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Description of kerosene / air combustion with Hybrid Transported-Tabulated Chemistry

Bastien Duboc, Guillaume Ribert*, Pascale Domingo

CORIA – CNRS, Normandie Univ., INSA de Rouen Normandie, 76000 Rouen, France

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ABSTRACT

A strategy to introduce the detailed chemistry of kerosene-air combustion into simulations of flames is reported. Despite the rise in computer power achieved during the last decade, simulations of combustion chambers using detailed chemistry mechanisms are still not possible because of 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, 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. HTTC has already been validated for light hydrocarbons such as methane. In this work, HTTC is extended to kerosene-air combustion showing that the number of species to be transported is unchanged compared to methane/air and that the self-similarity can still be applied. The chemistry of nitrogen oxides is also addressed with HTTC. The method allows for a reduction of the computational cost by around four orders of magnitude when computing laminar premixed flames. HTTC appears as a flexible tool since its prediction capabilities are maintained even if the table for intermediate species is generated in different conditions than those encountered in the simulation.

1. Introduction

Direct Numerical Simulation (DNS) of a reactive flow with detailed chemistry requires to solve the transport equations for energy, momentum and mass fractions of all chemical species. For the latter, the computation of many source terms, thermodynamical quantities and transport coefficients using the full set of species contained in the kinetic mechanism is needed. Solving for the mass fraction of the species leads to two main difficulties: the number of computing operations increases dramatically with the number of species, and the stiffness of the chemical system imposes fine mesh and time resolutions [1,2]. Implicit numerical schemes can be used to overcome this stiffness, and increase the stability limit of the time step [3–8]. However, those numerical schemes do not solve the issue raised by the first point: the computational cost does not scale linearly with the number of species and it may become very high for large chemical mechanisms [9]. In contrast, reduced kinetics feature smaller numbers of species and may be a solution to the two difficulties presented above [10], but at the cost of a lack of precision or a limited range of application for highly simplified mechanisms [9].

An alternative method able to take all the species of a full kinetic mechanism into account during a simulation, with a computational cost compatible with today's computer capabilities, has been proposed by Ribert et al. 11. It is called "Hybrid Transported-Tabulated Chemistry" (HTTC). With HTTC, the full set of species is split into two parts: the main species, carrying most of the mass, and the remaining minor species. The mass fractions of the main species are computed by solving a transport equation, using a detailed chemistry solver. Instead of being transported, the minor species are read in a look-up table which is built from self-similar flame profiles [12–14]. The standard momentum and energy transport equations are still solved. The basis of HTTC is to keep unaltered the detailed kinetic mechanisms without the suppression of species or reactions.

Radical and minor intermediate species are involved in chemical reactions that mostly take place in the flame front and which are responsible for the stiffness of the chemical system. Consequently, removing them from the set of transported species by reading their values in a table, makes the chemistry of combustion easier to solve. In the frame of explicit solvers, the chemical time step is then expected to be largely increased without any stability issue, thanks to the tabulation of the minor species. In the case of kinetic mechanisms for heavy fuels, the chemical time step is usually far below the convective time step [15], which leads to prohibitive computation costs. For such fuels, it could be increased by several orders of magnitude, to become larger than the convective time step when using HTTC. Simulations of reactive flows with very large detailed mechanisms using fully explicit numerical

* Corresponding author.
E-mail address: guillaume.ribert@coria.fr (G. Ribert).

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Nomenclature

Acronyms

DNS	Direct Numerical Simulation
FTC	fully transported chemistry
HTTC	Hybrid Transported-Tabulated Chemistry

Greek

ε	threshold
α_k	coefficients used to define the progress variable
β_k	coefficients used to define the mixture fraction
ϕ	equivalence ratio
ρ	density
$\dot{\omega}$	chemical source term

Latin

c_p	heat capacity at constant pressure
h	enthalpy
N_m	total number of tabulated species
N_M	total number of transported species
N_r	total number of elementary reactions
N_sp	total number of chemical species
P	pressure
S	set of conditions for fresh gases
S_L	laminar flame speed
t	time
T	temperature
u_i	ith component of the velocity
Z	mixture fraction
Y	mass fraction
Y_c	progress variable
$Y_{c,i}$	value of Y_c where Y has a minimum different from zero

Subscript

eq	equilibrium value
k	kth species
L	lean
m	minor or tabulated species
M	major or transported species
R	rich
u	unburnt

Superscript

lmin	local minimum in Y_c space
lmax	local maximum in Y_c space

schemes could then be considered.

