Simulating kerosene/air flames with hybrid transported-tabulated chemistry

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Abstract A strategy to introduce the detailed chemistry of kerosene combustion into direct numerical simulations of flames is reported. During the last decade, significant progress has been made to improve the chemical kinetic and turbulent combustion modeling as well as the high-performance computer power. However, a large-eddy simulation of an aeronautical combustion chamber using detailed chemistry mechanisms is still not possible because of the needed temporal resolution and the large number of species to be transported. The hybrid transported-tabulated chemistry method (HTTC) has been designed to overcome these obstacles and radically reduce the computational cost of such simulations, by transporting only a reduced set of major species and tabulating the intermediate species while making use of their self-similarity property to downsize the table. In this work, the application of HTTC to kerosene combustion is investigated. Although intermediate heavy species typical of kerosene combustion feature a particular behavior, making difficult the use of the self-similarity, the method allows a decrease of the timestep by three orders of magnitude. HTTC is quite flexible, since it leads to good results even if the table for intermediate species is generated in different conditions than those of the simulation.

Introduction

In a near future, aircraft engines are expected to respect more and more restrictive emission standards. They are also expected to feature low fuel consumption, low noise emission and high reliability. To fulfill these requirements, efficient CFD tools are developed to better understand the kerosene combustion. Dealing with ignition and pollutant emission implies to introduce detailed chemistry into the simulation codes. Indeed, simplified chemistry descriptions using optimized reduced kinetic schemes, such as the BFER two-step mechanism proposed by Franzelli *et al.* [1], are able to predict the ignition delay, the burnt gas temperature and the flame speed over given fresh gas temperature, equivalence ratio and pressure ranges, but generally fail when the operating conditions are out of these ranges. Besides they are unable to predict pollutant concentrations, since the polluting species are absent from these schemes.

Detailed mechanisms for kerosene combustion do not suffer from this lack of generic character and offer better prediction capabilities. Several of them can be found in an overview provided by Dagaut *et al.* [2]. Unfortunately, LES of practical burners using these schemes cannot be achieved, because the number of species and reactions is still too large, even for today's supercomputers. This work highlights another issue when a full-explicit solver is used to solve the transport equations : the intermediate species chemical timestep is too small to complete a simulation successfully, and implicit (or semi-implicit) numerical schemes have to be employed for the time advancement.

Along these lines, many approaches based on the tabulation of chemical responses of canonical combustion problems have been developed. For example, one-dimensional laminar flames can be projected into a progress variable and mixture fraction space, to build a look-up table which will be used during the simulation to extract some variables, such as the species mass fractions, instead of solving for them [3, 4]. Thus only the mixture fraction and the progress variable need to be transported with the flow, dramatically reducing the computation cost. These techniques have been successfully applied in LES of kerosene combustion in practical devices [5]. However, the use of such tables may lead to a significant lack of accuracy and flexibility, and may become too large when the dilution by burnt gases, heat transfers or multiple inlets are considered. The size of these multidimensional tables is often considerable, which is not well-adapted to the context of high-performance computing.

Hence, table downsizing methods have been discussed in the literature, using the self-similarity behavior of the radical species in laminar flamelets [6, 7]. This remarkable property has been exploited by Ribert *et al.* to develop a strategy combining the detailed-chemistry solving for the main species with the tabulation of the intermediate species, called Hybrid Transported-Tabulated Chemistry (HTTC) [8]. Thus, most of the detailed chemistry features are preserved, with a reduced chemical timestep. This method has been validated on methane/air flames. In the present work, the contribution of the HTTC method to the computation of kerosene/air flames is investigated.

