

Computations of Laminar Premixed Flames using Extended FPI Modeling

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Abstract

A new method to allow reacting flow computations using industrial type CFD solvers and detailed chemistry (through the FPI tabulation model) is introduced in this paper. Whereas FPI has already been extensively used in conjunction with laboratory CFD codes, its implementation in industrial solvers appears to be very challenging. In particular, species balance equations need to be solved with the corresponding chemical source terms being retrieved within the FPI databases. Among the difficulties arising from this weak coupling, it is noticeably shown that the interpolated reaction rates may not be coherent with the locally computed flame structure. A specific modeling of the chemical source terms is hence required to prevent species concentrations from drifting from their tabulated states. To validate this approach, freely propagating laminar premixed flames are successfully computed. Finally, the extension of the model to non-adiabatic combustion thanks to the addition of an extra dimension (h) is discussed.

Introduction

Predicting pollutant formation in industrial devices such as gas turbines or aeronautical combustion chambers has become in recent years a really concerning issue due to the increasingly restricting ecological norms. Within this context, Computational Fluid Dynamics (CFD) has raised as a very promising tool to help industrials develop more environment friendly technologies. However, predicting with accuracy the behavior of turbulent reacting flows in complex geometries remains a very challenging issue. In particular, the evaluation of minor species formation (especially NO_x and CO) requires a precise description of the chemical processes, generally involving hundreds of intermediate species. To make such computations feasible within a limited CPU time, kinetic reduction techniques are necessary to decrease the number of parametrizing variables defining the problem. In that way, different automatic strategies were developed, such as ILDM [1] or FPI [2, 3] (very similar to the FGM model [4]), based on the fact that low dimensional attracting chemical manifolds can be identified during the evolution of simplified reacting systems [1]. The existence of those manifolds allows the construction of look-up tables where the chemical responses of elementary flames are stored according to a limited number of progress variables (usually less than 3). Therefore, the CPU time required for complex reacting flow simulations including detailed chemistry with a CFD code is dramatically reduced as the resolution of the whole reacting system is replaced by simple interpolations in chemical databases. Those approaches seem very promising but computations of complex 3D geometries with industrial type CFD solvers and tabulated chemistry models are still very tedious.

Specific objectives

Few simulations of complex geometries using tabulated chemistry approaches were reported in the litera-

ture, mainly due to the difficulties related to their implementation in industrial CFD codes (the most recent and complete study on the subject was proposed by Galpin & al. [5]). Industrial codes are indeed designed to operate on real geometries and enable computations of various flow configurations (multiphase or supersonic flows, cryogenic combustion...). This requires a particular architecture, especially to allow the communications between the different modules and physical models (thermodynamics, chemistry, turbulence) of the software. Those specificities are generally not directly compatible with the use of tabulated chemistry models. The objective of this paper is thus to introduce an efficient coupling strategy to facilitate the use of chemical tables with industrial CFD codes.

In this work, CEDRE, the aerothermochemistry solver developed at the ONERA, was used. Besides, the chemical tabulation model FPI was retained. This model has already been successfully employed in various studies to predict premixed and partially-premixed reacting flows [6, 7, 8]. The implementation of FPI in CEDRE will ultimately allow premixed combustion simulations within various conditions, from the simplest canonical flames to more complex turbulent reacting flows.

In the following, the FPI approach is first shortly described. The coupling strategy retained is then introduced and its limitations and inherent difficulties are outlined. The necessary modifications of the original FPI method to ensure an efficient coupling are presented in the following section and validated on freely propagating laminar premixed flames with varying equivalence ratio. Numerical issues induced by the implementation of this coupling method are then discussed. The extension of the method to non-adiabatic flames is assessed in the final section.

The FPI approach and the coupling strategies

The FPI approach is based on the construction of chemical look-up tables using laminar freely propagating pre-

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mixed flames. To that end, the chemical responses of unstrained planar steady laminar premixed flames computed using a dedicated solver (here PREMIX [9]) are stored in databases according to a unique progress variable. This latter must vary monotonically across the flames so that only one set of chemical variables stored corresponds to each particular value of c . In this study, we chose to define c as in [3] :

$$c = \frac{Y_{CO_2} + Y_{CO}}{Y_{CO_2}^{eq} + Y_{CO}^{eq}} \quad (1)$$

where the superscript eq denotes quantities at the equilibrium. The evolution of the elementary chemical system thus reduces to a monodimensional manifold.

