

A flame surface density model including tabulated chemistry and heat losses

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Introduction

Reducing pollutant emissions is a very important and practical challenge in combustion applications. As numerical simulations are now widely used to design and optimise actual burners, pollutant levels should be predicted by models. Unfortunately, hydrocarbon combustion involves hundreds of species and thousands of chemical reaction that cannot be handled in simulations of industrial devices. Accordingly, adapted “low-cost” models, incorporating chemistry features, should be devised. Industrial furnaces are also devoted to heat a charge (glass, cement, iron,...) and the combustion cannot be considered as adiabatic, an assumption generally retained to develop combustion models.

Our objective is to propose a combustion model in the Reynolds averaged Navier-Stokes equations (RANS) framework, to predict the mean flow characteristics, including heat losses and chemistry features. This model combines a flame surface density balance equation to describe turbulence / combustion interactions (the so-called Coherent Flame Model, CFM) and a tabulated chemistry through the Flame Prolongation of ILDM (FPI) approach. In the FPI database, the reaction rates of chemical species are tabulated as a function of a progress variable, a mixture fraction and an enthalpy to incorporate mixing inhomogeneities and heat losses. Such databases have already been coupled to presumed probability density function approach [1; 2]. In the present work, we have implemented CFM balance equation FPI routines in the FLUENT solver. Preliminary results are successfully compared to experimental data obtained in a simplified lean partially premixed combustion chamber.

Turbulent combustion model

The turbulent combustion model proposed here combines the Coherent Flame Model (CFM), where the flame surface density is estimated by solving a balance equation and a tabulated chemistry generated in the FPI framework. The main elements of the model are briefly summarized in the following.

- The **Coherent Flame model (CFM)**, firstly proposed by Marble and Broadwell [3] for non-premixed flames, is a flamelet model based on the flame surface density concept [4; 5]. The turbulent flame is viewed as a collection of flame elements behaving as laminar flame. The mean reaction rate per unit volume of a species k , $\bar{\omega}_k$ is written as the product of the flame surface density (i.e. the available flame surface per unit volume), Σ , and the mean reaction rate per unit surface, $\langle \dot{\Omega}_k \rangle_s$:

$$\bar{\omega}_k = \langle \dot{\Omega}_k \rangle_s \Sigma \quad (1)$$

Chemistry features are incorporated into the mean reaction rate per unit surface $\langle \dot{\Omega} \rangle_s$ assuming to be the reaction rate of a laminar flame in the same condition and extracted from the chemical database. The interaction between the flame front and turbulent motions is described by the flame surface density Σ determined by solving a balance equation. An exact but unclosed balance equation may be derived [4] and various closure schemes are discussed in [5] and [6]. A simple version is:

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial \tilde{u}_i \Sigma}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\nu_t}{\sigma_\Sigma} \frac{\partial \Sigma}{\partial x_i} \right) + \alpha_0 \frac{\varepsilon}{k} \Sigma - \beta_0 S_L^0 \frac{\Sigma^2}{\tilde{c}(1 - \tilde{c})} \quad (2)$$

where k is the turbulent kinetic energy, and ε its dissipation rate. ν_t denotes the turbulent viscosity and σ_Σ a turbulent Schmidt number. S_L^0 is the laminar flame speed, α_0 and β_0 are two model parameters and \tilde{c} the mean progress variable ($\tilde{c} = 0$ in fresh gases and $\tilde{c} = 1$ in burnt gases). The three right-hand side terms in Eq. (2) correspond respectively to the turbulent transport of the flame surface density, the increase of flame surface area due to the strain rate induced by turbulent flow motions and the destruction of flame surface by consumption of the intervening reactants.

- The **tabulated chemistry** provides the mean reaction rate per unit surface $\langle \dot{\omega} \rangle_s$ and the laminar flame speed S_L^0 . Under the flamelet assumption, the flame is locally identified to a laminar flame element. Following the approach developed by Gicquel *et al.* [7] and Fiorina *et al.* [8], the chemical database is generated from laminar premixed flames computations using the CHEMKIN package [9] and the Qin *et al.* [10] propane / air mechanism including 70 species and 463 elementary chemical reactions, for various values of the mixture fraction and the total enthalpy. The local reaction rate per unit of flame area of species k is then extracted as:

$$\dot{\Omega}_k(z, h_t) = \int_{-\infty}^{+\infty} \dot{\omega}_k dn \quad (3)$$

where n denotes the coordinate along the normal direction to the flame front. Relation (1) requires that the mean reaction rate per unit flame area should take into account the possible variations of the mixture fraction and the enthalpy along the flame surface. Here we assumed that the mean reaction rate per unit flame area is the one of the laminar flame corresponding to $z = \tilde{z}$ and $h_t = \tilde{h}_t$:

$$\langle \dot{\Omega}_k \rangle_s \approx \dot{\Omega}_k(\tilde{z}, \tilde{h}_t) \quad (4)$$

The chemical database is then addressed as a function of two variables: the mixture fraction z and the total enthalpy h_t .