Hybrid transported-tabulated chemistry method

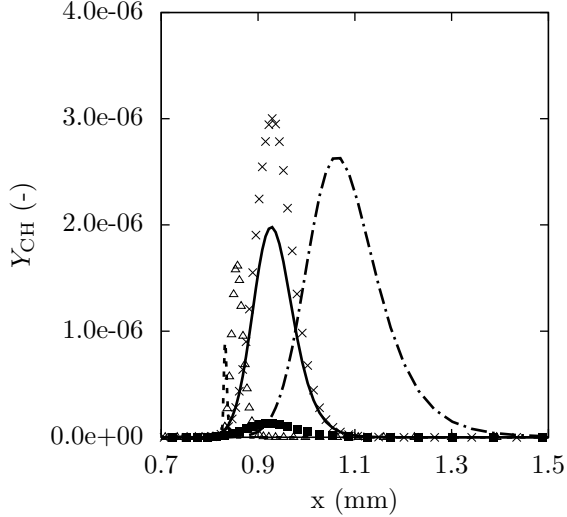The goal of the HTTC method is to preserve the precision of detailed chemistry, but with a dra-

Figure 1: CH mass fraction versus physical space for various S. —— (1.0 bar,1.0,500 K), ···· (20.0 bar,1.0,500 K), –·– (1.0 bar,1.4,500 K), $\triangle$ (3.5 bar,1.0,500 K), $\times$ (1.0 bar,1.0,700 K), ■ (1.0 bar,0.6,500 K)

matically reduced computational time. With this aim in mind, the main species of the flow (i.e. those which feature a non-zero mass fraction out of the flame front) are solved, while the intermediate species mass fractions are tabulated as a function of a progress variable, as well as the pressure, the inlet temperature and the equivalence ratio, to ensure the generic character of this approach. The progress variable is built from the main species. This tabulation leads to a decrease of the chemical timestep and of the number of equations to be solved. Nevertheless, the size of such tables would be gigantic if they were stored as they are. Consequently, the self-similar property of the hydrocarbon flames is used to provide light tables, as explained below in the case of methane/air flames [8].

Here the methane/air detailed mechanism of Linstedt *et al.* [9] (29 species, 141 reversible reactions) is used under the hypothesis of a unity Lewis number. The computations presented in this section and in the next one are performed with the laminar flame solver REGATH [10]. It is observed that intermediate species profiles, such as CH, keep a similar shape although their width and maximum is different for each set $S = (P, \phi, T_u)$, where P is the pressure, ϕ is the equivalence ratio and T_u is the unburnt gas temperature (Fig. 1). Every profile of jth intermediate species vanishing in both fresh and burnt gases may be normalized by its maximum ($Y_j^+ = Y_j/Y_j^{max}$) and expressed in a reduced progress variable $Y_{c,j}^+$ space:

$$Y_{c,j}^+(S) = \frac{Y_c - Y_{c,j}^A(S)}{Y_{c,j}^B(S) - Y_{c,j}^A(S)} \qquad (1)$$
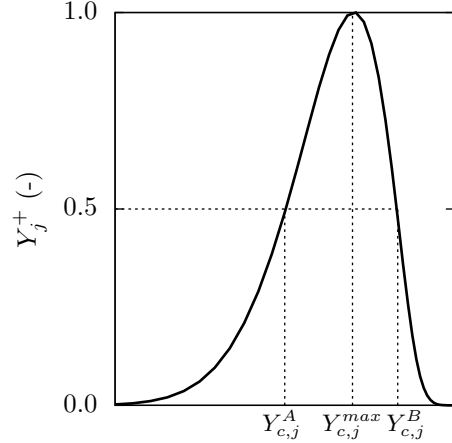

