Dynamics and Properties of 2D vs. 3D Ethylene-Air Detonations

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1 Introduction

Ethylene has been considered as a fuel of choice for detonation-based propulsion devices such as Rotating Detonation Engines (RDEs) [1]. In comparison with many other hydrocarbon fuels, ethylene is more reactive and hence it exhibits better detonatability. Ethylene is also formed as a main species during pyrolysis of real liquid fuels (e.g., Jet A and JP8). For these reasons, a close study of the dynamics of multi-dimensional detonations in ethylene-oxidizer mixtures is beneficial to both fundamental understanding of fuel-dependent detonation chemistry and detonation dynamics, and practical RDE design. Over the past decade, with the advent of high performance computing, significant progress has been made in numerical modeling of gas-phase detonations. Studies are however primarily limited to two-dimensional (2D) geometries [9–11, 21, 22]. To date, there are only a handful of studies that considered detonations in three-dimensional (3D) channels modeled using single-step [2–5, 10] and simplified multi-step [6–8] chemical kinetics. Further, all of these previous 3D studies have been restricted to H_2/air and H_2/O_2/Ar mixtures. Detailed dynamics of detonations in hydrocarbon fuels remain virtually unexplored using detailed chemistry with a notable exception of the work by Araki et al. [11]. Furthermore, for realistic hydrocarbon fuels, additional factors important to both detonation experiments and practical engines, including channel width, viscous wall losses, and wall heat transfer have not received proper attention.

Here, we present the first, realistic ethylene/air detonation simulations in channels, which employ complex, finite-rate, multi-step chemical kinetics and realistic no-slip, isothermal wall boundary conditions. While our key target is a 3D simulation of the detonation structure and dynamics, a 2D simulation is also performed to identify any similarity and contrast the difference. Numerical soot foils are used to compare the cellular structures and the flow field images are presented to illustrate the overall dynamics and structures.

2 Numerical Setup

We solve the unsteady, reactive, compressible Navier-Stokes equations to simulate the detonation dynamics in ethylene-air mixtures. The governing equations are solved on a uniform grid using a fully

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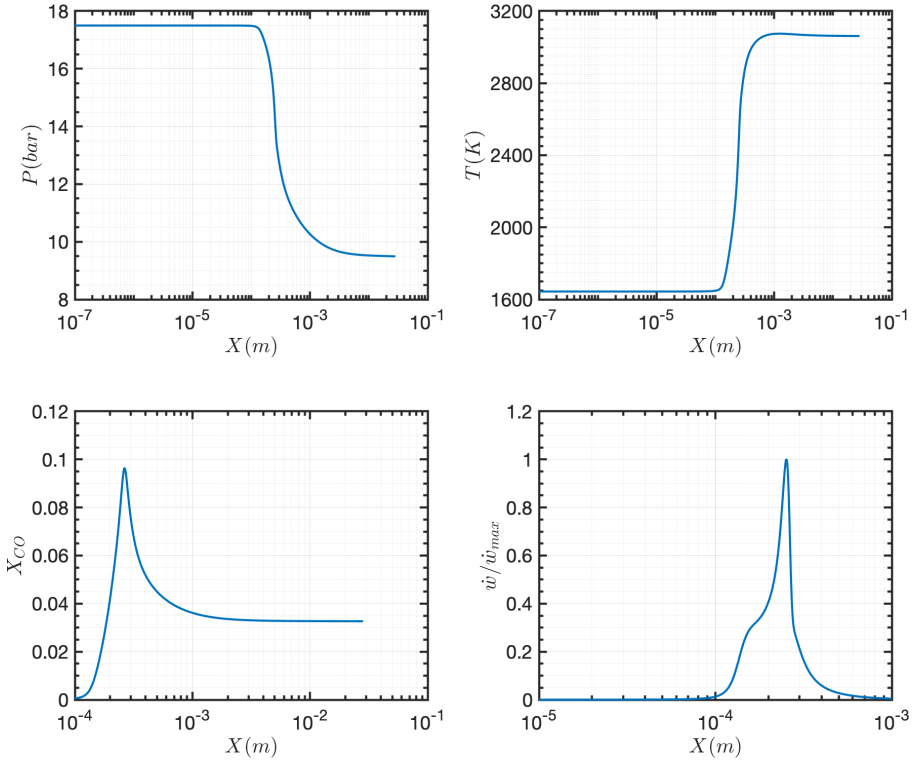

