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An improved high-order scheme for DNS of low Mach number turbulent reacting flows based on stiff chemistry solver

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ABSTRACT

We present an improved numerical scheme for numerical simulations of low Mach number turbulent reacting flows with detailed chemistry and transport. The method is based on a semi-implicit operator-splitting scheme with a stiff solver for integration of the chemical kinetic rates, developed by Knio et al. [O.M. Knio, H.N. Najm, P.S. Wyckoff, A semi-implicit numerical scheme for reacting flow II. Stiff, operator-split formulation, Journal of Computational Physics 154 (2) (1999) 428–467]. Using the material derivative form of continuity equation, we enhance the scheme to allow for large density ratio in the flow field. The scheme is developed for direct numerical simulation of turbulent reacting flow by employing high-order discretization for the spatial terms. The accuracy of the scheme in space and time is verified by examining the grid/time-step dependency on one-dimensional benchmark cases: a freely propagating premixed flame in an open environment and in an enclosure related to spark-ignition engines. The scheme is then examined in simulations of a two-dimensional laminar flame/vortex-pair interaction. Furthermore, we apply the scheme to direct numerical simulation of a homogeneous charge compression ignition (HCCI) process in an enclosure studied previously in the literature. Satisfactory agreement is found in terms of the overall ignition behavior, local reaction zone structures and statistical quantities. Finally, the scheme is used to study the development of intrinsic flame instabilities in a lean H_2/air premixed flame, where it is shown that the spatial and temporary accuracies of numerical schemes can have great impact on the prediction of the sensitive nonlinear evolution process of flame instability.

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1. Introduction

With the development in computational methods and the increasing availability of massive scientific computing resources in recent decades, detailed reacting flow simulation emerges as a promising approach for combustion research [1–3]. In turbulent reacting flows there exists a wide range of chemistry and flow scales. A detailed simulation should resolve accurately the relevant scales in both space and time; as such, it is desirable to develop high efficiency numerical schemes that can handle the multi-scale chemical and physical processes involved.

For numerical simulation of reacting flows the convection, diffusion and reaction processes can all be the limiting factor for the global computational time step. In an explicit method the convection terms limit the time step due to the well-known CFL constraint. The diffusion stability limit on the other hand requires that $D_{\max}\Delta t/\Delta x^2 < 1/2^q$, where $D_{\max}$ is the maximum diffusion coefficient, q is the space dimension number, and Δt and Δx are the time step and grid size, respectively. For an explicit integration of the chemical reacting rates, the time step should be less than the time scale of the fastest elementary

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reactions within the chemical kinetic mechanism. A full explicit solver satisfying all three constraints are relatively straightforward to implement with high spatial and temporal accuracy; this approach is widely adopted for compressible reacting flow simulations, e.g. [3–5]. However, for numerical simulations of low speed reacting flows the CPU demand with such solver can be very high due to the small time stepping. For such system one of the most limiting factors on time step size is usually the reaction terms. For example, Najm et al. [6] estimated that for a CH_4/air mechanism a 2 ns time step is required for an accurate chemistry integration. Another limit can be the CFL constraint due to the high acoustic speed. The acoustic speed can lead to a time step as small as the smallest reaction scales.

For numerical simulations of low Mach number reacting flows, a typical way to remove the reaction limits on time step is to use a stiff solver for integration of the chemical reaction rates. With a stiff solver the chemistry integration can be done in adaptive smaller time steps. The acoustic limit on time step can be circumvented using the Low Mach number assumption by which the high-speed acoustic wave is neglected. With both the stiff chemistry solver and the low Mach number assumption, the calculation of diffusion terms can still limit the time step size through the diffusion stability limit. For example, for a 2D CH_4/air flame the critical time step is around 20 ns with a cell size of 15.6 μm [6]. The problem becomes more severe if smaller cell size is used since the diffusion stability limit scales with the square of the cell size.