Figure 2: Sketch of an intermediate species profile versus the progress variable Y_c.
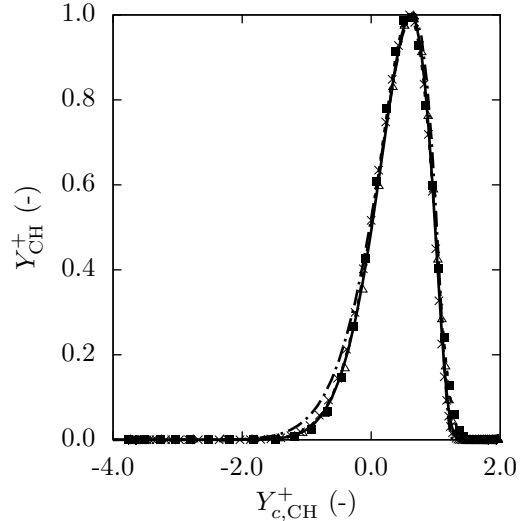

Figure 3: Reduced CH mass fraction profiles for the same sets S as Fig. 1.

where Y_c is the progress variable, simply defined in this work as $Y_c = Y_{CO} + Y_{CO_2}$. The parameters $Y_{c,j}^A$ and $Y_{c,j}^B$ are the two values of Y_c when $Y_j^+ = 0.5$ (Fig. 2).

As soon as they are expressed in this reduced progress variable space, every profiles are superimposed for each set S (Fig. 3). In the HTTC formalism, only one of these reduced profiles $Y_j^+(Y_{c,j}^+)$, plus $Y_{c,j}^A(S)$, $Y_{c,j}^B(S)$ and $Y_j^{max}(S)$, are tabulated, using the self-similar property highlighted above. The jth intermediate species mass fractions is thus computed as $Y_j = Y_j^+ \times Y_j^{max}$ using the look-up table instead of being transported with the flow.

Application of HTTC to kerosene/air flames

In order to apply the HTTC method to the combustion of kerosene, the transported species are separated from the tabulated species, and then the self-similar properties of kerosene/air flames are studied.

	Decane	Mixture
n-decane	1.0	0.74
n-propylbenzene	-	0.15
n-propylcyclohexane	-	0.11

Table 1: Species molar fraction of the kerosene surrogates used in this work

Transported $\mathcal{B}^1$			
H_2	O_2	CO	CO_2
CH_2O	$NC_{10}H_{22}$	H	O
OH	HO_2	H_2O	HCO
N_2			
Transported $\mathcal{B}^2$ (high pressures)			
CH_3	CH_4	CH_2OH	CH_3OH
Transported $\mathcal{B}^3$ (for *Mixture*)			
CYC_9H_{18}	PHC_3H_7		
Tabulated $\mathcal{C}^1$ (two-peak species)			
PC_4H_9	AC_5H_{11}	AC_6H_{13}	BC_6H_{13}
AC_8H_{17}	$AC_{10}H_{21}$	$CC_{10}H_{21}$	$DC_{10}H_{21}$
$EC_{10}H_{21}$	$APHC_3H_6$	$CPHC_3H_6$	$PHCH_2$
Tabulated $\mathcal{C}^2$ (self-similar species)			
$\mathcal{A} - (\mathcal{B} \cup \mathcal{C}^1)$			

Table 2: Sets of transported species. The species nomenclature is given in [13].

Kerosenes are usually composed of hundreds of different chemical species such as aliphatic and aromatic compounds, but also linear alkanes [11]. The development of a chemical mechanism including all of them is a task which has not been achieved yet. Therefore a surrogate should be used to make the combustion chemistry modeling possible. In this work, two surrogates will be considered (Table 1): the surrogate *Decane* (100% n-decane), and the surrogate *Mixture*, typical of commercial jet fuels, composed of n-decane, n-propylbenzene and n-propylcyclohexane, as proposed by Guéret *et al.* [12]. The Luche kinetic mechanism [13], which involves 91 species and 991 reactions, is employed. If the nitrous oxides are not taken into account, the mechanism is reduced to 74 species and 746 reactions. In this work, a unity Lewis number assumption is made.

