

Numerical Investigation of Cylindrical Detonation using a Multiscale Adaptive Reduced Chemistry Solver (MARCS)

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Abstract

This study carried out direct numerical simulations of hydrogen-air cylindrical detonation with a central ignition source at a stagnation temperature of 3000K and stagnation pressure of 5MPa, using a Multiscale Adaptive Reduced Chemistry Solver (MARCS). The MARCS was developed by integrating the Correlated Dynamic Adaptive Chemistry and Transport (CO-DACT) method with the Hybrid Multi-Timescale (HMTS) and the G-Scheme methods, and a full-speed flow solver to conduct the efficient combustion modeling with detailed chemical kinetics. In the final paper, two different reduced chemical kinetics mechanisms, a comprehensively reduced mechanism and a 2-step skeletal mechanism, are examined. Results from these computations are compared with experimental observations, enabling their reliable assessment through the detailed investigation of averaged velocities as well as pressure fluctuations. Several initial turbulence intensities are also considered. Importance of including accurate chemical kinetics in numerical simulations is demonstrated.

1 Introduction

Cylindrical detonation was found to have a complicated three-dimensional structure in both experiments and numerical simulations. Previous studies are limited to the generation and self-sustaining mechanisms of cylindrical detonation. The cell-detonation shock front consists of a series of Mach stems and incident waves with transverse waves behind. Triple points appear due to the intersection of the leading shock, Mach shock and transverse shock wave. At the diverging stage, Soloukhin observed that the transverse fronts generate such that the average distance between adjacent perturbations maintains nearly constant with the detonation propagation [1]. Jiang [2] found out four mechanisms of the transverse wave generation in detonations, by using direct numerical simulations coupled with a 2-step kinetic model. Han [3] further pointed out the role of global curvature on the structure and propagation of weakly unstable cylindrical detonations, with a single step kinetics model in his simulations. Note that initial turbulence intensity has not been considered in the published papers.

Moreover, it was found that even a small or moderate uncertainty in chemical kinetic rates could lead to gross errors in the detonation simulation results [4]. However, detailed reaction mechanisms are typically too computationally expensive due to the large number of species and reactions, as well as the stiffness induced by the vastly different time scales, which may span several orders of magnitudes, between the major species and the highly reactive radicals. To address these two issues, a Multiscale Adaptive Reduced Chemistry Solver (MARCS) [5] for computationally efficient reactive-flow modeling, has been proposed recently. It integrates a parallel PDE solver and a full-speed flow solver [6], with the CO-DACT (Correlated dynamic adaptive chemistry and transport) method [7] for on-the-fly mechanism simplification and transport property evaluation, and with both HMTS (Hybrid multi-timescale) [8] and G-Scheme [9] methods that are adaptively selected as chemistry solver according to the size of the reduced mechanisms and the local combustion regimes.

The objective of this work is to apply MARCS in a cylindrical detonation simulation to investigate chemistry modeling strategies as well as the effects of initial turbulence intensity. The chemical mechanism adopted here, including 10 species and 26 reactions, was reduced by the present authors from the detailed HP-Mech [10] using PFA (Path flux analysis) method for skeletal reduction. Moreover, a 2-step global kinetic model by Sichel [11] will be applied to the same case. The discrepancies among the results of different models as well as different initial turbulence intensity will be discussed.

2 Multiscale Adaptive Reduced Chemistry Solver (MARCS)

In this section a brief introduction to the methods forming MARCS is provided.

A. Correlated dynamic adaptive chemistry and transport method (CO-DACT)

In a combustion simulation, one cell in adjacent time steps or two different cells in the same time step may have similar thermodynamic conditions, which results in the same local reduced chemical mechanism and/or transport properties. Therefore, detailed calculation in similar cells is redundant. Based on this idea, the CO-DACT method examines computational cells in correlated space spanned by a few phase parameters. Similar cells in the correlated space will be grouped so that the detailed calculation is performed only once.

