



A chemical time scale approach for FPI modeling

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Abstract

In most reactive CFD codes, the set of resolved governing equations is not compatible with the original formulation of the “Flame Prolongation of ILDM” (so-called FPI) tabulation technique. In the absence of an explicit continuity equation, the total mass conservation may be expressed implicitly, through the transport of each species. The corresponding reaction rates are then to be evaluated in the FPI database. With this procedure, any chemical source term perturbation often results in very poor predictions of the flame inner structure. In the present work, we propose a chemical-time based formulation aimed at correcting the table interpolated species reaction rates. The very good agreement obtained by this modified approach on an elementary 1D premixed laminar flame bench-mark validates the effective improvement of the FPI model. *To cite this article: J. Savre et al., C. R. Mecanique 336 (2008).*

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Résumé

Une approche à temps caractéristiques chimiques pour le modèle FPI. Au sein de la plupart des codes de simulation numérique, capables de décrire des écoulements réactifs à cinétique complexe, les équations résolues ne sont pas compatibles avec la formulation originale de la méthode de tabulation FPI. Ces équations imposent en effet que la totalité de la masse soit conservée via le transport des fractions massiques de chaque espèce pour lesquelles les taux de réaction doivent être évalués dans la base de données FPI. En procédant ainsi, toute perturbation des termes sources chimiques se traduit par une mauvaise représentation de la structure interne des flammes. Nous proposons ici une formulation corrigeant les taux de réaction des espèces interpolés dans la table, et qui améliore notablement l'utilisation de ce modèle dans les codes de simulation. Les bons résultats obtenus sur le cas élémentaire d'une flamme laminaire de prémélange monodimensionnelle tendent à valider l'efficacité de cette nouvelle approche.

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1. Introduction

Present reactive CFD codes are able to simulate quite complex industrial reacting flows, including intricate geometries and multiphysical phenomena. However, precise pollutant emission prediction still remains a particularly challenging issue. Its numerical solution may require a complete description of the detailed chemical phenomena, that may involve hundreds of intermediate radicals (e.g. for hydrocarbons). Mainly due to the high number of dependent variables, the large scale disparity (in both time and space) and strong and coupled non-linearities (arising e.g. from fluid mechanics and/or chemical kinetics), industrial simulations of those complex flows with detailed chemical mechanisms are still out of reach, even with nowadays extremely powerful computers.

Within this context, the use of *automatic* reduction methods is very attractive. They allow the construction of tables that can be coupled in a modular way to the CFD software. Using this strategy may result in a dramatic decrease of the overall CPU cost. This kind of approach was first considered in the early 1990s with the development of the “Intrinsic Low Dimensional Manifolds” method or ILDM [1], a method for identifying invariant manifolds of the slow dynamics of a simple kinetic system — originally a homogeneous chemical reactor. The analysis of the Jacobian matrix eigenvalues enables the identification of the n_f fast varying species that may be considered as being in a quasi steady state, while the n_s “slow” others define the attracting manifold. The manifold is finally stored in a computational database. The ILDM strategy has shown to be able to reproduce academic flame behaviors such as planar laminar premixed flames [2]. However, a major issue of this modeling concerns the relevance of the manifold in the low temperature region where the system eigenvalues are all of the same order of magnitude. This yields ambiguous identification of slow and fast chemical time scales. The manifold is usually extended to this domain as proposed by Maas and Pope [1] by using linear interpolations. However, this approach seems not completely satisfactory, since the species may have non-linear behaviors in this domain. The FPI tabulation technique of Gicquel et al. [4], or the equivalent FGM model, [3], were proposed to provide a physical prolongation of the ILDM method in the domain of low temperatures. In this model, the structure of a 1D unstretched laminar premixed flame is used to build the subspace, where all the species mass fractions and the chemical source terms are mapped according to a unique progress variable c . The latter must evolve monotonically along the flame, so that each value of c corresponds to only one particular set of tabulated scalars. This recent model seems to be very promising for industrial reacting flows simulations. Tabulated chemistry models are currently used in research codes, but the constraints imposed by industrial solvers are quite different. In the present work, we propose a methodology that seems to be able to overcome most of the difficulties appearing when trying to use FPI within this framework. It must be noticed here that a slightly different method, developed within a similar context, was recently proposed in [13].