Two way of coupling FPI with a CFD software can be distinguished. This distinction has already been made by Poinot & Veynante [10] in the framework of the SLFM model for diffusion flames :

- 1– The "direct coupling" consists in solving equations for momentum, density, energy and the FPI input variable : c . The species mass fractions, and possibly the temperature, are then recovered using interpolations in the flamelet libraries (this approach was successfully used to compute complex turbulent reacting flows [6, 8]).
- 2– The "indirect coupling" consists in solving equations for momentum, energy and the species mass fractions. The density is then recovered using $\rho = \sum_{i=1}^{N_{sp}} \rho_i$, and the progress variable is computed with relation 1. The species chemical source terms $\dot{\omega}_i$ are interpolated in the FPI look-up tables. This method was used in [5] to compute a swirled premixed turbulent burner.

Considering the specific restrictions imposed by industrial CFD codes such as CEDRE, the second option was employed in this work. This approach possesses however some major drawbacks that make its implementation into CFD solvers very difficult.

Mass conservation issue

The application of the "indirect coupling" method implies the solving for a balance equation for each species described by the detailed reaction scheme used by the database generator. Provided that this would lead to unaffordable computational times if every species were transported, we chose to solve only a few species balance equations. The transported species are then selected so that most of the total mass is represented (say, more than 99% of the entire mass). For instance, for methane/air combustion, this represents 6 species : CH_4 , O_2 , H_2O , CO_2 , CO and N_2 . Nevertheless, to avoid possible drifts of the concentrations across the flame due to mass losses, we defined a procedure based on atom conservation to verify the mass balance.

This procedure consists in adding one virtual species for each element present in the flow (C , H , O and N

for usual hydrocarbons). The reaction rates of those new species are then reconstructed so that atom conservation is verified. A simple manipulation of the mass conservation relations leads to the following expression :

$$\dot{\omega}_j = -\frac{M_j}{\mu_j^k} \sum_{i=1}^N \mu_i^k \frac{\dot{\omega}_i}{M_i} \quad (2)$$

Where N is the number of transported species, μ_j^k represents the number of atom k in the j th virtual species and μ_i^k represents the number of atom k in the i th real species. Finally, the virtual species are given the physical properties of real species. CH_3 is chosen to represent the balance of C , OH for O and H_2 for H . Those species were retained because their formation enthalpies are low enough to have a limited impact on the global heat release rate. The adiabatic temperature of the burnt gases is hence not altered.

Coherence of the chemical reaction rates

When the FPI model is used in that way, discrepancies into the computed premixed flame structures may still be observed, even in the simple test case of a freely propagating laminar premixed flame. In such a flame for instance, where the effects of strain and curvature are negligible, the observed drifts are due to incoherences of the interpolated chemical reaction rates with the local structure of the computed flame. The origin of those disparities is easily identified when the balance equations for each species are rewritten in the phase space. In the physical space, these equations read :

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho u Y_i) = \nabla \cdot (\rho D \nabla Y_i) + \rho \dot{\omega}_i(x, t) \quad (3)$$

Where the Lewis numbers are assumed constant. We now apply the following transformation :

$$\nabla Y_i = \frac{\partial Y_i}{\partial c} \nabla c \quad (4)$$

$$\nabla^2 Y_i = \frac{\partial^2 Y_i}{\partial c^2} |\nabla c|^2 + \frac{\partial Y_i}{\partial c} \nabla^2 c \quad (5)$$