Two databases (one for each surrogate) of 1D steady freely propagating flames are generated on a large range of pressure P, equivalence ratio ϕ, and temperature of fresh gases T_u. The following ranges are chosen :

$$\begin{cases} P \in [1, 20] \text{ bar} \\ \phi \in [0.6, 1.4] \\ T_u \in [500, 700] \text{ K} \end{cases} \quad (2)$$

A numerical criterion is used to divide the full set of species $\mathcal{A}$ into transported species $\mathcal{B}$ and tabulated species $\mathcal{C}$. The species j belongs to $\mathcal{C}$ if $Y_j < \varepsilon$ out of the flame front. In this work, $\varepsilon = 10^{-10}$ but this value could be increased to reduce the set $\mathcal{B}$ if needed, but at the cost of a precision lost. For decane/air flames at low pressure, a set $\mathcal{B}^1$ of 13 species has to be transported (Tab. 2). At high pressure ($P > 14$ bar), the set $\mathcal{B}^2$ is added so that ($\mathcal{B}^1 \cup \mathcal{B}^2$) is transported. For the *Mixture*/air flames, the two other components of the surrogate are simply added (set $\mathcal{B}^3$). The set $\mathcal{B}^1$ is almost identical for methane/air flames [8], and thus can be expected to be similar for every alkanes. Thanks to this property of interest, the computational time spent for the species transportation should be comparable.

The reduced mass fraction profiles of the tabulated species can be split into two groups, depending on the shape of their profile across the flame. The light species included in $\mathcal{C}^2$ (from C_1 to C_4 species) feature a classic self-similar behavior, as shown in Fig. 4 for CH, just as for the Lindstedt mechanism methane/air flames [8]. The reduced mass fraction profiles are well superimposed for the *Decane* and the *Mixture* surrogates. For the light species, Y_c^A, Y_c^B and Y^{max} are nearly identical (the mean difference is around 5%) on the whole (P, ϕ, T_u) domain (Fig. 5), defined in Eq. (2).
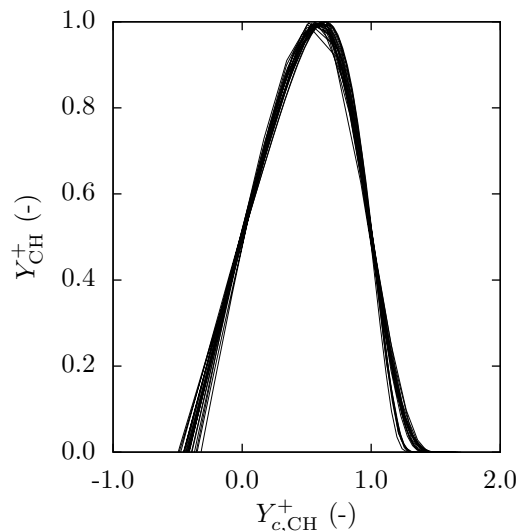

Figure 4: Reduced CH mass fraction profile in decane/air and *Mixture*/air flames, for several sets S of the domain defined in Eq. (2).

