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ScienceDirect
Proceedings of the Combustion Institute 32 (2009) 1687–1694
Proceedings of the Combustion Institute
www.elsevier.com/locate/proci

Turbulent flame simulation taking advantage of tabulated chemistry self-similar properties

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Abstract

Predicting the flame shape, its stabilization process, and pollutant emissions in practical combustion devices requires to incorporate complex chemistry features. As detailed chemical schemes are too voluminous for practical numerical simulations, tabulated chemistry techniques have been proposed to account for the complexity of kinetics in turbulent flame simulations. Unfortunately, the size of these databases may become a crucial issue for efficient implementation on massively parallel computers. A reduction strategy that takes advantage of self-similar properties of tabulated chemistry is proposed for turbulent combustion modeling. A reduction of the database size by a factor of 1000 is achieved. This procedure is successfully applied to a RANS simulation of a turbulent jet flame.

Keywords: Turbulent combustion; Modeling; Tabulated chemistry; PDF

1. Introduction

Thanks to the emergence of super-computer, simulations of highly complex realistic turbulent reacting flow become feasible. For example, numerical simulation of a 20 degree sector of an entire gas turbine engine has been recently performed using up to 700 processors [1]. During the same period, the ignition of a full gas turbine combustion chamber has been simulated using 4096 processors [2]. Flame ignition and extinction or prediction of pollutant formation are crucial issues in such simulations and are strongly influenced by the chemistry. Unfortunately, despite the rapid advance in computational power, to perform turbulent simulations of industrial configurations including detailed mechanism remains out of reach.

A large variety of approaches exist to tackle the interaction of chemistry with fluid dynamics at reduced computational cost. Most of them consist of tabulating trajectories effectively accessed in a chemical space during realistic turbulent reactive flow. Chemical reaction rates are then stored in a look-up table. The Intrinsic Low Dimensional Manifold (ILDM) is based on a direct mathematical analysis of the dynamic behavior of the nonlinear chemical system response [3]. Relevant subspaces are determined by separating chemical evolutions between fast and slow time scales. ILDM allows an exact description of the chemical system and has been successfully applied to turbulent jet flames [4]. However, a large number of dimension, around four or five, is required when hydrocarbons fuels are considered. Alternatives to ILDM that requires less dimensions are Flame Prolongation of ILDM (FPI) [5] or Flamelet

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doi:10.1016/j.proci.2008.06.004

Generated Manifold (FGM) [6]. Both techniques assumes that the chemical flame structure can be described in a reduced phase subspace from elementary combustion configurations. For example, the chemical subspace of partially premixed flames or self-igniting mixtures can be approximated from a collection of 1D laminar flames [7] or 0D auto-ignition stirred reactors computations [8], respectively. Efficiency of the FPI tabulation procedure has been demonstrated for laminar premixed and partially premixed flames [5,7,9]. In Refs. [10,11], this technique has been used to successfully compute a turbulent premixed flame and a turbulent jet flame, respectively.

In parallel computation framework, chemical databases are loaded in the local memory of each processor to minimize data exchanges. Then, the chemical database size may become a problem when handling with a large number of coordinates. This issues is of crucial importance when running on massively parallel computers having a limited memory per processor. For instance, the memory per processor available on the super-computer IBM BlueGene/L located at DOE comprising 212,992 processors is limited to 346 Mb.[1]

Some strategies has been developed to limit the chemical database sizes. For example, ISAT (In Situ Adaptive Tabulation) [12] is based on the in situ generation of look-up tables, which are constructed from the direct solving of time evolution of species concentrations. Only the chemical compositions effectively accessed during the computation are computed and included in the chemical table. An alternative to reduce the database size is to introduce optimal neural networks to approximate chemical tables [13,14].

In the framework of FPI (or FGM), Ribert et al. have exploited self-similar properties of laminar premixed flames to reduce the database size [15]. They show that species reaction rates expressed as a function of a progress variable reduce to single curves when using suitable scaling rules. For example, an initial 2D FPI chemical database for partially premixed flames is reduced to four vectors. This technique has been successfully applied to premixed laminar flames computations. This strategy has been recently extended to turbulent regimes by taking advantage of self-similar properties of mean FPI chemical quantities under a presumed probability density function formalism [16,17]. The 4D chemical database has been reduced to two 2D tables. The required memory is then dramatically reduced while, because each quadrilinear interpolation is replaced by two bilinear interpolations, access times to look-up tables are reduced by about 60%. This reduction procedure gives very good agreement with the 4D original database on a priori tests but has not been applied yet in practical turbulent flame simulations.

The objective of the present work is to investigate the performance of this reduction procedure for actual RANS flame simulations. In the first section, the turbulent combustion model that combines FPI and presumed PDF modeling is presented. This modeling strategy has been successfully applied in RANS simulations of turbulent premixed [10] and jet diffusion flames [11]. Then, details are given for the reduction of the chemical database size using self-similar properties of tabulated mean chemical reaction rates. Finally simulation of a jet flame is proposed. A comparison between experimental data and computational results obtained with the original and the reduced database is provided.

2. Modeling turbulent combustion using tabulated chemistry

2.1. Chemistry tabulation

The FPI approach [5] assumes that the chemical subspaces accessed by a partially premixed flame in a complex geometry configuration can be mapped by a collection of 1D premixed laminar flames computed for various equivalence ratios using detailed chemistry. This assumption is relevant for premixed and partially premixed flames [7]. However, errors are introduced in non-premixed regions, when mass diffusion through iso-equivalence ratio surfaces dominates. Nevertheless, these errors are limited when the fuel feeding stream is close to the rich mixture flammability limits [7], as in the flame investigated here (equivalence ratio of the fuel stream is 3 whereas the rich flammability limit of methane/air is about 2).

One-dimensional laminar premixed flames are computed for equivalence ratios evolving within the mixture flammability limits of methane-air combustion under unity Lewis assumption. The PREMIX [18] solver is combined with the chemical mechanism of Lindstedt [19], involving 29 species and 300 elementary reactions. A look-up table stores chemical reaction rates as a function of two coordinates: $Y_c = Y_{CO} + Y_{CO_2}$, combines CO and CO_2 mass fractions to measure the reaction progress [9] and the nitrogen mass fraction $Y_z = Y_{N_2}$, corresponds to a mixture fraction as NO_x formation is not considered. These two coordinates are normalized as:

$$z = \frac{Y_z - Y_{z_o}}{Y_{z_f} - Y_{z_o}}; \quad c = \frac{Y_c - Y_{c_f}(Y_z)}{Y_{c_b}(Y_z) - Y_{c_f}(Y_z)} \tag{1}$$

where z and c vary between zero and unity. Y_{c_f} and Y_{c_b} are, respectively, the values of Y_c in fresh

[1] DOE IBM BlueGene/L is first ranked on the TOP500 list released on November, 2007 (http://www.top500.org).