Due to space limitation, only the implementation of the correlated groups is presented here, the details of phase parameter selection and the validation of the method can be found in [7]. Assuming the phase parameters are: (z_1, z_2, \dots, z_M) , in which each z_i ($i = 1, 2, \dots, M$) is a non-negative parameter in thermodynamic states, such as the temperature and mass or molar fractions, and M is the dimension of the phase space. The phase space, \mathbf{S} , can be constructed by taking the logarithm of the phase parameters: $\mathbf{S} = (\ln(z_1), \ln(z_2), \dots, \ln(z_M))^T$.

As shown in Figure 1, the computation cells in physical domain can be mapped into correlated groups by the following two procedures, time correlation and space correlation.

Time correlation: The time correlation between current and previous time step is examined and applied first. For any cell, if the thermodynamic states in the current and the previous time step fall into the same correlated group in the phase space, the cell at the adjacent time steps is correlated. So, the local reduced mechanism or the transport properties at previous step will be directly passed to the current time step. Here we only consider the time correlation between two adjacent time steps to limit the memory and CPU-time cost of data storage.

Space correlation: For the cells which are not in the time correlated groups, we apply the space correlation. A set of group indexes, (l_1, l_2, \dots, l_M) will be assigned to each cell, where $l_i = [(\ln(z_i) - \ln(z_{i,\min}))/2\varepsilon] + 1$, ($i = 1, 2, \dots, M$), and ε is a user specified threshold value to discretize the phase space.

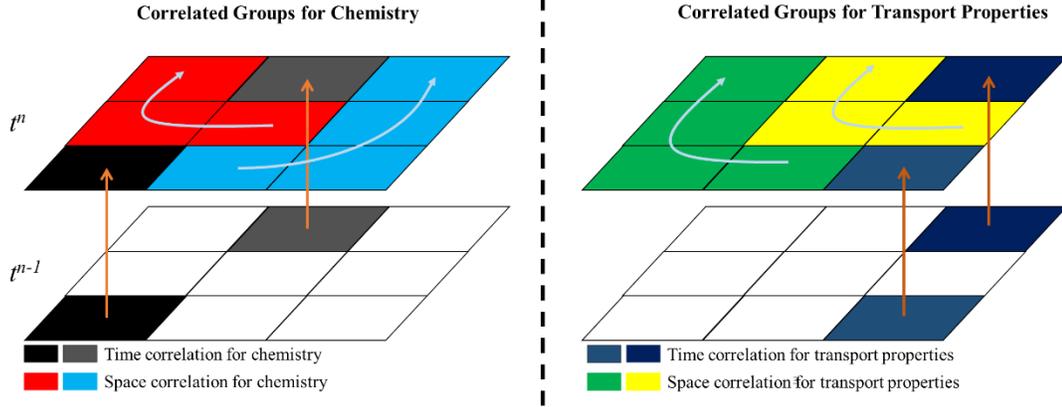


Figure 1. Schematic of time and space correlations in chemistry and transport properties.

According to the group index in phase space, the existing correlated groups will be recorded by a hash table. The key in the hash table is the group index l and the corresponding value, v , is the physical index of the first cell in this group. If the group index of a computation cell already exists, this cell will use the local reduced mechanism or the transport properties in cell v . Otherwise, the reduced mechanism or the transport properties in this cell will be calculated by the detailed model and a new key-value mapping will be added in the hash table.

B. Hybrid Multi-Timescale (HMTS) and G-Scheme methods

Based on the locally reduced mechanism from the CO-DACT method, the chemical reactions are integrated by HMTS or G-Scheme method. The solver automatically determines which method to use based on the combustion regime and the size of mechanism.

In the HMTS method, the species equations are integrated with their own characteristic time scales. The timescale of n -th species, τ_n , is estimated as [8]:

$$\tau_n = -\frac{\partial \ln Y_n}{\partial t} \frac{\partial \ln D_n}{\partial Y_n}^{-1} = \frac{\partial \ln D_n}{\partial Y_n} \frac{\partial \ln Y_n}{\partial t}^{-1} \quad (1)$$

where Y_n and D_n are the mass fraction and the destruction rate of n -th species, respectively. The species having a difference of timescale in one order of magnitude, are grouped into an integration group. The group index of the n -th species, G_n can be obtained as:

$$G_n = \left\lceil \log_{10} \frac{\tau_n}{t_{base}} \right\rceil + 1 \quad (2)$$

where t_{base} is the base time step in DNS calculations.