The reduced mass fraction profile shape of heavy species contained in $\mathcal{C}^1$, produced by the decane breakdown, differs from what can be observed for the light species. Two local maxima are present (Fig. 6), and their positions and values are different for every sets S. Consequently, the profiles of these species cannot be self-similar, and some error is expected to appear if the self-similarity were
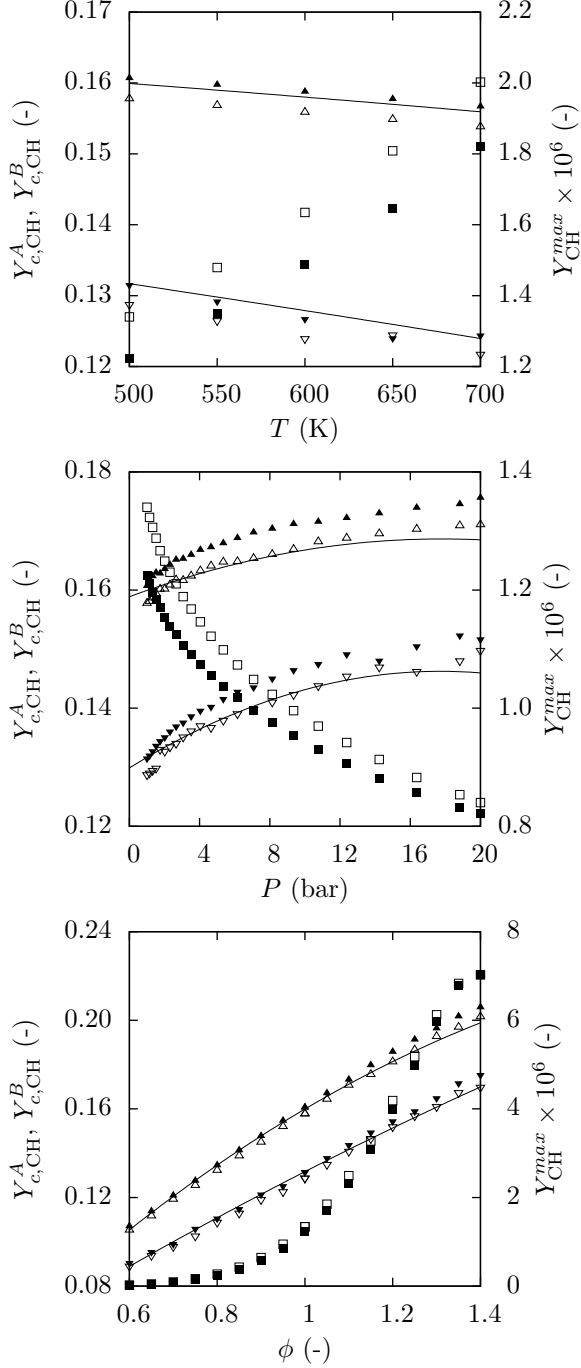
Figure 6: Reduced mass fraction profiles of the intermediate species $AC_{10}H_{22}$ for various sets S (surrogate *Decane*).

Figure 5: Y_c^A, Y_c^B and Y^{max} vs. P, ϕ and T_u for the species CH. $\triangledown$ Y_c^A, $\triangle$ Y_c^B, $\square$ Y^{max}. Open symbols: *Decane*, solid: *Mixture*. Lines: interpolating functions of Y_c^A and Y_c^B for *Decane*.
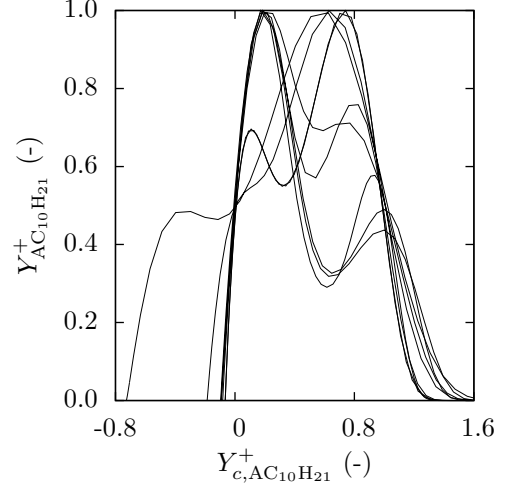
used anyway in the simulation, using a table containing only one reduced profile for each species. The error amount which would be induced on the main variables of the flow in that case is assessed in the next section. Moreover, the chemical behavior of heavy species during the decane breakdown is different between *Decane* and *Mixture* surrogate, thus the value of Y_c^A, Y_c^B and Y^{max} are not equal as found for the light species.

