Structure of Conical Oblique Detonation Waves at an Angle of Attack

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1 Introduction

Oblique detonation waves (ODWs) have garnered considerable attention due to their significance in high-speed propulsion and the innovation of advanced engine designs [30, 13, 7]. These ODWs arise when fuel-air mixtures encounter a wedge, which generates a shock wave, providing the conditions for chemical reactions. When the shock compression is sufficiently intense, heat release may occur in close proximity to the shock wave, resulting in thermal choking along the shock-normal axis, thereby producing a detonation wave. Historically, ODWs have been broadly analyzed through computational simulations [16, 1, 9, 32, 6, 29, 27, 25] and through experimentation [15, 23, 20, 28, 19, 34, 11, 33]. Former research has predominantly concentrated on two-dimensional wedge configurations, contrasting with practical systems which are more likely to be cylindrical, thus forming shocks on conical surfaces with diminished shock losses [2]. The present investigation aims to apply a theoretical basis for conditions following oblique detonation, derived from inflow conditions, to inform highly detailed numerical simulations of conical detonations occurring at an angle of attack, thereby illustrating the detonation structure and the cellular instabilities that develop in this regime.

Experimental efforts in conical detonation waves has concentrated on initiation and criticality, both essential for designing efficient hypersonic engines [18]. Various studies have demonstrated that wave curvature (induced by blunt projectiles), the thickness of the reaction zone, and the size of detonation cells significantly influence the stability of oblique detonation waves [14, 12]. Verreault and Higgins [26] conducted experiments with conical projectiles with varying cone angles and identified different combustion regimes. In addition, they estimated the wave angle based on the CJ speed and the projectile velocity. In some cases, angle deficits of up to 20% were found. Due to challenging experimental conditions, only limited measurements that characterize wave angle and possible secondary wave structures such as oscillations or combustion-induced instabilities could be identified [18].

High-fidelity simulations of such conical detonations are inherently challenging due to the high computational cost. Earlier studies have considered axisymmetric configurations (for instance [32, 24, 5, 27]), where surface instabilities cannot be fully captured. However, the coupling between the reaction zone and the leading shock has been explored. Three-dimensional simulations have been performed using single-step chemistry, which have shown the formation of surface instabilities for a specific range of heat release [10]. The heat release parameter (Q in [10]) uniquely determines the CJ velocity and is used to characterize the detonation structure. Similar to two-dimensional wedges, increasing Q led to the formation of cellular instabilities. However, for a given inflow velocity, a higher Q also implied a lower overdrive factor, which contributed to steeper wave angles with increasing heat release. In the condition with the highest Q, it was observed that the transition to detonations from a conical shock occurred very close to the leading edge, and the instabilities, although present, displayed a fine structure. In other words, there exists an intermediate heat release value with sufficient overdrive to generate observable cellular instabilities.

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Ultimately, using a nominal set of operating conditions, induction-region-resolved numerical simulation with multistep chemical kinetics is performed. This work presents the first three-dimensional numerical simulation of conical detonation at an angle of attack, allowing the study of instability formation and variation along the detonation surface.

2 Flow Configuration

Figure 1 presents the three-dimensional cone geometry schematic used in this study. The inflow conditions are specified at Mach 7, with pressure and temperature matching the standard atmosphere (1 atm and 298.15 K, respectively) and an angle of attack of 3°. A stoichiometric ethylene-air mixture is implemented. Figure 1 underlines key characteristics of conical detonation waves. It is important to note that the cone half-angle is fixed at 45°; however, due to the 3°angle of attack, the wave angle on the topside, β_1, exceeds that on the underside, β_2. Through a one-dimensional analysis, these values fall within the weakly overdriven regime. The computational domain measures L_x = 1.125 cm, L_y = 2.0625 cm, and L_z = 2.0625 cm.