One way to use a larger time step while still maintaining stability is to solve all the diffusion terms implicitly, as did in Day and Bell [7]. However, it is a challenge to design an efficient implicit algorithm when a large number of species equations are employed to take into account detailed chemistry mechanisms. Another difficulty stems from the large discretization stencils when high-order schemes are used in direct numerical simulations (DNS) of turbulent reactive flows. A feasible solution is to split a large time step calculation into multiple sub-steps of explicit integration of the diffusion terms, as in Knio et al. [8]. The fractional step splitting approach is stable and simple to implement even for high order discretization of diffusion terms, as long as a sub-time-step size satisfies the diffusion stability limit.

To integrate a stiff chemistry solver to a large time-step method for calculation of convection and diffusion terms an operator-splitting technique can be used. While simple splitting procedure is easier to implement it often leads to low-order discretization errors. It is still a research topic to devise high order accuracy and stable splitting methods [9–11] for the convection–diffusion-reaction (CDR) problems. To the best knowledge of the authors only a 2nd order symmetrical Strang splitting scheme [12] has been reported for multidimensional combustion simulations with complex chemistry as in Day and Bell [7] and Knio et al. [8]. For a CDR problem the Strang splitting method employs typically a full time step integration of either the diffusion terms or the reaction rates in between two half-time-step integrations of the other process. While keeping the stiff solver in the first and the last fractional steps is suggested in [13], it is more efficient to place the computationally heavy stiff solver in the center to avoid executing the stiff solver at each time step twice [8].

In reacting flow simulations the density field is varying in space. A well-known issue of numerical instability in flows with large density ratio (between the burned and unburned gases) has been addressed by several authors [7,14–17]. When the density change across the flame is large, the time derivative of density in the continuity equation can be very large if it is directly approximated with the density values at new time step and the previous time step. This can lead to numerical instability. An approach to remedy this instability is to use a predictor/corrector method [6,8,17]. This method was used in the work of Knio et al. [8], who employed a second corrector step in addition to the conventional predictor step. With only the predictor step, the stability can only be maintained at a lower density ratio of 2–3. By adding a corrector step numerical stability can be maintained for a rather high density ratio of 7–8. However, an absolute stability can not be guarantied for higher density ratio. An heuristic argument has given by Pierce [16] who speculated the cause of instability is the spurious heat release introduced by the numerical discretization error of the convective terms. This has motivated the development of another approach: using the material derivative (also known as advective derivative) form of continuity equation and estimating the material derivate of density, which is free of numerical errors in the discretization of convective terms. This method was used by Bell et al. [18] to simulate nuclear flames of a density ratio over 1000. With this approach the corrector step is no longer needed. The trade-off goes into the projection step, which involves the solution of a variable coefficient Poisson equation instead of a constant-coefficient one.

In this paper we propose an improved numerical scheme for simulation of low Mach number reacting flow. The method is based on the Strang operator splitting method with stiff chemistry solver placed in the middle step in between the two half-time-step integrations of the flow transport terms, as in the work of Knio et al. [8]. The numerical instability at large density ratios is addressed by employing the material derivative formulation of the continuity equation, as in Day and Bell's work [7]. We further incorporate the later development for efficient calculation of detailed transports coefficients of Najm et al. [19]. The proposed scheme is extended for direct numerical simulation of turbulent reacting flow by applying high order spatial scheme. While the previous works [6–8,19] were developed for constant pressure system, we further extend the scheme for simulating non-constant pressure reacting system.

The paper is organized as follow: Section 2 describes the governing equation for low Mach number reacting flows with the material derivative formulation of the continuity equation. Section 3 discusses the operator splitting method and the overall solving procedure, where the difference of the present scheme with the previous one [8] will be explained. In Section 4 the temporal and spatial accuracy of the proposed scheme will be examined in open and closed one-dimensional reacting flows. The scheme is further examined in numerical simulation of two well-known cases: the first is a laminar vortex-pair/flame interaction and the second is direct numerical simulation of auto-ignition of premixed fuel/air mixture in a constant volume enclosure with an initial temperature inhomogenity. Finally, the numerical scheme is employed to simulate the

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