Figure 1: 1D ZND structure of a stoichiometric C_2H_4/air mixture at 5 bar and 298 K.

compressible reactive flow solver `Athena-RFX` [12–15]. The solver uses a directionally unsplit corner transport upwind (CTU) [16] integrator with the piecewise-linear method (PLM) for spatial reconstruction. The interface fluxes are computed using the HLLC-ADC [17] Riemann solver, which avoids the carbuncle phenomenon in the presence of strong shocks. The stiff system of ODEs that represent the chemical kinetics is solved using YASS ODE integrator [9]. The chemical reactions are coupled to the flow equations using Strang splitting [18] providing the overall 2^{nd}-order accuracy in both space and time. The chemical reaction model, comprised of 30 species and 231 reactions, is a reduced version of the Foundational Fuel Chemistry Model (FFCM) series of reaction models [19, 20]. The equation of state is that of an ideal gas with the thermodynamic functions computed using NASA seven-coefficient format. The molecular transport is treated with mixture-averaged formulations.

The numerical simulation of a 3D stoichiometric premixed ethylene/air mixture is carried out in a rectangular domain with size $5.7 \times 1 \times 1$ cm, while the domain size for the 2D simulation is 5.7×1 cm. Initial pressure, P, and temperature, T, are set to 5 bar and 298 K respectively in both 2D and 3D cases. The boundary conditions in the transverse directions are set to isothermal no-slip walls with wall temperature of 298 K in both calculations. The left streamwise boundary is set to a zero-order extrapolation (outflow) boundary condition, while the right boundary is held fixed at the Chapman-Jouguet (CJ) state calculated from the Zeldovich-von Neumann-Döring (ZND) solution. The ZND structure is obtained using CalTech Shock and Detonation Toolbox [23]. The problem is solved in the laboratory frame of reference with a moving grid to limit the streamwise length of the domain. Figure 1 shows the corresponding ZND structure of a stoichiometric ethylene/air mixture. Salient features of the ZND structure include the dual-stage heat release (the characteristic "knee" in the normalized thermicity profile, $\dot{\omega}$, Fig. 1d), and the presence of significant amounts of CO in the product state at chemical equilibrium (Fig. 1c) due to high-temperature dissociation of CO_2.

The CJ detonation speed of the mixture is 1,863 m/s with an induction length, defined as the distance

