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Simulations of a turbulent non-premixed flame using combined dimension reduction and tabulation for combustion chemistry

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HIGHLIGHTS

- Advanced methods are needed for the use of detailed hydrocarbon chemistry in simulations.
- We demonstrate a method for accelerating chemistry calculations in CFD.
- We simulate a bluff-body-stabilized non-premixed turbulent methane/air flame.
- NOx and CO emissions have been accurately and efficiently modeled.
- Combustion models have no impacts on reduced description of reactive flows.

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ABSTRACT

The use of large chemical mechanisms of hydrocarbon fuels in turbulent flame simulations is computationally expensive due to the large number of chemical species and the wide range of chemical time scales involved. The reduced description of reactive flows in combination with chemistry tabulation can effectively reduce the simulation time when detailed chemical kinetics is employed in multi-dimensional Computational Fluid Dynamics (CFDs). In this study, this approach is applied to simulate a bluff-body-stabilized non-premixed flame with the eddy dissipation concept (EDC) and transported probability density function (PDF) combustion models. In the calculations, the 31 chemical species in the GRI-Mech 1.2 mechanism are partitioned into represented species and unrepresented species. The reactive system is described in terms of a smaller number of represented species instead of the full set of chemical species in the mechanism; and the evolution equations are solved only for the represented species. The *In Situ* Adaptive Tabulation (ISAT) approach is employed to speed the chemistry calculation by tabulating information of the reduced system. The simulations show that a reduced description with 13 represented species and three atomic elements in the unrepresented species agrees well with the full description that has 31 species while achieving a speed-up factor of up to three. Compared to experimental data, the PDF model yields more accurate predictions in the composition fields of upstream locations than EDC. The impact of the reduced description on NOx emissions is also studied by performing the full and reduced descriptions of the flame with GRI-Mech 3.0. The study shows that a reduced description with a total 16 represented species, including three nitrogen-containing species, agrees well with the full description and incurs less than 5% error in NO predictions. Moreover, in this study, an efficient initialization procedure is first demonstrated for the CFD calculations with detailed chemistry.

1. Introduction

Realistic modeling of chemically reactive flows burning hydrocarbon fuels involves a large number of chemical species, which participate in tens to thousands of chemical reactions occurring simultaneously within a complex flow field [1]. For example, a detailed mechanism for iso-octane [2] contains more than eight hundred species that participate in more than three thousand reactions. Currently, it is computationally prohibitive to directly incorporate detailed chemical kinetics in multi-dimensional simulations due principally to the large number of species involved and the wide range of chemical time scales present, although its use is essential for a reliable prediction of ignition and extinction phenomena, and emissions such as CO and NOx. To meet this challenge, significant progress has been made in methodologies and

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algorithms that rationally reduce the computational burden imposed by the use of detailed chemical kinetics in CFD [1,3–32]. Among the available techniques, three frequently used in the literature are: the development of skeletal mechanisms from large detailed mechanisms by the elimination of inconsequential species and reactions [9–13]; dimension-reduction techniques [14–27]; and storage/retrieval methodologies such as *in situ* adaptive tabulation (ISAT) [28,29], repro-modeling [30], piecewise implementation of solution mapping (PRISM) [31], and artificial neural networks (ANNs) [32].

In recent years, combined methodologies have also been developed, wherein reduced mechanisms or dimension reduction methods are used in conjunction with storage/retrieval methods [18,33–35]. For example, a reduced description of reactive flows was recently developed by Ren et al. [35] by exploiting, in combination, techniques of dimension reduction and storage retrieval to effectively reduce the computational cost of detailed chemical kinetics in CFD. It can be implemented in a species-transport-equation-based CFD solver or a particle-based (such as PDF methods) CFD solver. In this approach, the full set of n_s chemical species in mechanism are partitioned into n_{rs} represented species and n_{us} unrepresented species (with $n_{rs} + n_{us} = n_s$). A flow solver solves the evolution equations only for the n_{rs} represented species instead of for the full set of n_s chemical species. Only when necessary, the n_{us} unrepresented species are reconstructed assuming that they are in constrained chemical equilibrium. The ISAT method is employed to speed the chemistry calculation by tabulating information of the reduced system. Hence the approach determines and tabulates *in situ* the necessary information of the reduced system based on the n_s-species detailed mechanism. In [35], the approach was validated in both premixed and non-premixed methane/air laminar flames. With the GRI-Mech 1.2 mechanism consisting of 31 species, with a relatively moderate decrease in accuracy, the reduced descriptions (with 12–16 represented species) achieve an additional speedup factor of up to three compared to the full description with ISAT, which has already achieved at least one order of magnitude speed up compared to the ones without ISAT.

In this work, this reduced description approach is further investigated in turbulent flame calculations in the context of different combustion models. Specifically, reduced descriptions of a bluff-body-stabilized non-premixed turbulent flame [36] are performed with the eddy dissipation concept (EDC) [37] and transported probability density function (PDF) combustion models [38]. The accuracy and efficiency of the reduced descriptions are assessed against the full descriptions in which all the chemical species are transported. Particularly, the impact of the combustion models on the accuracy of the reduced description will be investigated and the impact of reduced description on NOx emission prediction will be quantified. Moreover a computationally efficient initialization procedure is first demonstrated for numerical calculations with detailed chemistry. The outline of the remainder of the paper is as follows. In Section 2, the reduced description of reactive flows with tabulation of chemistry is briefly reviewed. The calculation details and results are reported in Sections 3, and Section 4 provides conclusions.