This model is supplemented with usual balance equations for the mean mixture fraction \tilde{z} , the mean total enthalpy \tilde{h}_t including heat losses and the mean mass fractions of the chemical species \tilde{Y}_k . In the following, we only consider the mass fraction $Y_c = Y_{CO} + Y_{CO_2}$ which has been found suitable to define a progress variable [7]. The mean progress variable is estimated as:

$$\tilde{c} = \frac{\tilde{Y}_c - Y_c^0(\tilde{h}_t)}{Y_c^e(\tilde{z}, \tilde{h}_t) - Y_c^0(\tilde{h}_t)} \quad (5)$$

where $Y_c^0(\tilde{h}_t)$ corresponds to the initial mass fraction of Y_c and $Y_c^e(\tilde{z}, \tilde{h}_t)$ the equilibrium value of Y_c for the given total enthalpy \tilde{h}_t . The mean reaction rate per unit flame surface of Y_c and the laminar flame speed S_L^0 are relied on as:

$$\langle \dot{\Omega}_c \rangle_s = \rho_0 S_L^0(\tilde{z}, \tilde{h}_t) \left(Y_c^e(\tilde{z}, \tilde{h}_t) - Y_c^0(\tilde{h}_t) \right) \quad (6)$$

and are extracted from the FPI chemical database.

Simulation

The model described in the previous section has been implemented in the FLUENT solver [11] through user defined functions (UDF). In the experimental configuration retained to validate the simulation [12], two parallel turbulent premixed propane / air flows, having different equivalent ratios $\phi_1 = 0.85$ and $\phi_2 = 0.65$ are injected into the combustion chamber where a flame is stabilized by two backward-facing steps (see Fig. 1). Uniformed mesh with 19600 cells is used, a typical calculation requires two hours on PC Athlon of 1.8 GHz. Inlet velocity profiles are specified in the numerical simulations according to experimental data [13]. As a first step, no heat losses are taken into account in the present simulations. Unfortunately, no data are available about the chemical reaction (mass fractions, temperature) and only a qualitative agreement can be evidenced from direct flame visualization (Fig. 2a) and the mean temperature field extracted from the simulation (Fig. 2b). The model is able to reproduce both the flame location and the flame shape. Fig 3 compares experimental and numerical transverse profiles of the mean axial velocity for two downstream locations expressed in terms of the height h of the backward facing step ($h = 0.0299$ m). The agreement is found to be very satisfactory. The model will be validated in the future work to predict heat losses and non-premixed turbulent combustion. Numerical simulations of an industrial furnace will then be performed.

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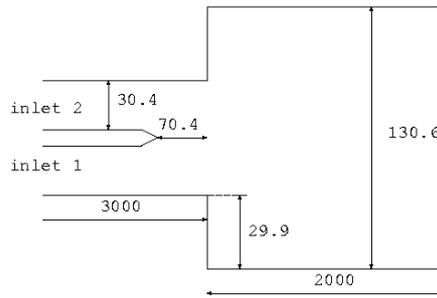


Fig 1: Experimental configuration (dimensions are in millimeters)

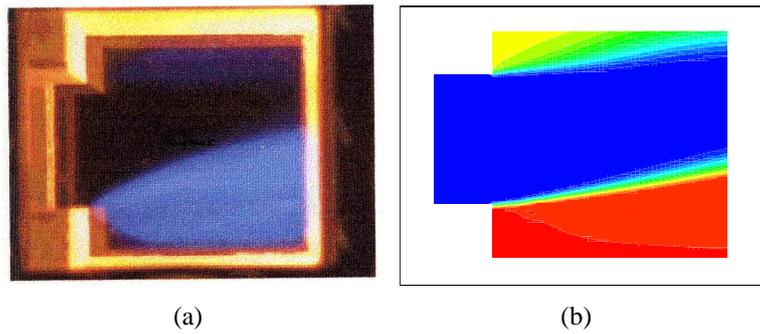


Fig 2: (a) Direct visualization of the flame front, (b) Numerical mean temperature field

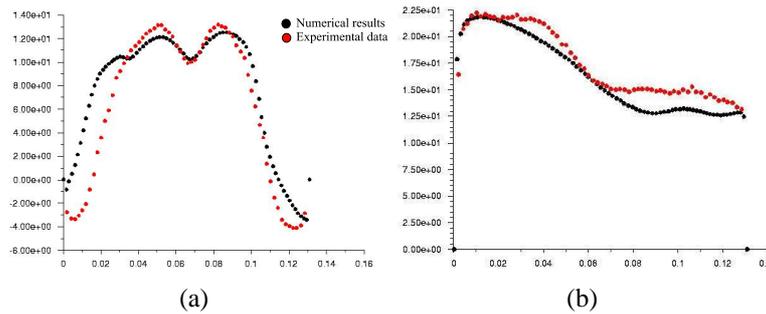


Fig 3: Transverse profiles of the mean axial velocity for two downstream locations: (a) 1 h; (b) 7 h

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