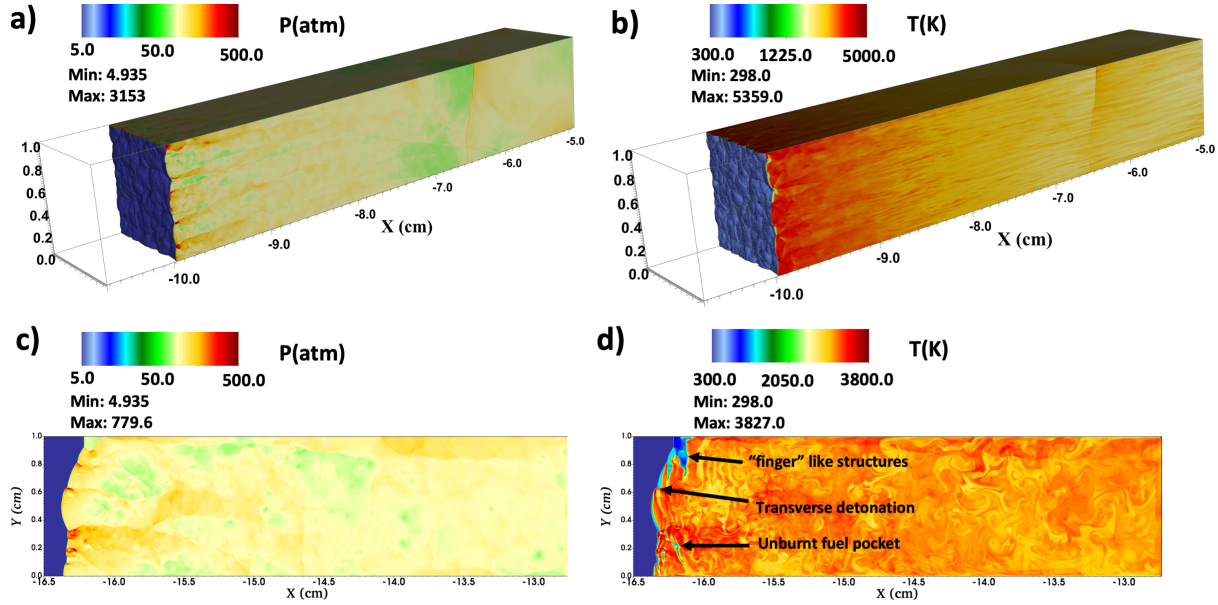

Figure 2: Comparison of the 2D and 3D detonation flow-fields for a stoichiometric ethylene-air mixture at 298 K and 5 bar. Panels (a) and (c): pressure in the 3D and 2D case, respectively. Panels (b) and (d): temperature fields in the 3D and 2D cases, respectively. Note the different colormaps, and different maximum values, in 2D vs. 3D simulations.

from the shock to peak thermicity, equal to 253 μm, and an exothermic pulse width, defined as the full width at half maximum of the thermicity profile, equal to 51.6 μm. The computational cell size is set to 12 μm, which gives 20 cells per induction length and 3 cells per exothermic pulse width. This results in 2.8 billion computational cells for the 3D case and 3.5 million cells for the 2D case. Resolution was limited to reduce the high computational cost of the 3D calculation, which still required $\approx$ 15 million CPU hours on a Cray XC40/50.

3 Results and Discussion

Figure 2 shows the flow fields of pressure and temperature in the 3D and 2D cases. Overall, the 2D detonation is significantly less stable with the front being much more irregular than the 3D case. Most notably, the 2D detonation exhibits a wider variety of flow features such as transverse detonation waves, multiple "finger"-like structures, and pockets of unburnt fuel (Fig. 2d) that are absent in the 3D detonation. On the other hand, the detonation in the 3D channel produces more extreme pressures and temperatures than in a 2D case (cf. Fig. 2). In particular, in 3D, static pressures reach values over 3,000 atm, while the temperature in the triple point collisions exceed 5,000 K. This is in contrast with maximum pressures of $\sim$800 atm and temperatures of $\sim$3,800 K in 2D under the comparable condition. The drastic difference in local maximum temperature and pressure indicates that while a 2D simulation may be useful for understanding the global dynamics of detonation waves, it does not provide accurate information about local dynamics in actual detonations in 3D. Other related issues revealed through the current simulation include the need to consider extreme thermodynamic conditions (primarily driven by hydrodynamics), which poses a significant challenge for testing chemical kinetic models for detonation simulations. In addition, the overall validity of the underlying physical model becomes questionable for detonation simulations. Further investigation is required of the importance of thermal non-equilibrium [22], real-gas effects in the equation of state, and the accuracy of the rigid-rotor,

