Development of a chemical kinetics tabulation method for the prediction of Diesel engine pollutants

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1   Introduction

In order to describe the chemical processes with a high level of accuracy in ICE, the kinetic model for a relevant practical fuel should contain hundreds of species N_{sp} and thousands of reactions. In spite of TFLOPS performance in the parallel supercomputer arena, 3-D simulation of ICE with detailed chemistry description remains out of reach. As CPU-time requirements are extremely stringent, tabulated chemistry techniques have been developed to describe turbulent combustion regimes [1–5] . Thermochemical quantities are expressed as a function of a reduced set of n variables. If n is sufficiently small compared to N_{sp} , this hypothesis will reduce drastically the number of balance equations to be solved, simplifying turbulent combustion modeling. The aim of the present paper is to develop a chemistry tabulation method valid simultaneously in the compression stroke, the reaction phase and the power stroke of an ICE. First, the database construction is briefly presented and a solution to take into account the low energy regions of the compression stroke is proposed. The tabulated chemistry strategy is first validated by 0-D simulations. Then the engine-adapted tabulated chemistry methodology is coupled with the Large Eddy Simulations compressible solver AVBP following the Tabulated Thermo Chemistry (TTC) formalism [6]. Preliminary homogenous auto-ignition simulations are presented.

2   Tabulated chemistry of ICE

2.1   Methodology

N-heptane ($n - C_7H_{16}$) is used to represent the Diesel fuel as it has the ability to properly foretell the auto-ignition delay, cetane numbers which are approximately 56 for both of them, as well as the cool flame regime. The following definition of the progress variable (Eq. 1) enables to tackle initial fuel decomposition, the cool flame and the main flame.

$$c = \frac{Y_{CO_2} + Y_{CO} - Y_{C_7H_{16}} + Y^0_{C_7H_{16}}}{Y^{eq}_{CO_2} + Y^{eq}_{CO} - Y^{eq}_{C_7H_{16}} + Y^0_{C_7H_{16}}} \tag{1}$$

where Y^{eq} and Y^0 corresponds to the equilibrium and initial mass fractions respectively.

Because of work exchanges during the piston displacement, the configuration of the engine causes changes in the chemical and sensible energy $e = \int_{T_0}^{T} C_v dT - \frac{RT_0}{W} + \sum_{k=1}^{N_{sp}} \triangle h_{f,k}^0 Y_k$ value. Similarly, as the system is closed during the ignition cycle of ICE, density ρ varies with time because of the changes in the volume of the combustion chamber. For these reasons, ρ and e must be considered as additional coordinates of the chemical database.

Density and energy ranges covered by realistic engine computations are $[\rho^-, \rho^+]$ and $[e^-, e^+]$. ρ^- and ρ^+ are respectively the minimal and maximal densities that correspond to the maximal and minimal combustion chamber volume. e^- and e^+ are the minimal and maximal energies encountered during the compression and power strokes, respectively. To build-up the database, a set of 0-D reactors at constant volume and constant energy is computed and then thermochemical parameters are tabulated as a function of specified coordinates (ρ, e, c) [1, 7]. However, constant volume calculations cannot cover the entire range of energy. Indeed a minimal energy e_i exists below which the auto-ignition will not occur under realistic delay time. This point was also mentioned by Colin et al. [7] who found that the energies during the power stroke of an engine would become too low to be tabulated using a constant volume reactor.
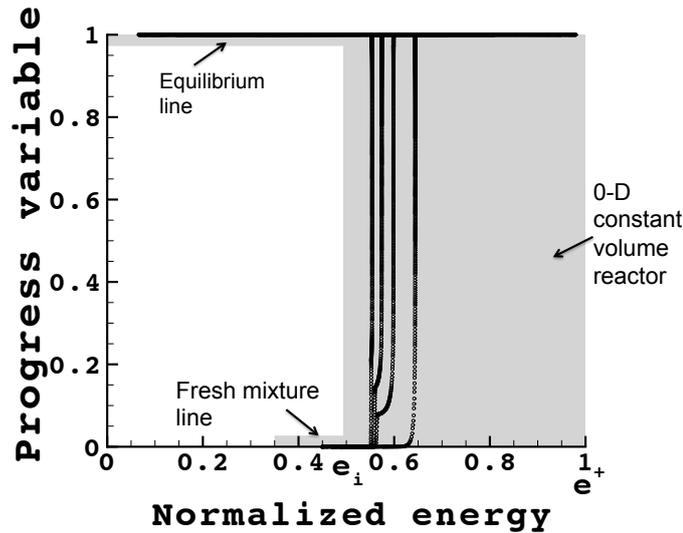
Figure 1: Grey region: 2-D projection in (c, e) subspace of the chemical database. Symbols: trajectories accessed by 0-D variable volume computations.