Replacing equations 4 and 5 into 3 leads to :

$$\frac{\partial \rho c}{\partial t} + \nabla \cdot (\rho u c) = \nabla \cdot (\rho D \nabla c) + \frac{1}{\partial Y_i / \partial c} \left(\rho \dot{\omega}_i(c) + \rho \chi_c \frac{\partial^2 Y_i}{\partial c^2} \right) \quad (6)$$

where $\chi_c = D |\nabla c|^2$ is the scalar dissipation rate of c . This relation is written within the phase space so that the chemical reaction rates are functions of the only progress variable c . By identification with the balance equation of c , one may now write :

$$\rho \dot{\omega}_i(c) = \rho \dot{\omega}_c(c) \frac{\partial Y_i}{\partial c} - \rho \chi_c \frac{\partial^2 Y_i}{\partial c^2} \quad (7)$$

Equation 7 represents the exact evolution of $\dot{\omega}_i$ in the phase space, as a function of c (the direct use of this expression in the CFD code should ensure a perfect match

between the tabulated and the transported species concentrations). If we now compare the phase space reaction rates driven by equation 7 and the actual chemical source terms in the physical space, one may find :

$$\rho(\dot{\omega}_i(x, t) - \dot{\omega}_i(c)) = (\rho\dot{\omega}_i(x, t) + \nabla(\rho D \nabla Y_i)) - \frac{\partial Y_i}{\partial c}(\rho\dot{\omega}_c(c) + \nabla(\rho D \nabla c)) \quad (8)$$

which leads to :

$$\rho(\dot{\omega}_i(x, t) - \dot{\omega}_i(c)) = \rho \left(S_d^i \frac{|\nabla Y_i|}{\nabla Y_i} - S_d^c \frac{|\nabla c|}{\nabla c} \right) \cdot \nabla Y_i \quad (9)$$

where S_d^i and S_d^c denote respectively the local propagation speeds of Y_i and c iso-surfaces. Those velocities are defined according to : $S_d^i = \frac{\dot{\omega}_i + \nabla(\rho D_i \nabla Y_i)}{|\nabla Y_i|}$. Finally, we define $n_i = \frac{\nabla Y_i}{|\nabla Y_i|}$ and $n_c = \frac{\nabla c}{|\nabla c|}$ the unit normal vectors respectively to Y_i and c iso-surfaces so that :

$$\rho(\dot{\omega}_i(x, t) - \dot{\omega}_i(c)) = \rho (S_d^i n_i - S_d^c n_c) \cdot \nabla Y_i = Q_i \quad (10)$$

The term Q_i was previously introduced by De Goeij & al. [12] to account for the fact that Y_i and c iso-surfaces generally do not coincide due to the diffusion of Y_i across c iso-surfaces. The existence of Q_i may induce disparities between the transported mass fractions and the tabulated trajectories leading to poor flame structure predictions. Those perturbations may ultimately lead to predicted burnt gas compositions different from the equilibrium.

Figure 1 presents the profiles of major species mass fractions across methane/air freely propagating laminar premixed flames computed using FPI, for 4 different equivalence ratios. The FPI look-up tables were built using the detailed reaction scheme of Smooke & Giovangigli [11]. The disparities arising within the flame front between the computed flames and the detailed chemistry solutions are clearly evidenced on those graphs.

This issue requires an adaptation of the current model to ensure an accurate convergence of the species concentrations toward their prescribed trajectories. We first assume that Q_i acts as a chemical perturbation of the source terms. The response of the species reaction rates to chemical perturbations is given by a simple linear analysis :

$$\dot{\omega}_i = \dot{\omega}_i^0 + \sum_{j=1}^{N_{sp}} \frac{\partial \dot{\omega}_i}{\partial Y_j} \Big|_0 (Y_j - Y_j^0) + \mathcal{O}(\Delta Y_j^2) \quad (11)$$

The reference state denoted by 0 corresponds to the tabulated state. If one assumes that the concentrations of each species only depend on the single progress variable c , then the off-diagonal terms of the Jacobian matrix

are negligible (the Y_i are assumed independent from each others). Relation 11 then gives :

$$\dot{\omega}_i^* = \dot{\omega}_i^{tab} + \frac{1}{\tau_{c,i}} (Y_i^{tab} - Y_i) \quad (12)$$

The diagonal terms of the jacobian matrix represent the rates of relaxation of the species concentrations toward the reference trajectories after a chemical perturbation [13]. The corresponding time scales are given by :

$$\tau_{c,i} = -\frac{1}{J_{ii}^{tab}} \quad (13)$$

In 12, the $\dot{\omega}_i^*$ define effective reaction rates that should be used in the CFD code instead of the directly interpolated ones. These source terms ensure a quick relaxation of the transported mass fractions toward their tabulated trajectories. Rao & Rutland [14] derived a similar expression for unsteady laminar flamelet modeling of diffusion flames.

