Auto-Ignition Probability of Ethylene/Air Mixture: Comparison Between Detailed Chemistry and Tabulated Chemistry

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***Abstract*— The current work will ultimately evaluate the ability of tabulated chemistry to predict the auto-ignition probability of ethylene/air mixtures. The evaluation is first performed by comparing the obtained flame structure and required computational efforts associated to tabulated chemistry with results produced by a detailed chemistry approach relying on Cantera.**

I. Introduction

The tabulated chemistry approach called FPI relies on detailed chemistry evaluations as first described by Gicquel *et al.* [1]. The capability of FPI to provide accurate predictions at low computational costs has been demonstrated for many combustion applications, e.g. [2]–[5]. This makes FPI one of the most promising reduced models for laminar and turbulent combustion applications. The advantage of FPI becomes even more important when working with complex fuels, i.e., methane, ethylene, diethyl ether, n-heptane, etc. For our project, the auto-ignition of a turbulent ethylene/air mixture is of particular interest. Resolving all turbulence and flame scales in a Direct Numerical Simulation (DNS) using detailed chemistry (solving all reaction and species equations during the simulation) leads to unacceptable computational times. The current work evaluates and discusses the behavior of FPI concerning autoignition of ethylene/air mixtures, comparing the obtained accuracy and the required computational time associated to a detailed chemistry DNS (relying on Cantera) with those obtained with FPI. To the authors' knowledge, a comparison between detailed chemistry and FPI has never been provided yet for such a complex fuel in a DNS.

II. FPI Principle

The FPI approach relies on a pre-tabulated detailed chemistry solution, usually based on one-dimensional laminar premixed flames. In this approach, every thermodynamic/physical/chemical quantity, φ is expressed as a function of two independent variables: mixture fraction, Y_z, and progress variable Y_c:

$$\varphi^{FPI} = \varphi(Y_z(\phi), Y_c). \tag{1}$$

Here, Y_z describes the state of the mixture through the equivalence ratio ϕ. Hence, it should be based on a suitable combination of non-reactive species. In the present work, Y_z is simply equal to the nitrogen mass fraction Y_{N_2}. On the other hand, Y_c must show a monotonic behavior representing the overall process of the chemical reactions. Here, the progress variable has been chosen as a combination of CO and CO_2, following [6], [7]:

$$Y_c = Y_{CO_2} + \alpha\, Y_{CO}, \quad \alpha \geq 0 \tag{2}$$

III. Numerics

In order to evaluate the FPI behavior for an ethylene/air system, a 2D look-up table has been generated by using an in-house Fortran code based on Cantera version 1.8. The table is computed starting from a skeletal mechanism developed by Luo *et al.* [8] that contains 32 species and 206 reactions. In the present work, Y_z, Y_c and all species mass fractions Y_k, mole fractions X_k, mixture-averaged diffusion coefficients D_k, mass production rates $\dot{\omega}_k$ are saved into the table. The temperature, density, dynamic viscosity, specific heat, thermal conductivity of the mixture are stored as well in the table.

All comparisons have been performed by using the in-house DNS low-Mach number solver DINOSOARS. This code can handle both techniques: 1) detailed chemistry (based on Cantera) or tabulated chemistry (based on FPI tables). In case of detailed chemistry, 37 conservation equation are finally solved: the low-Mach number Navier-Stokes equations, Poisson equation for pressure, temperature, and 32 species equations, the system being closed by the equation of state. On the other hand, in case of FPI, just six equations need to be solved: again, the low Mach number Navier-Stokes equations, Poisson equation for pressure, two conservation equation for Y_z and Y_c, using the equation of state to close the system.

IV. Results

In this section, first results and comparisons concerning planar premixed flames for stoichiometric conditions, $\phi = 1$, are presented. For the present results, $\alpha = 0$ is used in (2). During the conference, the structure of 3D turbulent premixed flames will be compared.

Figs. 1, 2 show the comparison of temperature and heat release for the ethylene/air laminar flame as obtained by detailed chemistry (Cantera, red line) vs. tabulated chemistry (FPI, dash black line), respectively. These figures reveal that the FPI simulations are able to reproduce the correct flame behavior.

Fig. 3 shows the comparison of computation time for the DNS simulation, using Cantera and FPI, using the Cantera simulation as a reference. It can be observed that the DNS

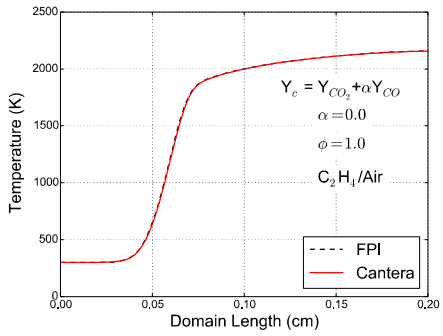

Fig. 1. Comparison of temperature.

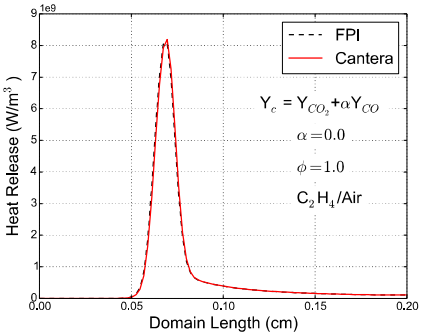

Fig. 2. Comparison of heat release.

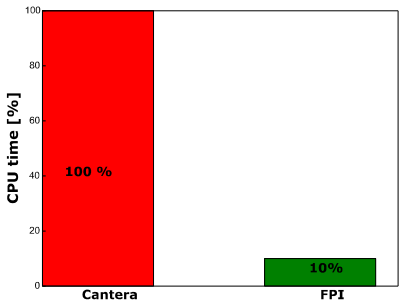

Fig. 3. Computational time for flame simulation relying on Cantera or FPI.

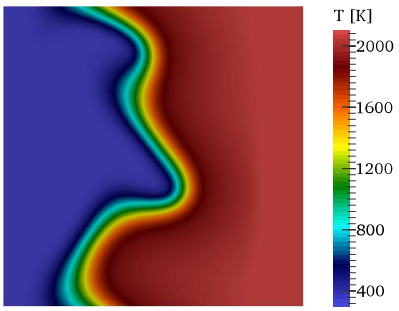

Fig. 4. Temperature field of the turbulent mixture, computed by FPI.

simulation relying on tabulated chemistry saves 90% of the total CPU time, highlighting the interest of this approach. Using FPI, systematic studies based on DNS become possible, opening the door for quantitative estimations of all relevant properties with a reasonable computational time.

The preliminary result of simulating turbulent ethylene/air mixture by FPI is shown in Fig. 4 which shows the temperature of the mixture. This figure shows the ability of FPI to work robustly with turbulent cases as well. The quantitative and qualitative comparison between the detailed chemistry and FPI will be shown during the conference.

V. Conclusion

The comparison of results obtained for premixed flames burning ethylene in air under atmospheric conditions reveals that tabulated chemistry (FPI approach) delivers results comparable to those obtained with detailed chemistry (relying on Cantera) at a fraction of the cost. Corresponding computations with FPI are typically one order of magnitude faster than those involving the complete reaction scheme. Finally, relying on tabulated chemistry in DNS should open the door for systematic studies of autoignition for turbulent ethylene/air mixture relying on DNS.

Acknowledgment

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