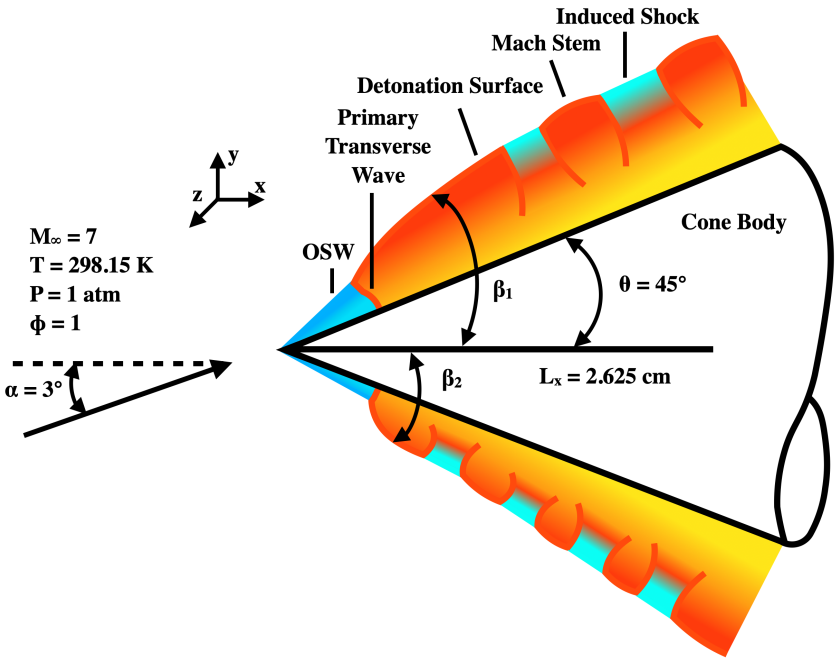


Figure 1: Schematic of simulation domain.

3 Numerical Methods

The reacting compressible Navier-Stokes equations are solved using a block-structured AMReX-based finite-volume solver to study the conical detonation system. In this work, the Strang operator splitting is used to split the time integration of the chemical and fluid systems [17]. In this setting, the limiting chemical timescale is assumed to be sufficiently smaller than the flow timescales, allowing the flow to be considered frozen during the evaluation of chemical kinetics. Multistep chemistry is solved using a matrix-based algorithm [3]. The inviscid fluxes are evaluated using a MUSCL (Monotonic Upwind Scheme for Conservation Laws) approximate Riemann solver and limited linear reconstruction. A shock-stable variant of the well-known HLLC (Harten- Lax-van Leer-Contact) solver, the approximate HLLC-LM [8] Riemann solver, is used to compute convective fluxes. The HLLC-LM scheme introduces

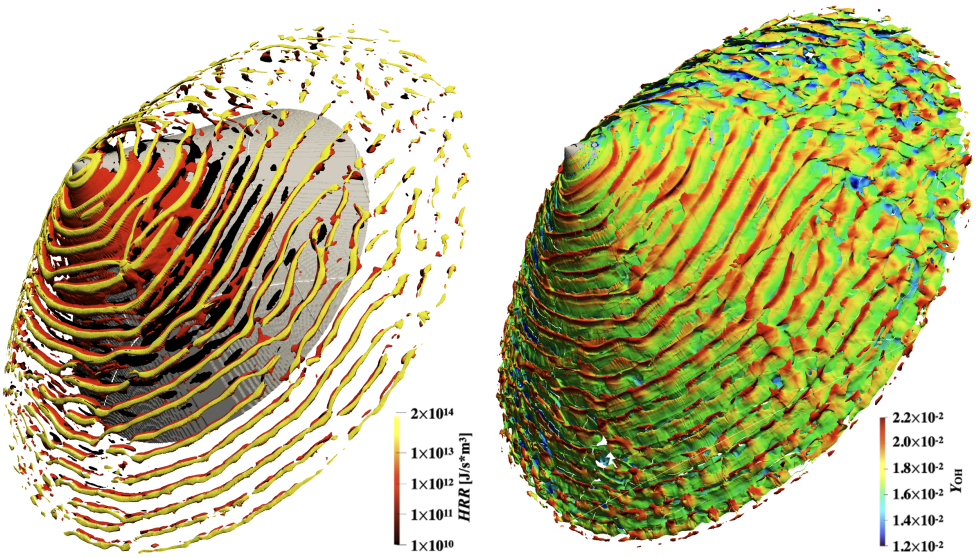
a smooth decay of the acoustic dissipation in the low Mach regime, thereby providing sufficient dissipation to limit grid-aligned instabilities. The viscous fluxes are evaluated using a second-order central scheme, and time integration is performed using the RK-3ssp scheme. Further discussion of numerical methods can be found in the works of Bielawski et al.[4] and Sharma et al. [21]. The modeling of multistep chemistry is crucial for understanding the development of instabilities within detonation waves, due to their wide range of compositions and thermodynamic states [1]. This multistep chemistry is represented using a skeletal mechanism derived from the FFCM-1 chemical kinetics model [22]. Tailored for C_2H_4 oxidation in the supersonic combustion environments typical of detonations and scramjets, the skeletal model comprises 30 species and 231 reactions [31]. The ODW simulation's maximum resolution is 14.6 μm, encompassing around 500 million cells. This highest spatial resolution corresponds to 42 cells per induction length for the given conditions. The simulation utilized 90 H100 NVIDIA GPUs, running for 72 hours.