The systems of governing equations effectively solved by the CFD code and to create the database are first described in Section 2. Section 3 introduces the discrepancies arising when using FPI in combination with an industrial CFD solver and the suggested corrections. The proposed corrective strategy efficiency is assessed in Section 4 on an elementary but very discriminating test case, namely a 1D methane/air laminar premixed flame. Some concluding remarks are finally given in Section 5.

2. Governing equations

Here, we simply give the set of governing equations solved in order to construct the tables and then the conservation equations implemented in the CFD software. For a mixture of N_{sp} gaseous species, tables are pre-processed by using a standard code for 1D premixed flames with complex chemistry and detailed transport as, e.g., PREMIX [5]. The solved balance equations correspond to the steady, quasi-isobaric (i.e. small Mach number approximation) 1D multi-component reactive Navier–Stokes equations, which solution yields a laminar unstretched premixed flame:

$$\dot{m} \frac{dY_i}{dx} + \frac{d}{dx}(\rho Y_i V_i) - \rho \dot{\omega}_i = 0 \quad (1)$$

$$\rho u - \dot{m} = 0 \quad (2)$$

$$\dot{m} \frac{dT}{dx} - \frac{1}{c_p} \frac{d}{dx} \left(\lambda \frac{dT}{dx} \right) + \frac{1}{c_p} \sum_{i=1}^{N_{sp}} \rho Y_i V_i c_{p,i} \frac{dT}{dx} + \frac{1}{c_p} \sum_{i=1}^{N_{sp}} \rho \dot{\omega}_i h_i = 0 \quad (3)$$

where \dot{m} is the mass flow rate, ρ the density, u the velocity, $c_{p,i}$ and c_p denote respectively the i th-species and mean specific heats at constant pressure, λ is the mean thermal conductivity, Y_i are the species mass fractions, V_i the diffusion velocities, h_i the species enthalpies, and T the temperature. The chemical source terms, $\dot{\omega}_i$, are evaluated using Arrhenius laws with detailed chemical mechanisms [6]. Finally, the system is closed by a gas state law as well as relations for the transport fluxes and thermodynamic properties.

The model assumes that the solutions of this system may be lumped into a unique table, as a function of the progress variable c . When considering hydrocarbon combustion, an appropriate definition of the progress variable is: $c = (Y_{\text{CO}_2} + Y_{\text{CO}})/(Y_{\text{CO}_2}^{\text{eq}} + Y_{\text{CO}}^{\text{eq}})$. With this construction, from a given local value of c , it is possible to extract (in a unique way) the corresponding values of $Y_i(c)$ and $\dot{\omega}_i(c)$ from the database.

In order to test our proposed corrective strategy (see Sections 3 and 4) we made use of a CFD industrial code, namely CEDRE, the ONERA solver for aerothermochemistry problems [7]. This code is able to solve the complete multidimensional and multi-component reactive NS system, using a cell-centered finite-volume approach. Those equations can be written as:

$$\frac{\partial \rho Y_i}{\partial t} + \frac{\partial \rho u_j Y_i}{\partial x_j} + \frac{\partial \rho Y_i V_{i,j}}{\partial x_j} - \rho \dot{\omega}_i = 0 \quad (4)$$

$$\frac{\partial \rho u_k}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_k u_j) + \frac{\partial p}{\partial x_k} + \frac{\partial \tau_{kj}}{\partial x_j} = 0 \quad (5)$$

$$\frac{\partial \rho e_t}{\partial t} + \frac{\partial}{\partial x_k} [(\rho e_t + p)u_k] + \frac{\partial}{\partial x_j} (\tau_{kj}u_k) + \frac{\partial q_k}{\partial x_k} = 0 \quad (6)$$

where $V_{i,j}$ is the j th component of the diffusion velocity of species i , τ_{kj} is the viscous tensor, defined by $\sigma_{kj} = -p\delta_{kj} + \tau_{kj}$ (σ_{kj} being the Cauchy stress tensor), e_t the total energy, and q_k the heat flux. Again, these equations are closed by a gas state law and relations for transport and thermodynamic properties. Solving for the density equation is not needed here as it can be recovered by summing up all the species balance equations written under conservative forms (4).