2. Reduced description of reactive flows with tabulation of chemistry

In this section we briefly describe the notions and steps in the reduced description; full details are provided in [35]. We consider a reacting gas-phase mixture consisting of n_s chemical species, composed of n_e elements. The thermo-chemical state of the mixture (at a given position and time) is completely characterized by the pressure p, the mixture enthalpy h, and the n_s-vector $\boldsymbol{z}$ of specific moles of the species. (The specific moles of species i is given as $z_i = Y_i/w_i$, where Y_i and w_i are the mass fraction and molecular weight of the species i, respectively. In reactive flow calculations, the species concentrations are governed by two processes: chemical reaction and transport. We consider the important class of solution methods in which a splitting scheme is used, where the chemical reaction and transport processes are accounted for in two separate sub-steps. Due to chemical reactions, the composition $\boldsymbol{z}$ evolves in time according to the following set of ordinary differential equations (ODEs):

$$\frac{dz}{dt} = s(\mathbf{z}) \tag{1}$$

where $\boldsymbol{S}$ is the n_s-vector of chemical production rates determined by the chemical mechanism used to represent the chemistry.

2.1. Reduced representation of chemistry

In the reduced description via dimension reduction, species are decomposed as $\boldsymbol{z} = \{\boldsymbol{z}^r, \boldsymbol{z}^u\}$, where $\boldsymbol{z}^r$ is an n_{rs}-vector of "represented" species, and $\boldsymbol{z}^u$ is an n_{us}-vector of "unrepresented" species (with $n_{rs} + n_{us} = n_s$ and $n_{rs} < n_s - n_e$). The reduced representation of the chemistry is $\boldsymbol{r} \equiv \{\boldsymbol{z}^r, \boldsymbol{z}^{u,e}\}$, where $\boldsymbol{z}^{u,e}$ is an n_e-vector giving the specific moles of the elements in the unrepresented species (for atom conservation). The elements in the unrepresented species are needed when reconstructing the unrepresented species using constrained equilibrium. Thus $\boldsymbol{r}$ is a vector of length $n_r = n_{rs} + n_e$, and the dimension of the system is reduced from n_s to n_r. At any time, the reduced representation $\boldsymbol{r}$ is related to the full composition $\boldsymbol{z}$ by $\boldsymbol{r} = \boldsymbol{B}^T\boldsymbol{z}$, where $\boldsymbol{B}$ is a known constant $n_s \times n_r$ matrix which can be determined for a specified set of represented species. The thermo-chemical state of the reduced reactive system is represented by $\{\boldsymbol{r}(\boldsymbol{x}, t); h(\boldsymbol{x}, t); p(\boldsymbol{x}, t))\}$. With assigned thermal and transport properties, the elements in the unrepresented species $\boldsymbol{z}^{u,e}$ are treated as "notional" species in the reduced description.

2.2. Steps in reduced description

In the reduced description, only the transport equations for the reduced composition $\tilde{\boldsymbol{r}} = \{\boldsymbol{r}; h\}$ are solved. Note that the unrepresented elements $\boldsymbol{z}^{u,e}$ do not have chemical reaction source terms. Chemical reactions are separated into a single reaction fractional step, where the effect of chemical reactions on the reduced composition is addressed through "species reconstruction" using constrained equilibrium [16–21] and the evaluation of reaction mapping in the full composition space. Specifically, the change in reduced composition due to chemical reactions is addressed through the following three major steps. The first step is the species reconstruction, i.e. given the initial reduced composition $\tilde{\boldsymbol{r}}(0)$, the initial full composition before reaction, denoted by $\Phi^{CE}(0) = \{\boldsymbol{z}^{CE}, h, p\}$ is obtained by assuming that the unrepresented species are in constrained chemical equilibrium at the cell (or particle) pressure and enthalpy, subject to the constraints of the represented species and the unrepresented elements. The constrained-equilibrium composition is computed using the CEQ [39] code. The second step is to obtain the reaction mapping. The set of ODEs Eq. (1) (together with the energy variable) is integrated numerically in the full space for a reaction time step Δt to obtain the reaction mapping (i.e. the composition after reaction) of all the species, $\boldsymbol{\Phi}(\Delta t)$. The final step is reduction, i.e. from the obtained reaction mapping, $\boldsymbol{\Phi}(\Delta t)$, extract the reaction mapping of the reduced composition denoted by $\boldsymbol{R}(\tilde{\boldsymbol{r}}) \equiv \tilde{\boldsymbol{r}}(\Delta t)$ using $\boldsymbol{r} = \boldsymbol{B}^T\boldsymbol{z}$. Note that a different approach for the second step [18,33] is to integrate the rate equations for the constraint potentials, which is more economical than integrating the ODEs (Eq. (1)) directly. In our