A methodology to tabulate the chemistry over the whole range of energy $[e^-, e^+]$ is proposed. A chemical database made of 0-D constant volume reactors is first computed over the range $[\rho^-, \rho^+]$ and $[e_i, e^+]$ by solving the following set of equations:

$$\begin{cases} \rho \dfrac{dY_k}{dt} = \dot{\omega}_k W_k, k = 1, ..., N_{sp} \\ \dfrac{de}{dt} = 0 \end{cases} \tag{2}$$

The grey region of the Fig. 1 represents the 2-D projection of the chemical table on the normalized (c, e) subspace. As the carbon chemistry characteristic time is very fast ($\sim 10^{-9}s$) compared to the piston motion (1 degree of crank angle is covered in $\sim 10^{-4}s$ at 1500 rpm) the composition state is in practice

very close to thermodynamic equilibrium during the power stroke. Then it can be assumed that the gas state bellow e_i is either the fresh mixture or the equilibrium. In fact intermediate states ($0 < c < 1$) are never accessed for $e < e_i$ in realistic engines. These limits are represented by the bold horizontal grey lines defined by $c = 1$ and $c = 0$.

2.2   Validation

To verify that the domain covered by the table is sufficient, computations of 0-D variable volumes engines are now performed by solving the following set of equations:

$$\begin{cases} \rho = \rho(t) \\ \rho\dfrac{dY_k}{dt} = \dot{\omega}_k W_k, k = 1, ..., N_{sp} \\ \dfrac{de}{dt} = \dfrac{P}{\rho}\dfrac{d\rho}{dt} \end{cases} \tag{3}$$

The calculations have been performed for $n - C_7H_{16}$ / air stoichiometric conditions using Golovichev's mechanism [8] with 53 species and 281 reactions. The density $\rho(t)$ is given for an engine with the following characteristics: bore = 85 mm, stroke = 88 mm, rpm = 1500.

Trajectories in (c, e) subspace followed by these computations are plotted in Fig. 1. It shows that for $e < e_i$, the domain between $0 < c < 1$ is never accessed by the variable volume chemical trajectories.

(a) Temperature   (b) Pressure

(c) CO_2 (d) CO
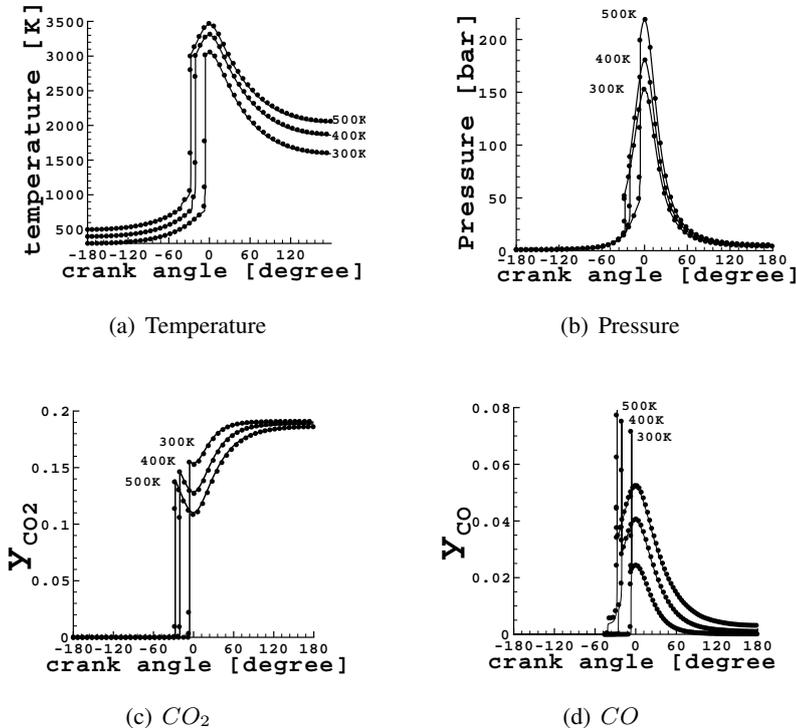
Figure 2:   0-D variable volume computations for various initial temperature conditions. Tabulated chemistry (symbols) is compared to detailed chemistry (line)