One particular issue of the model concerns the evaluation of the relaxation time scale $\tau_{c,i}$. Simplified definitions of this time scale must often be used for practical reasons, as in [14]. After several tests, the following definition was retained, based on the minimum of the reciprocal jacobian matrix diagonal terms across the flame. It was shown that this is the only modeled time scale that leads to a perfect convergence of the results.

$$\tau_{c,i} \approx \min(1/|J_{ii}^{tab}|) \quad (14)$$

Figure 1 presents for 4 laminar premixed flames the results obtained after correction of the chemical source terms. Perfect agreements for each transported major species are found between the corrected results and the detailed chemistry solutions, which completely validates the approach.

The FPI databases required for such computations must contain the reaction rates of each transported species as well as the corresponding mass fractions, for each value of c . This multiplies by a factor 2 the size of the databases compared with the "direct coupling" approach. Linear interpolations are then used to extract the chemical datas from the look-up tables.

Finally, the global coupling procedure between the FPI databases and an industrial CFD code following the "indirect coupling" method can be summarized by the sketch on figure 2. An equivalent approach was previously proposed by Colin & al. [15] and Galpin & al. [5] in similar contexts, but with noticeable differences (especially for the correction of the chemical source terms).

Numerical issues

The numerical stiffness and stability of the reacting problem may be altered by the correction of the chemical source terms. The stability of the model can be assessed by considering the following simple equation representing the evolution of a perfectly stirred reactor (the equations are cast into a matricial form) :