3. Discrepancies, proposed corrections

The FPI model is a tabulated chemistry reduction model based on premixed flame calculations. Evolutions of species mass fractions and reaction rates as well as temperature and density across planar laminar premixed flames are collected in a database according to a unique progress variable c . This approach was extended to non-premixed combustion and non-adiabatic flames through the addition of extra parameters — for instance the mixture fraction z and the total enthalpy h [8]. We are here interested in difficulties arising in the simple test case of a planar laminar premixed flame. Only the perfectly premixed case — characterized by a unique progress variable c — will be discussed here. In the original version of FPI [4], only a balance equation for the progress variable — and for some possible extra parameters — are solved along with the momentum and the density equations. The temperature and the species mass fractions are then deduced from the FPI database. The system of governing equations solved is then quite different from system (4)–(6).

When continuity equation is not explicitly included in the solved system, conservation of total mass is a consequence of species conservations. However, in order to decrease computational effort, industrial CFD codes do not wish to solve for the full set of species involved in the detailed reaction mechanism used to build the table. Only a reduced number of chemical species are to be transported. We impose that the choice of the transported species is such that almost all of the entire mass, typically more than 99%, be represented in the transported species. For instance, for a methane/air combustion, the chosen species will be CH_4 , O_2 , N_2 , H_2O , CO_2 and CO . It hence becomes necessary to consider some more species, as relation $\sum_{i=1}^{N_{sp}} \dot{\omega}_i = 0$ is no more exactly verified. The chemical reaction rates of those additional species are no longer evaluated in the FPI table, but are reconstructed to ensure atom conservation — only one species is added per element. Furthermore, the additional species should be chosen so that the global heat release rate is not much affected. When non-adiabatic flames are considered, it may be necessary to modify the procedure in order to enforce energy conservation. This procedure to ensure total mass conservation is equivalent to the one proposed by Galpin et al. [13].

Further difficulties may arise since the coupling between FPI and the CFD code is only made through the progress variable c and the (extracted) chemical reaction rates. Any perturbation to the chemical source terms may induce

irreversible deviations of the mass fractions from their “ideal” trajectories $Y_i^{\text{tab}}(c)$. This may finally bring very poor species profiles across the flame (see Fig. 2 in Section 4). These perturbations may stem from several contributions. As pointed out by De Goey and Ten Thije Boonkkamp [9], from the set of NS equations, a new conservation system (7), (8), cast into a quasi 1D form, and written in a referential linked to the flame iso-surfaces, can be derived:

$$F_i = \dot{m}_b Y_i - \rho D_i \frac{\partial Y_i}{\partial n} \quad (7)$$

$$\frac{\partial F_i}{\partial n} - \rho \dot{\omega}_i(c) = -\rho K Y_i + \kappa F_i + Q_i \quad (8)$$

where \dot{m}_b is a mass burning rate, D_i are the mean species diffusion coefficients, n denotes the arc-length normal to the flame surface; K and κ denote respectively the stretch rate and the curvature of the flame surface. If the chemical reaction rates are assumed to depend on a single progress variable c (as for the FPI model), then the additional term Q_i must be considered. The first two terms on the right-hand side of Eq. (8) respectively account for stretching and curvature effects. Transport phenomena along flame surfaces due to the fact that Y_i and c iso-surfaces do not generally coincide — the flame iso-surfaces propagation speeds are not correctly predicted — are expressed by the extra term Q_i (see [3] for details). In a planar steady laminar flame calculation, the first two terms (stretching and curvature) are usually negligible but the contribution of the last one may be significant and lead to discrepancies between computed and tabulated flame inner structures. Those terms can be viewed as an external modification of the reaction rates.