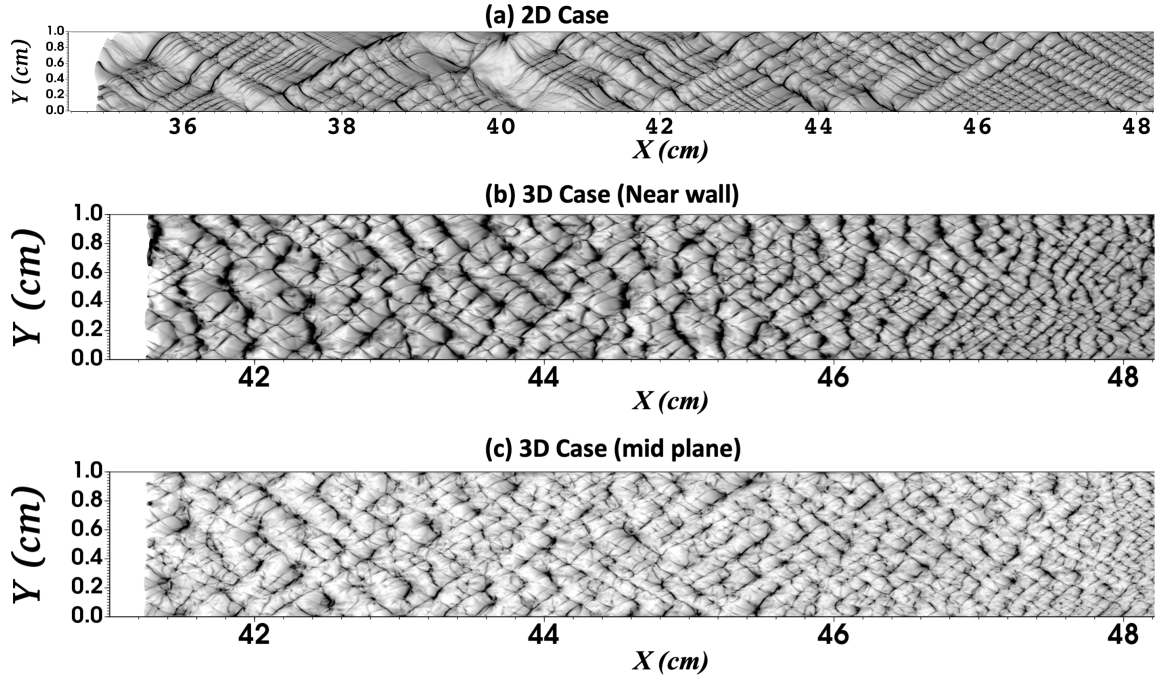

Figure 3: Numerical soot foils obtained by recording the maximum pressure in each computational cell from the simulation of detonation of a stoichiometric ethylene-air mixture at 298 K and 5 bar. Panel (a) shows the soot foil in the 2D case. Panels (b) and (c) show the soot foil near the wall and at the mid plane, respectively, for the 3D case.

harmonic oscillator assumption in the treatment of the thermochemical properties.

Figure 3 compares the numerical soot foils obtained in the 2D and 3D detonations. Figures 3b and 3c show the soot foils from the near-wall and mid-plane regions, respectively, for the 3D case. These soot foils are generated by recording the maximum pressure in each computational cell. The detonation cells in 2D (Fig. 3a) are irregular with a hierarchy of cells characteristic of an unstable mixture. Their evolution, however, appears to show spatial correlations in the diagonal direction of the channel. Previous studies [9, 21], which modeled detonations using single-step chemical kinetics, reported that the cell irregularity is related to the effective activation energy of the mixture. Cell irregularity results from frequent quasi-failure/re-ignition events during detonation propagation especially when the activation energy is large. When the detonation is about to undergo a failure, the incident shock weakens, creating a large induction zone behind the primary detonation front. The large induction zone causes a transverse detonation wave, which burns most of the compressed reactive mixture in the induction zone and at the same time, it could leave pockets of unburnt fuel behind. Such transverse detonations appear on the soot foil as the darker, thicker inclined streaks (Fig. 3a). The formation and subsequent propagation of a transverse detonation creates a series of smaller detonation cells across the domain width, re-energizes the detonation, and produces heat release necessary for the propagation of the primary front. Therefore, in such unstable mixtures, the periodic appearance of transverse detonations is crucial for continued detonation propagation. Similar transverse detonation dynamics was previously reported by Taylor et. al. [22] in H_2/air mixtures using detailed chemistry.

In comparison to the soot foil in the 2D channel, the 3D counterpart does not show evidence of periodic detonation failure and re-ignition, even though the cells are still irregular. Overall, cells have more uniform sizes than in 2D. The detonation is more stable in spite of wall losses due to the isothermal, no-slip transverse boundary condition.

4 Concluding Remarks

In this work, we present the comparison of the structures and dynamics of 2D and 3D gas-phase detonations of a stoichiometric ethylene/air mixture in a channel using realistic boundary conditions and finite-rate, multi-step reaction chemistry. We observe that the detonations in 2D undergo periodic failure/re-ignition events, which cause a periodic formation of transverse detonation waves propagating in extended regions of the compressed unburnt mixture. This leads to a hierarchy of detonation cell sizes with pronounced cell irregularity. In contrast, in a 3D channel, under the same conditions, the detonation does not exhibit such behavior with no failure/re-ignition events recorded. These differences indicate that the 2D structure and dynamics do not approximate the 3D structure and dynamics well, both qualitatively and quantitatively, and that for the mixture considered, 2D detonations do not sufficiently exhibit real detonation dynamics. To this end, it is useful to understand whether such 2D behavior can be representative of the dynamics of realistic detonations in narrow 3D channels, and how the transition from a quasi-2D to a fully 3D dynamics occurs. Such analysis will be presented in subsequent papers.

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