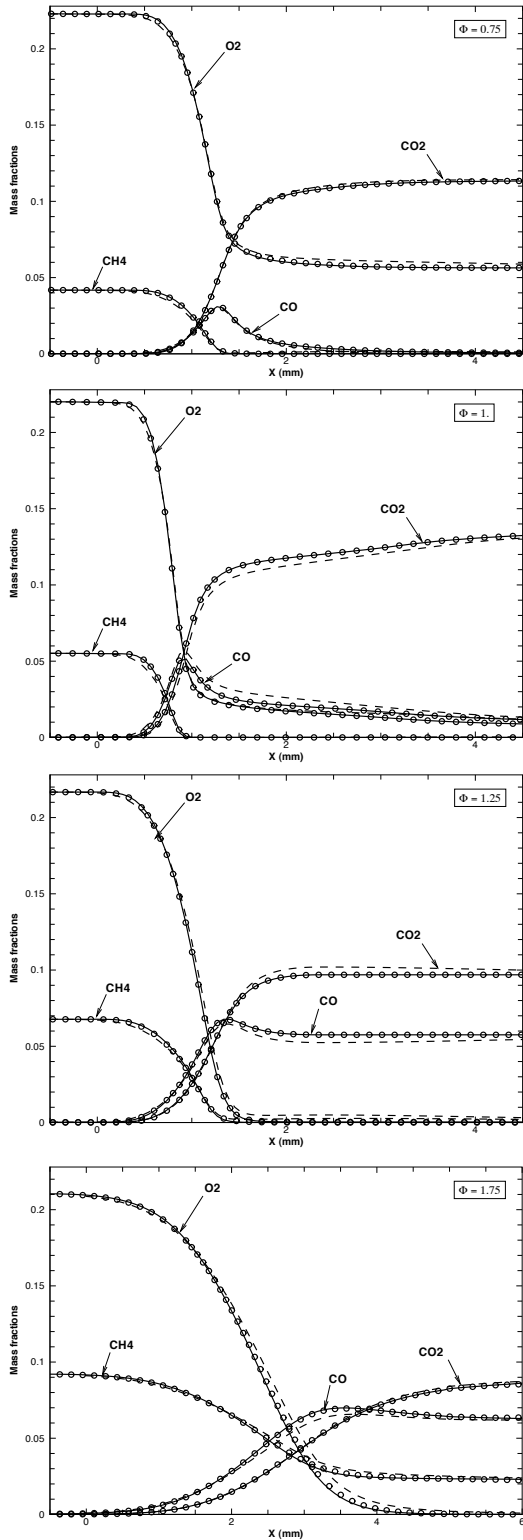


Figure 1: Freely propagating laminar premixed flames computed with CEDRE and FPI for 4 different equivalence ratios. Full lines, detailed chemistry (PREMIX), dashed lines, non-corrected reaction rates, symbols, corrected reaction rates.

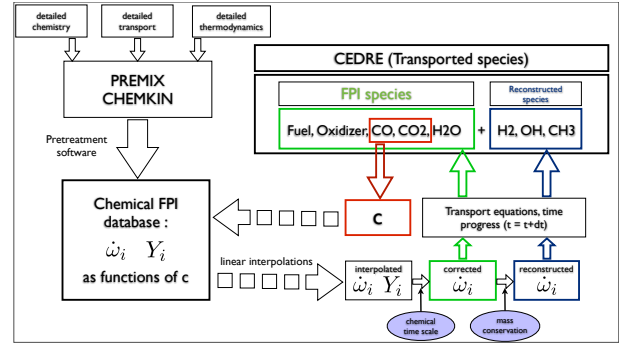


Figure 2: Sketch representing the coupling procedure between CEDRE and FPI look-up tables.

$$\frac{d\mathbf{Y}}{dt} = \dot{\omega}^* \quad (15)$$

$$= \underbrace{(\mathbf{J} - \text{diag}(|\mathbf{J}|))}_{\mathcal{J}} \mathbf{Y} + \text{diag}(|\mathbf{J}|) \mathbf{Y}^{\text{tab}} \quad (16)$$

where $\text{diag}(|\mathbf{J}|)$ should be approximated by $\tau_{c,i}$. It is usually admitted that to ensure the numerical stability of the reacting system, all the scales related to the chemical processes have to be resolved. In other words, the timestep used must be smaller than the minimum reciprocal real part of the eigenvalues of \mathcal{J} : $\Delta t \ll \frac{1}{|\text{Re}(\lambda_1)|}$ (where the eigenvalues are ordered in descending order so that λ_1 represents the largest eigenvalue).

Figures 3 and 4 present the evolution of the minimum reciprocal real parts of the eigenvalues of \mathcal{J} , across a stoichiometric methane/air flame.

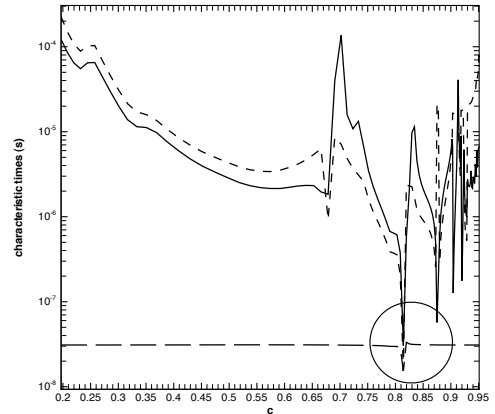


Figure 3: Minimum reciprocal real parts of the eigenvalues of \mathcal{J} across a stoichiometric methane/air flame. Full line, without correction, dashed line, correction with the exact time scales, long dashed line, correction with the approximated time scales (relation 14).