In order to downsize again the table, Y_c^A and Y_c^B are expressed as a function of P, ϕ and T_u using a second-order polynomial (Eq. (3)).

$$Y_{c,j}^A = aP + bP^2 + c\phi + d\phi^2 + eT_u + fT_u^2 + g \quad (3)$$

Thus, for each species j, only 14 coefficients are stored instead of 2 three-dimensional arrays. The error between the polynomial and the array is negligible (around 2%). However, Y^{max} features a more complicated behavior and cannot be expressed so simply with such a polynomial, and should be fully tabulated.

Results

This section presents the results obtained for the simulation of 1D premixed kerosene/air flames, simulated with the DNS compressible code SiTCom-B [14], using the HTTC solver. Here the surrogate *Decane* is used, and the Lewis number is set to 1 for every species. The following conditions (P, ϕ, T_u) are investigated: (1.0 bar, 1.0, 500 K), (3.5 bar, 1.0, 500 K), (1.0 bar, 1.0, 700 K), (1.0 bar, 0.6, 500 K), (1.0 bar, 1.4, 500 K), (20.0 bar, 1.0, 500 K).

Three types of tables are used to perform the same simulations with the HTTC solver (Tab. 3). The table *Full* contains the reduced profiles computed for all the different simulated conditions.

Table	Reduced profiles	Y_c^A, Y_c^B, Y^{max}
Full	Same conditions as simulations	Same conditions as simulations
Self	1.0 bar, $\phi = 1.0$, 500 K	Same conditions as simulations
Standard	1.0 bar, $\phi = 1.0$, 500 K	1.0 bar, $\phi = 1.0$, 500 K

Table 3: HTTC tables used to perform the simulations of decane/air flames.

In other words, the self-similarity property is not used here. With this table, the agreement between the SiTCom-B results with HTTC and the detailed chemistry solution computed by REGATH is very good for all the simulated sets, as expected (Fig. 7). Similar results are observed for every major species. In every cases, the chemical timestep value varies from 10^{-9} s at 1 bar to 10^{-10} s at high pressures. If the simulation had to be performed using detailed chemistry, values from 10^{-12} s at 1 bar to 10^{-13} s would be observed (using a classic timestep computation approach such as $\Delta t = \rho Y / |\dot{\omega}_Y|$, where $\dot{\omega}_Y$ is the species source term). Thus, the chemical timestep is increased by 3 orders of magnitude, so that the overall value is increased up to the CFL convective timestep.

The table *Self* is used to assess the error induced if only one reduced profile per species is tabulated, neglecting the fact that several species do not feature any self-similar behavior. The reduced profile is computed in "standard" conditions (1 bar, $\phi = 1$, 500 K). Large deviations from the detailed chemistry solution are observed in the flame structure (Fig. 7). Indeed, in this case $Y_c^{A,B}$ and Y^{max} values are set according to the simulation conditions, whereas the reduced profiles are tabulated at (1 bar, $\phi = 1$, 500 K). Thus the chemical reactions of the heavy species cannot be consistent because of their lack of self-similarity.