We shall now present a simple strategy to correct these perturbations. The idea consists in relaxing the perturbed mass fractions toward the ideal trajectory. By linearizing the reaction rates around a reference state, denoted by the 0 superscript, one can write $\dot{\omega}(Y) \simeq \dot{\omega}(Y^0) + \mathbf{J}(Y - Y^0)$. The Jacobian matrix \mathbf{J} (with $J_{ij} = \frac{\partial \dot{\omega}_i}{\partial Y_j}|_0$) corresponds to the response to small perturbations of $\dot{\omega}_i$ along each direction in the phase space. As stated before, these perturbations mainly proceed from uncorrect flame velocity evaluations including diffusive and reactive phenomena. In laminar flames, characteristic time scales associated to diffusion and chemistry are of the same order; thus these perturbations may be balanced considering only chemical processes. Following the assumptions of the FPI model, the reaction rate associated to a species i mainly depends on mass fraction Y_i , which could be traduced by $J_{ij} \approx 0$ for $i \neq j$. The Jacobian matrix diagonal terms define the chemical time scales for each species: $\tau_{c,i} = 1/|J_{ii}|$. They are measures of the relaxation speed toward equilibrium of Y_i , after a concentration perturbation [10]. We can now define a corrective term that may be added to the interpolated reaction rates to prevent mass fractions from drifting away from their tabulated trajectories. An effective chemical source term $\dot{\omega}_i^{\text{eff}}$ is thus defined depending on the corresponding tabulated source term $\dot{\omega}_i^{\text{tab}} = \dot{\omega}_i^{\text{tab}} - (Y_i - Y_i^{\text{tab}})/\tau_{c,i}$. In the present work, we shall define $\tau_{c,i}$ for each species as the minimum reached by the inverse of $|J_{ii}|$ along the flame. This minimum is attained within the reaction zone, where the evolutions of the considered species are the stiffest. Fig. 1 shows the evolution of major species time scales, with respect to the abscissa x , for a stoichiometric methane/air flame. There may be several other ways of choosing the relaxation time $\tau_{c,i}$ [10,11]. The precise way of defining the chemical time scale used is currently further investigated as it clearly plays a crucial part in the numerical behavior of the method — stiffness and/or stability of the system may be affected.

4. Validation on a 1D laminar premixed flame

The test case retained here consists in a methane/air 1D unstretched laminar premixed flame under stoichiometric and atmospheric conditions. The diffusion fluxes were evaluated using Fourier and Fick’s laws, with non unit Lewis numbers. It is well known that these assumptions do not ensure mass conservation. Usually, only $N_{\text{sp}} - 1$ species are transported, the last one being deduced from total mass conservation. The main transported species are CH_4 , O_2 , N_2 , H_2O , CO_2 and CO . To ensure mass conservation, we added three more species: CH_3 , H_2 and OH . We insist upon the fact that these 3 last species are “reconstructed species” — their reactions rates are not interpolated in the FPI table — and do not correspond to real physical species. They are added to enforce atom conservation and thus total mass conservation — CH_3 for C, H_2 for H and OH for O. In addition, density must be evaluated in the CFD computation from species conservation equations — and not directly in the FPI database — in order to verify $\rho = \sum_{i=1}^{N_{\text{sp}}} \rho_i$. This point is particularly relevant in order to compute consistent thermodynamic properties. In our calculations, the reaction zone was meshed using ≈ 15 points and temporal integration was performed using an explicit two-step RK scheme, with a timestep of 10^{-8} s. The database was built using the PREMIX code along with

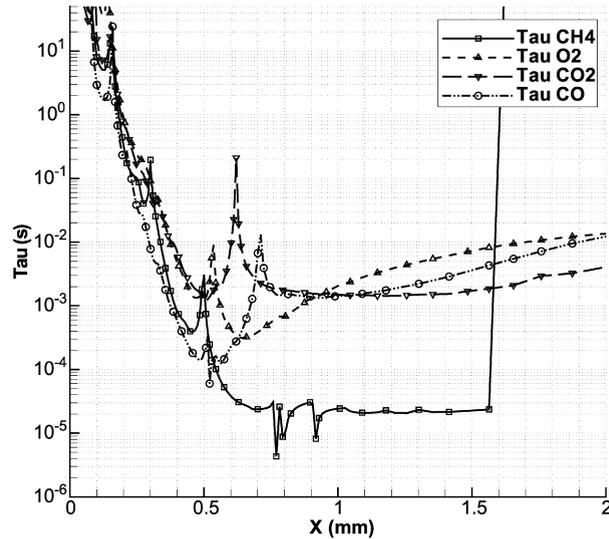


Fig. 1. Evolutions of the chemical time scales, associated to mixture major species, for a stoichiometric methane/air laminar premixed flame.