As shown on figure 4, the correction of the chemical source terms before their use in the CFD solver tends to artificially stiffen the problem. The minimum value reached by the reciprocal eigenvalues of the simplified system, corresponding to the limiting eigenvalue for the

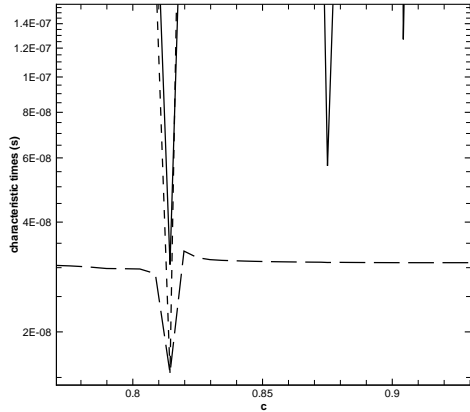


Figure 4: Zoom around the region where the minimum reciprocal real parts of the eigenvalues of \mathcal{J} reach their lowest values (same legend as 3).

stability, is indeed divided by a factor 2 (at this location, the local chemical time scale is equal to the relaxation time scale). Everywhere else, the relaxation time scale retained is lower than the local chemical time scales. The relaxation term in relation 12 becomes thus dominant so that the minimum reciprocal eigenvalue remains equal to the relaxation time scale. Therefore, to ensure the stability of the new corrected system, a time step divided by a factor 2 compared with a non corrected simulation must be employed.

Extension to non-adiabatic flames

The FPI model described in the previous sections of this paper is only valid for perfectly premixed, adiabatic and isobaric flames because of the strong assumptions made to build the databases. The extension of the original FPI model to non-adiabatic flames and partially premixed combustion was already discussed by Fiorina & al. [3]. We propose here to extend and to validate the present FPI model coupled with the CFD code CEDRE to non-adiabatic flames.

Building FPI look-up tables for non-adiabatic flames requires the addition of a new parametrizing dimension to take into account the energy losses. It is common to parametrize non-adiabatic flames using the total enthalpy of the mixture h (sometimes normalized). Two dimensional databases are thus created where the chemical responses of various freely propagating laminar premixed flames submitted to heat losses are tabulated according to the progress variable c and the mixture enthalpy h .

Different methods exist to build non-adiabatic FPI tables. We retained in this work the approach employed by Van Oijen & al. [4] based on the computation of a set of freely propagating laminar premixed flames with varying initial enthalpies. For the first flamelets, the modification of the enthalpy is simply obtained by varying the initial temperature of the flame. In the following flamelets, the enthalpy is adjusted by altering the initial composition of the mixture. Part of the reactants is transformed into com-

busion products (for instance H_2O and CO_2) so that the atomic balance is verified. Figure 5 illustrates a database obtained for premixed stoichiometric methane/air flames calculations. In this example, the temperature of the first 3 flames was varied from 250 K to 400 K. The initial composition of the mixture was varied for the following flames.

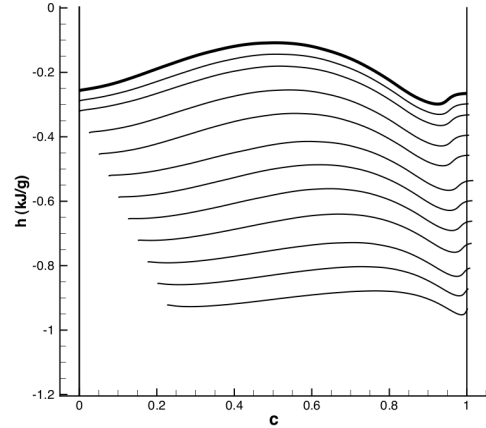


Figure 5: Example of a database for non-adiabatic methane/air stoichiometric flames.

As stated before, major species mass fraction transport equations are solved by the CFD code, which does not allow total mass and enthalpy conservation. We previously defined a procedure to enable mass conservation through the atomic balance. However, within the framework of non-adiabatic combustion, the enthalpy of the mixture must be accurately predicted as it defines one of the control variables of the model.

The enthalpy is related to the local heat release rate through $\dot{\omega}_T = -\sum_{i=1}^N \dot{\omega}_i h_i^0$, with h_i^0 the formation enthalpy of species i . A new procedure is necessary to ensure the coherence between the computed heat release rate and the tabulated one. In this work, two extra virtual species were added to the transported set of species : the first one (with a negative h_i^0) balances the enthalpy losses and the second one (with a positive h_i^0) balances the enthalpy gains (in the present example, H and H_2O_2 were selected). Their chemical source terms are then reconstructed in order to balance the differences between the local heat release rate in the flow field and the corresponding one in the FPI database.