With the definitions of the timescale and group index, each of the groups is integrated separately based on its own timescale. Moreover, when it is not interested in the detailed history of the fast modes, the implicit Euler method can applied to further increase the efficiency. The HMTS method has been demonstrated to be more efficient than the VODE solver [8].

In the G-Scheme method [9], projects the system of ODEs in a phase space and exploits the possibility for reduction from the manifestation of spectral gaps. The modes are automatically spited into slow, active and fast modes by evaluating their own timescale and the relative contribution to the vector field. For slow and fast modes, the regular perturbation and standard perturbation are applied, respectively, to correct the results. The detailed integrations are only applied to the active modes. By doing this, the G-Scheme method removes the stiffness of the system using the time scale of the active modes for time integration.

The HMTS and G-Scheme methods have their own advantages depending on the mechanism size and the combustion regimes. Therefore, adaptively selecting the locally most efficient solver is according to the local conditions, so that higher computational efficiency can be achieved.

C. Full Speed Flow Solver

The HMTS and G-Scheme methods are implemented into an in-house parallelized full-speed flow solver [12] to simulate unsteady, compressible and reactive flows. The code is based on curvilinear coordinates and uses cell-centered collocated storage arrangement on semi-block structured grid for all quantities. The convection and diffusion terms are discretized with 3rd-order AUSMPW+ and central difference schemes respectively. A modified fully implicit lower-upper symmetric Gauss-Seidel (LU-SGS) scheme with Newton-like sub-iterations in pseudo time is taken as time marching method for solving the Navier-Stokes equations. The corresponding Courant number is under unit for most of the grid cells. Ten steps of sub-iteration are performed in each computational step, which guarantees that the residual decreases of about three orders of magnitude in the inner iteration so that the LU-SGS can achieve second order accuracy. This solver has been validated with several real-geometric cases [12, 13].

3 Numerical Setup

In the numerical experiments, Cartesian coordinates were used. The computational domain is a two-dimensional quarter area ($0 \leq x \leq 2\text{cm}$, $0 \leq y \leq 2\text{cm}$). We set a symmetric boundary condition at the lines $x=0$ and $y=0$ and a free outflow boundary condition at $x=2\text{cm}$ and $y=2\text{cm}$. A stoichiometric hydrogen-oxygen mixture filled the domain with an initial temperature $T_0=300\text{K}$ and pressure $P_0=1\text{MPa}$. A central ignition source was set with a stagnation temperature $T_s=3000\text{K}$ and a stagnation pressure $P_s=5\text{MPa}$ in the region with $R=\sqrt{x^2+y^2} \leq 2\text{mm}$. The computational domain was divided into 1000×1000 grids uniformly with the grid size $dx=dy=10\mu\text{m}$.

Two simulations: without (Case 1) and with (Case 2) initial turbulence intensity have been carried out. A detailed kinetics model including 10 species and 26 reactions is used adopted in both cases.

4 Preliminary Results

Figure 2 gives the pressure contours for Case 1 at $t=1.205\mu\text{s}$, $3.395\mu\text{s}$, $5.586\mu\text{s}$ and $7.776\mu\text{s}$ respectively. The detonation structure was successfully resolved by the MARCS solver. Figure 3 further shows the evolution of cellular structure and cylindrical front for Case 1 and Case 2. It is seen that initial turbulence intensity breaks the symmetry of the detonation front structure and promotes the generation of the transverse wave. At $t=9.96\mu\text{s}$, it appears a significant increase of the number of transverse waves in Case 2, which indicates the importance of turbulence in the generation of transverse waves.