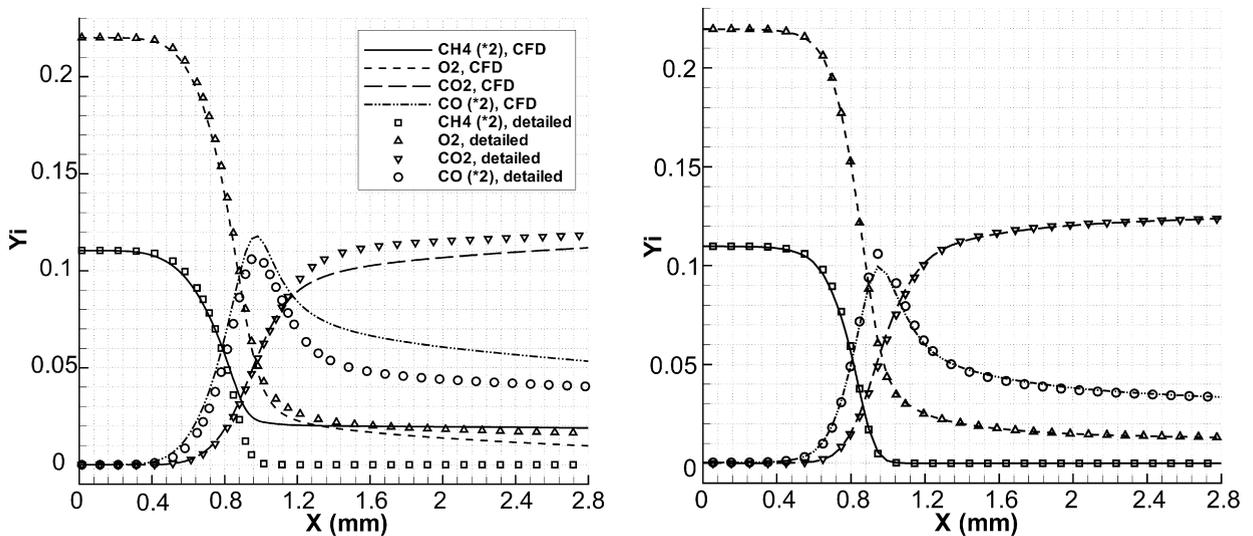


Fig. 2. Major species profiles along a stoichiometric methane/air premixed laminar flame — the perturbed case is on the left, the corrected case on the right—. The very good agreement of the corrected profiles — compared to the uncorrected ones — is worth noticing.

the simplified reaction mechanism proposed by Smooke and Giovangigli [12] including 16 species and 25 reactions, and was mapped using 250 points along c . Space profiles of the main species mass fractions along the flame in the perturbed and the corrected case are shown in Fig. 2. The non-corrected case results clearly show a marked deviation between the reference trajectory and the simulated one. On the other hand, the graph on the right presents very good agreements between CFD computations and complex chemistry results. We can hence clearly identify the contribution of our method compared with the non-modified FPI. Other tests were carried out on this flame with equivalence ratios ranging from 0.6 to 1.8. Similar trends were observed in each case.

5. Conclusion

A simple methodology was proposed to couple the FPI tabulation model with an industrial CFD code. We first analysed why the original FPI/CFD coupling may lead to uncorrect results. A simple corrective term — based on

a relaxation chemical time — was then introduced to enforce the perturbed species mass fractions to relax toward their reference trajectories. This strategy was successfully validated on a canonical 1D laminar premixed methane/air flame. The results obtained using the introduced correction show a very good agreement with those obtained using full chemistry modeling. Being able to accurately compute laminar flame profiles is a compulsory prerequisite before trying to simulate more complex flows. In that case, the capacity of the model to describe non-planar premixed flames has to be assessed. For non-planar premixed flames, stretch and curvature are no more negligible and should be taken into account in the modeling.

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