widetilde{T}}(\overline{u}_{jp} - \widetilde{u}_j)\frac{\partial\overline{P}_p}{\partial x_i} + \sum_{p=1}^{4}\alpha_p\frac{T_p}{\widetilde{T}}\left(-\overline{u_{jp}'\frac{\partial P_p'}{\partial x_i}}\right) \qquad (17)$$

Where p characterizes the conditional value at each Dirac delta peak.
The gradient of mean conditional pressures are split into two different parts: a non-reactive contribution and a reactive contribution:

$$\frac{\partial\overline{P_p}}{\partial x_i} = \left[\frac{\partial\overline{P_p}}{\partial x_i}\right]_{NR} + \left[\frac{\partial\overline{P_p}}{\partial x_i}\right]_{R} \qquad (18)$$

The non-reactive part is modeled by introducing the simplified conditional mean equation of motion already proposed by Domingo and Bray [3], Eq.(19). The reactive part is modeled by introducing a premixed planar laminar flame relationship, Eq.(20).

$$\left[\frac{\partial\overline{P}_p}{\partial x_i}\right]_{NR} = \rho_p\frac{\partial\overline{u}_{ip}}{\partial t} + \rho_p\overline{u}_{jp}\frac{\partial\overline{u}_{ip}}{\partial x_j} \qquad (19)$$

$$\left[\frac{\partial\overline{P}_p}{\partial x_i}\right]_{R} = -\omega_p\left(\frac{\partial u_i}{\partial Y}\right)_p \qquad (20)$$

The velocity gradient that appears in Eq.(20) is assumed to be constant across the local flame but conditioned by the mixture fraction and can be again evaluated thanks to the PDF.

4 Results

The second-order model described in the previous section is applied to the calculation of a turbulent reactive flow of propane and air stabilized by a plane sudden expansion of a 2-D channel [5]. The reaction zone is fed by two streams of mixtures of different equivalence ratio (Fig.1). This experimental configuration exhibits a large scale coherent motion that cannot be handled by using the steady RANS approach. Numerical results are then compared to experimental data corresponding to the highest Reynolds number for which the energy of the large scale motion is the weakest.

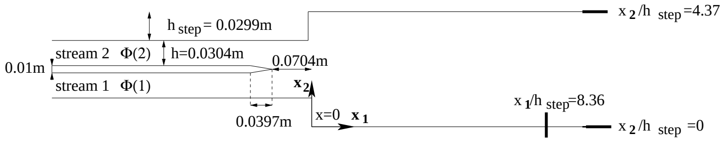

Figure 1: Experimental configuration

Two calculations are performed: the first uses the first-order model described by Robin et al. [1] and the second uses the full second-order model described here. As an example of result Fig.(2) compares experimental and numerical profiles of turbulent kinetic energy in the combustion chamber at $x_1/h_{step} = 8.36$. This result shows the ability of the second-order LW-P model to represent the flame generated turbulence phenomena whereas the first-order model does not take this effect into account.

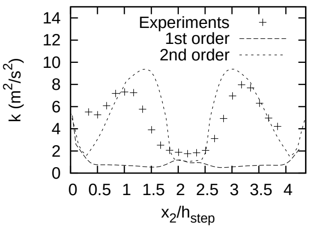

Figure 2: Turbulent kinetic energy at $x_1/h_{step} = 8.36$

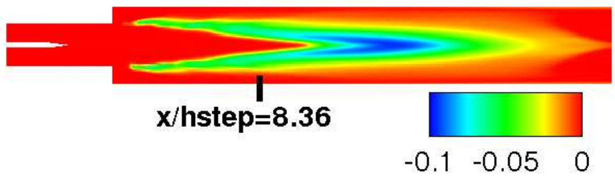

Figure 3: Turbulent fluxes $\overline{\rho u_1'' Y''}/\overline{\rho}$ (m/s)

Figure (3) provides the numerical field of the turbulent flux $\overline{\rho u_1'' Y''}/\overline{\rho}$ for the fully premixed situation using the second-order model. As shown by the figure the turbulent flux $\overline{\rho u_1'' Y''}/\overline{\rho}$ is found to be negative in the flame brush, contrary to the sign deduced from the gradient assumption $-\partial\widetilde{Y}/\partial x_1$. This result highlights the counter-gradient diffusion phenomena and confirms that gradient hypothesis used in RANS first-order models are not valid in the present case. Other simulations have been carried out in the more generalized case of partially premixed flows as those studied in reference [1].

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