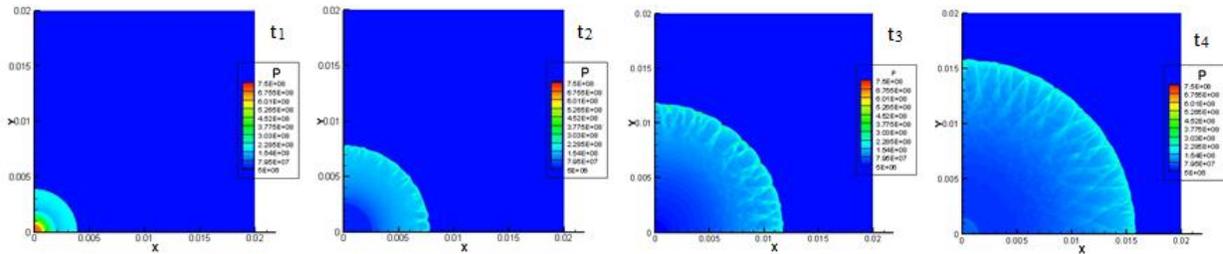


Figure 2. The pressure contours for Case 1 at $t=1.205\mu\text{s}$, $3.395\mu\text{s}$, $5.586\mu\text{s}$ and $7.776\mu\text{s}$ respectively.

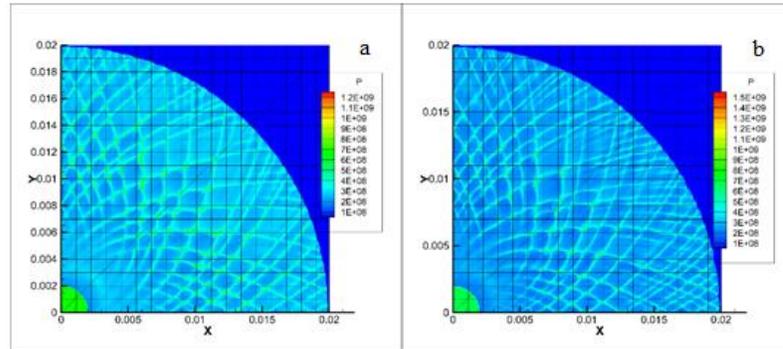


Figure 3. Evolution of cellular structure and cylindrical front with Case 1 (a) and Case 2 (b).

In Figure 4, we further compared the maximum pressure distribution on the diagonal line of Figure 3. It is seen that for both cases, pressure jump due to the evolution of cellular structure along with the movement of triple points. The peaks were dramatically shifted downstream with the initial turbulent intensity. The asymmetry leads to the split of peaks in Case 1 into two sub-peaks which indicates higher intensity in triple points than the Mach stems and incident waves.

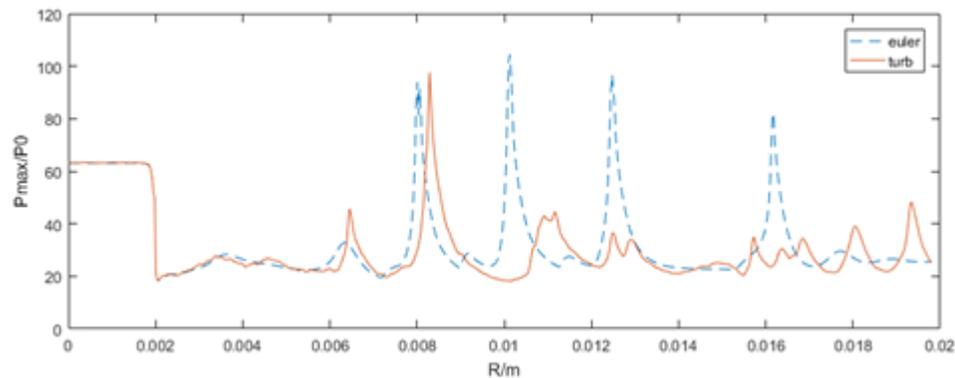


Figure 4. Maximum pressure distribution on the diagonal line of Figure 3

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