The HTTC method was proposed by Ribert et al. [11] and validated in the context of the simulation of mono-dimensional laminar freely propagating premixed methane/air flames. Its extension to heavy hydrocarbons such as kerosene is presented in this study. Validations are performed with a fully compressible solver. The paper is organized as follows: next section describes the methodology of HTTC. The self-similarity of hydrocarbon flames is reinforced in Section 3. The procedure is extended to kerosene-air flames featuring NO_x emission. The time step used in HTTC simulations becomes then four orders of magnitude larger than for a simulation with detailed chemistry, confirming the potentiality of the proposed method.

2. Hybrid Transported-Tabulated Chemistry

In the original work of Ribert et al.n HTTC [11], the method was implemented and tested in the steady, isobaric one-dimensional numerical code REGATH [16,17] for methane-air flames only. Its implementation into a fully compressible DNS numerical code requires additional developments that are now briefly explained. The HTTC solver shares many features with any fully transported chemistry solver (shortened by the acronym “FTC”): for example, the chemistry integration or the treatment of boundary conditions are unchanged. Only the number of transported species and the handling of the look-up table for minor species are different and require special cares.

The following notations are introduced:

- The subscript M (for “Major”) will refer to the transported species, and the subscript m (for “minor”) will refer to the tabulated species.
- The total number of transported and tabulated species are denoted N_M and N_m, respectively. The total number of species present in the detailed kinetic mechanism is denoted N_{sp}, and the total number of chemical reactions is N_r. We have $N_\mathrm{sp} = N_M + N_m$.
- The letters M and m will also be used to refer to the set of indices of the transported and tabulated species, respectively. Then, $M = \{k|\text{species } k \text{ is transported}\}$, $m = \{k|\text{species } k \text{ is tabulated}\}$, and $m \cup M = [1, N_{sp}]$.
- The mass fraction of any species k is denoted Y_k. The full vector of species is denoted Y: $Y = (Y_1, ..., Y_{N_\mathrm{sp}})$. The vectors Y_M and Y_m are built with the mass fractions of the transported and tabulated species, respectively. We have $Y_M = (Y_k|k \in M)$ and $Y_m = (Y_k|k \in m)$.
- Classic notations are used for the time (t), spatial coordinates (x_i), density (ρ), pressure (P), temperature (T) and velocity components (u_i) in the x_i-axis.

Neglecting external forces and energy sources, any fully transported chemistry solver considers the balance equations of momentum, species density k, ρ_k ($\rho_k = \rho Y_k$) and energy. The total non chemical energy is presently used and corresponds to the sum of the kinetic energy and sensible energy. The diffusion velocity is modeled with the Hirschfelder and Curtiss approximation [18] and a correction velocity [19] is used to ensure mass conservation. The reaction rate of species k ($\dot{\omega}_k$) is evaluated from Arrhenius rate expressions.

Introducing the HTTC approach into a numerical code is simplified if a FTC solver is already present. With HTTC [11], the major species (Y_M) are transported with the flow whereas the mass fraction of minor species (Y_m) are extracted from a look-up table. Then, the focus is on tasks that differ from the FTC solver.

The initialization step is nearly identical for the two solvers (FTC and HTTC). The thermodynamical data of species involved in the kinetic mechanism and the Arrhenius coefficients of the chemical reaction are fetched in a data file and the primitive variables (P, T, U and Y) are read from an initial solution. The HTTC solver requires an additional step, to read and store in the memory of every MPI process the look-up table that contains the tabulated minor species mass fractions (Y_m). The data Y_m is accessible via the parameters or coordinates of the look-up table and represent physical phenomena (progress of reaction, mixing, etc.). By following the classic approach of tabulated chemistry [20,21], it is common to use the progress variable (Y_c), mixture fraction (Z), enthalpy (h), etc. as table coordinates. Building the look-up table is detailed in Section 3.

However, to ensure the mass conservation with the solver HTTC, ρ at the current time step n, is given by:

$$\rho^n = \sum_{k\in M} \rho_k^n + \sum_{k\in m} \rho_k^{n-1} = \sum_{k\in M} \rho_k^n + \sum_{k\in m} \rho^{n-1} Y_k^{n-1}, \quad (1)$$

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