Computations of monodimensional radiating laminar premixed flames were performed to validate the approach. To model the heat losses, a simple model based on the optically thin gases assumption was used. The heat loss term appearing in the energy balance equation is then approximated by :

$$\dot{Q}_T = -4\sigma\alpha(T^4 - T_0^4) \quad (17)$$

where T_0 represents the external temperature (here 300 K), σ is the Stefan-Boltzmann constant and α is the mean Planck absorption coefficient. Three radiating

flames were computed with different absorption coefficient values. Figure 6 presents a comparison between the computed temperature across the three flames and the detailed chemistry results. Very good overall agreements are found, even if slight discrepancies are observed when the absorption coefficient is increased (these errors remain however very small, $< 1\%$).

The ability of the model to account for heat losses is particularly important when considering pollutant formation as it is well known that the production of NO_x strongly depends on the local temperature of the flow.

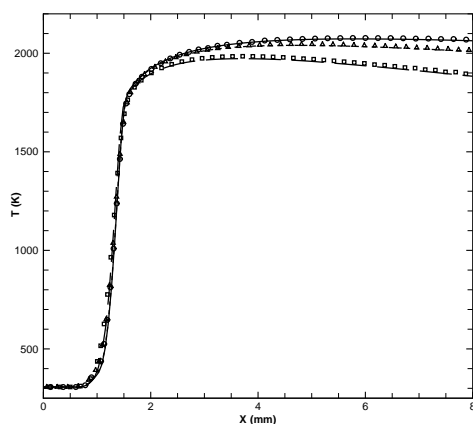


Figure 6: Radiating freely propagating premixed flames computed using CEDRE and non-adiabatic FPI databases for different absorption coefficients. Symbols : computed flames. Lines : Detailed chemistry. Full line and circle, $\alpha = 10m^{-1}$, dashed line and triangles, $\alpha = 20m^{-1}$, long dashed line and squares, $\alpha = 40m^{-1}$.

Conclusion and future works

The "indirect coupling" between an industrial type CFD code, and the FPI chemistry tabulation model was assessed in this work. This new coupling approach requires the solving for the major species balance equations in the CFD code, which imposes several adaptations of the model. In particular, as only a few species are transported among those described in the chemical databases, a specific procedure to ensure mass conservation must be employed. This procedure is based on the addition of virtual species to the transported set of species, whose chemical source terms are reconstructed to preserve the atomic balance. Moreover, it was evidenced that the reaction rates interpolated in the phase space manifolds may not be coherent with the local structure of the computed flames in the physical space. This issue requires a correction of the interpolated reaction rates to enforce the transported species mass fractions to follow their tabulated trajectories. This new model includes the evaluation of species relaxation time scales for which it was shown that one accurate definition is given by the minimum reciprocal diagonal terms of the chemical jacobian matrix. This model however leads to an artificial stiffening of the problem which requires lower time steps to ensure the

numerical stability.

The approach proposed here was validated on freely propagating laminar premixed methane/air flames at various equivalence ratios (the ONERA CFD code CEDRE was used). Excellent agreements with the detailed chemistry results obtained with PREMIX were observed. This validates completely our strategy, and especially the chemical source term relaxation method. The model was then extended to non-adiabatic combustion thanks to the addition of an extra dimension to the FPI manifolds : h . Here again, excellent agreements were found between PREMIX calculations of radiating laminar premixed flames and CEDRE computations using the FPI model for non-adiabatic flames.

In this work, the validity of the coupling strategy was only assessed within a laminar context. Future works will thus be dedicated to the extension of the model to turbulent combustion using a presumed PDF approach as in [5, 8]. Within this framework, a special attention must be given to the definition of the chemical reaction rate correction as it is clear that turbulence will affect the relaxation term. LES computations of turbulent reacting flows using CEDRE and FPI are currently in progress.

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