4 Results and Discussion

Based on the detailed simulation approach described in Sec. 3, a representative condition of $M = 7$ at STP is simulated with a premixed mixture of ethylene-air for a cone with a half angle of 45°at an angle of attack of 3°. The subsequent discussion elaborates on the details of the detonation structure.

Figure 2a presents the local heat release rate superimposed on the isosurfaces of the sonic flow conditions. These regions represent a strong overdrive factor, where the post-detonation flow locally is sufficiently compressed to reach subsonic flow in the wave normal direction. The observed heat release rates are comparable to strong detonations, with values reaching a peak of 2×10^{14} J/s·m^3 near triple points. It is important to highlight the regularized structure of the triple points azimuthally along the underside compared to the topside, where the triple point structure is fragmented. This is due to the increased compression along the underside with the inflow angle of attack. In prior research on detonations, increased compression has been shown to increase the frequency of instability formation in a similar manner. The spatial distribution of chemical reactions, marked by the OH mass fraction, is shown in Fig. 2b where increased OH formation is prominent at overdriven triple point locations. This lower heat release rate surface represents chemical reactions in the post-shock deflagration state rather than at locally overdriven high heat release rates.

When observing detonation instability formation along the cone axis, a wide range of instability states can be observed as shown in Fig. 3. The sonic regions are colored by angular velocity with clockwise and counter-clockwise instabilities marked in red and blue respectively. Instabilities on the underside are more regularized, but move rapidly away from each other until they collide intensely yet infrequently on the topside in a fragmented instability pattern. Moreover, the contrasting velocity contours in the vicinity of the triple points emphasize the interactions occurring at the collision sites and the resulting velocity conditions following the collisions. The triple points along the underside, while azimuthally uniform locally, display a mixing of clockwise and counter-clockwise modes with few significant triple point collisions. This may present a unique form of triple-point formation distinct from other detonation configurations, such as channel detonation, where external geometric effects significantly inform formation. It is also important to note that the collisional frequency of triple points along the left and right sides of the detonation surface are qualitatively similar to that of conical detonation without an angle of attack, which may be explained by the fact that the angle of attack may present as a local sideslip rather than increased or reduced shock compression.



(a) (b)

Figure 2: (a) $M = 1$ isosurface colored by heat release rate (*HRR*). (b) *HRR* = 1×10^{12} J/s·m^3 isosurface colored by Y_{OH}.

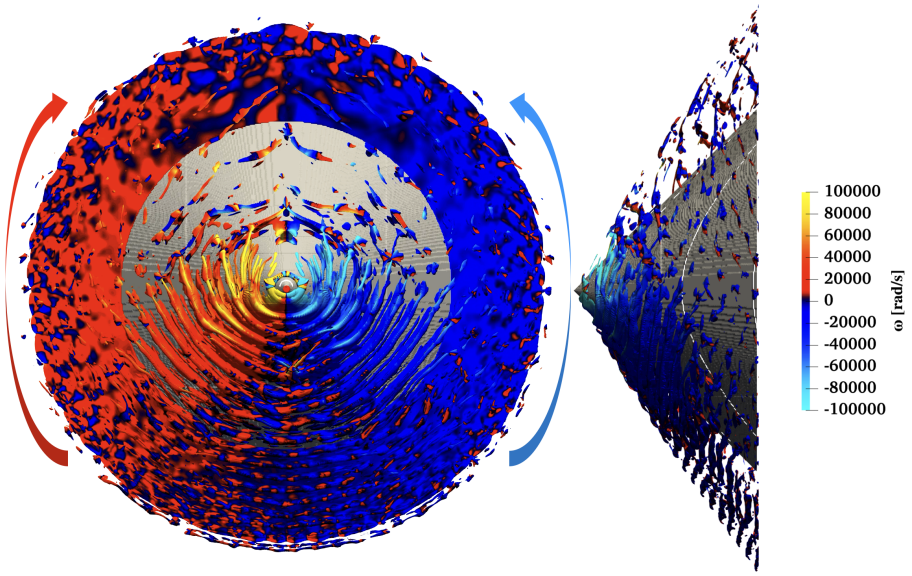


Figure 3: $M = 1$ isosurface colored by angular velocity

5 Conclusion

The high-fidelity simulations with multistep chemical kinetics presents cellular instabilities formed on the detonation surface that lead to locally intense heat release, even for a conical system at an angle of attack that has significant isentropic expansion and nominally weaker initial shock compared to a two-dimensional wedge. Overall, the detonation structure is similar to two-dimensional wedge-based oblique detonations and planar cellular detonations. The simulations indicate that the transverse waves reflecting from the surface of the cone lead to the formation of triple points on the detonation surface, which could lead to the formation of further instabilities.

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