The table *Standard* includes only the reduced profiles, $Y_c^{A,B}$ and Y^{max} in "standard" conditions. Figure 7 shows that a good agreement is observed with the detailed chemistry solution for the flame at $P = 3.5$ bar and the flame at $T_u = 700$ K. Hence the HTTC method is quite flexible since it allows pressure and fresh gas temperature variations, using a table generated for a single set S. In particular, this property is convenient to avoid building and storing a full flame database. Equivalence ratio variations have not been tried, since they are expected to cause significant errors on the flame speed [8]. A better robustness than *Self* is achieved. Indeed the reduced profiles, $Y_c^{A,B}$ and Y^{max} are computed using the same conditions, which keep the chemical mechanism coherent.
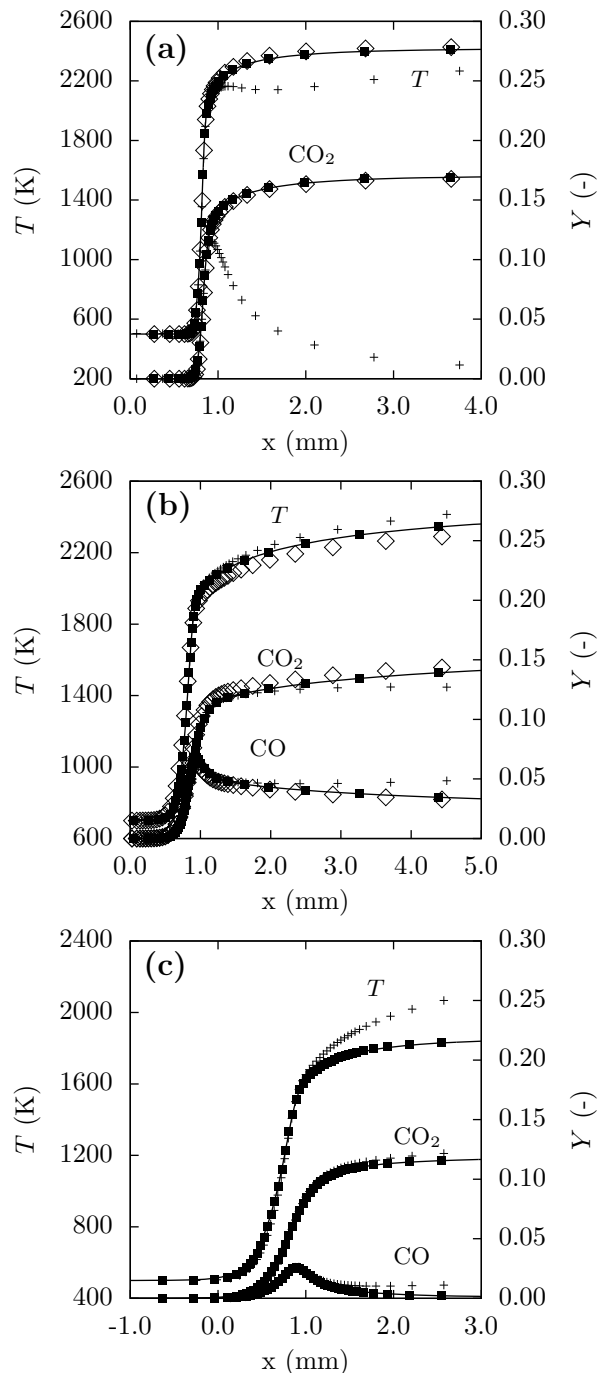

Figure 7: Temperature, Y_{CO} and Y_{CO_2} profiles. (a) $P = 3.5$ bar, $\phi = 1.0$, $T_u = 500$ K; (b) $P = 1.0$ bar, $\phi = 1.0$, $T_u = 700$ K; (c) $P = 1.0$ bar, $\phi = 0.6$, $T_u = 500$ K. Lines: detailed chemistry. Symbols: HTTC. ■ *Full*, + *Self*, ◇ *Standard*.

Conclusion

In this work, the HTTC method has been applied to kerosene/air flames. The set of species to be transported is nearly identical as found for methane/air flames. However, heavy species produced by the decane breakdown feature a "double-peak" reduced mass fraction profile, resulting on large errors during the simulation when trying to systematically use the self-similarity property. A table containing only one reduced mass fraction profile for the self-similar species and several profiles for every simulated conditions for the double-peak species can avoid this error, but the size of the table would be increased. An alternative method to reduce the species profiles and then achieve a correct auto-similarity (as in [15] for example) will be investigated in a future work. However, HTTC gives results in good agreement with detailed chemistry, when used with tables generated at fixed conditions. With HTTC, the timestep is increased by three orders of magnitude compared with detailed chemistry, and reach values usually encountered for non-reactive flows with compressible solvers. The error on the main variables (temperature, main species) stays at low levels when the pressure or the fresh gas temperature moderately varies around the values used to build the table.

Acknowledgments

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