0-D computations using the previously defined chemical table are now performed to validate the tabulation methodology. The following set of equations is solved:

$$\begin{cases} \rho = \rho(t) \\ \rho\dfrac{dY_c}{dt} = \dot{\omega}_c \\ \dfrac{de}{dt} = \dfrac{P}{\rho}\dfrac{d\rho}{dt} \end{cases} \qquad (4)$$

Solutions of this set of equations are compared to the detailed chemistry computations in Fig. 2. Time evolution of temperature, pressure, CO_2 and CO mass fractions are plotted for different initial temperature conditions. For all variables and configurations, the tabulated chemistry solution (symbols) is in very good agreement with the detailed chemistry reference solution (lines). The (ρ, e, c) tabulated chemistry is therefore able to predict at reduced CPU time the main behavior of the combustion process in an ICE engine.

3 Coupling the chemical table in a compressible CFD solver

Large Eddy Simulations (LES) of 3-D combustion engine with a tabulated chemistry strategy require the coupling of the previously defined database in a compressible solver. A new strategy, called Tabulated Thermochemistry for Compressible flows (TTC), has been proposed by Vicquelin et al. [6] for introducing tabulated chemistry in compressible code for low mach number flow regimes. The methodology has been proposed for isobar chemical database where the perturbations due to compressible effects are not considered during the database generation.

As detailed in section 2, due to the strong compressible effects that occur in ICE, energy is considered as a database coordinate. In the present work, the TTC formalism has been extended to account for 3-D (ρ, e, c) look-up table. It has been implemented in the AVBP LES code [9]. 0-D constant volume with

(a) Low temperature regime

(b) High temperature regime
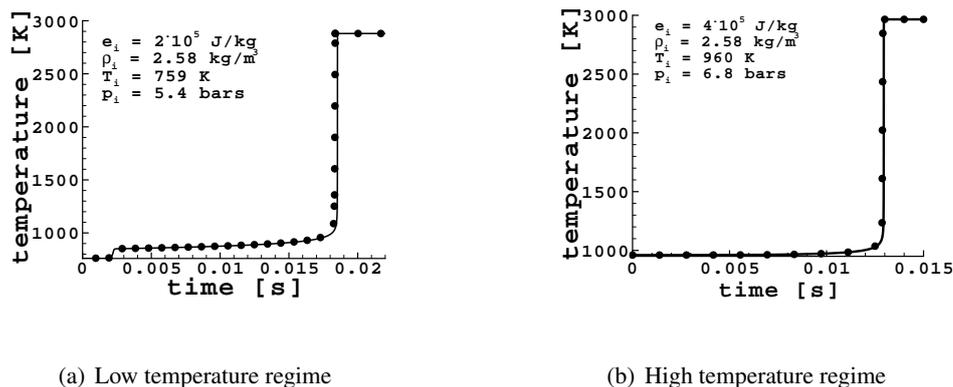
Figure 3: 0-D constant volume computations. AVBP TTC Tabulated chemistry (symbols) is compared to detailed chemistry (line)

variable pressure simulations have been performed with the present tabulated chemistry strategy implemented into AVBP. Temperature evolution is presented in Fig. 3. The AVBP TTC solution (symbols) is compared with the detailed kinetics calculations for a low and a high temperature regimes. The good agreement demonstrates the table's ability to account for variable pressure configurations.

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