High-Fidelity Numerical Analysis of the Detonation Wave Structure

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Introduction & objectives

One of the fundamental challenges in the successful operation of rotating detonation engines (RDEs) is the design of a robust fuel-oxidizer injection system. To minimize pressure losses while ensuring efficient mixing that promotes stable detonation, the injection has to satisfy many different constraints. In this work, the impact of discrete injection on wave propagation is studied in an effort to understand the impact of fuel stratification on detonation stability. The physics of wave propagation are a function of the fuel-oxidizer mixture's chemical composition and the geometric configuration of the combustor annulus and injector system. The development of turbulence is vastly different from the fully three-dimensional turbulence found in gas turbine combustors. This study is primarily motivated by the need to better understand the flow-field within the RDE system. In most chemical compositions and flow conditions, the detonation wave, which consists of the pressure/shock wave followed by the reaction zone, is on the order of a few micrometers in length. Thus, the complex combustion processes require a massively-parallel direct numerical simulation (DNS) approach with multistep chemical mechanisms to study the detonation wave propagation accurately. The DNS studies were performed using UTCOMP, a parallel compressible flow solver with detailed chemical kinetics provided through Chemkin integration.

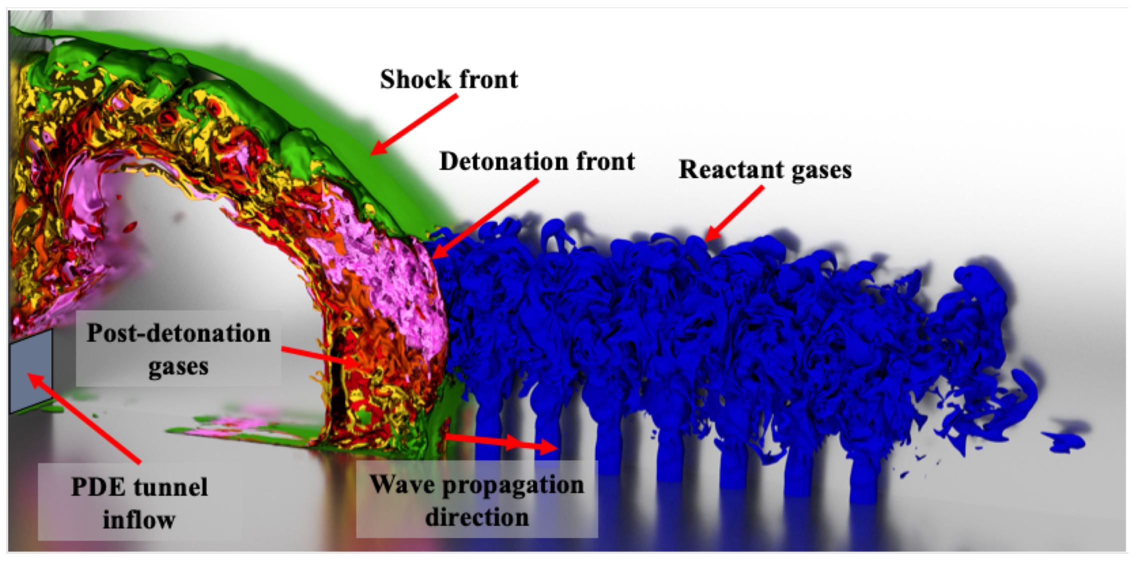

Figure 1: Detonation wave structure and features.

Linearized RDE simulations

The detonation wave is studied with a canonical flow configuration – a linearized model detonation engine (LMDE) – corresponding to a small section of a typical RDE. The LMDE simulates the interaction between the fuel-oxidizer mixture injected transversely into the channel and the detonation wave, while removing the effects of curvature. A detonation wave generated by a pulse detonation engine (PDE) expands radially through the channel, consuming the fuel-oxidizer mixture. The LMDE consists of 15 injectors with 2.5 mm diameter and 6.4 mm center-to-center spacing. The simulation configuration is shown in Fig. 2.

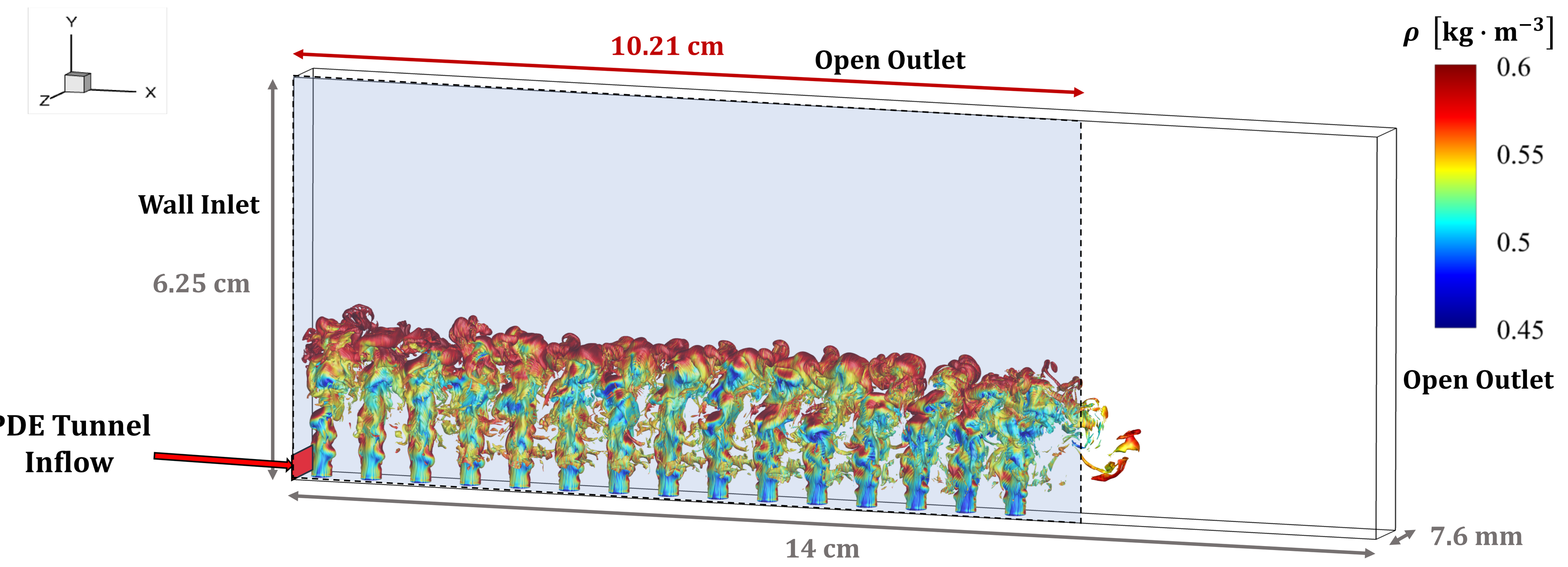

Figure 2: Simulation configuration with fully-developed injector jets in the LMDE; isosurface of $Y_{H_2} = 0.016$, colored by density.

The effects of fuel composition and equivalence ratio on the wave structure are studied with mixtures of H_2-air and H_2-O_2. Figure 3 depicts the sequence of numerical schlieren images of the detonation wave entering the channel. The wave diffracts as its axial kinetic energy is distributed into both the axial and transverse directions.

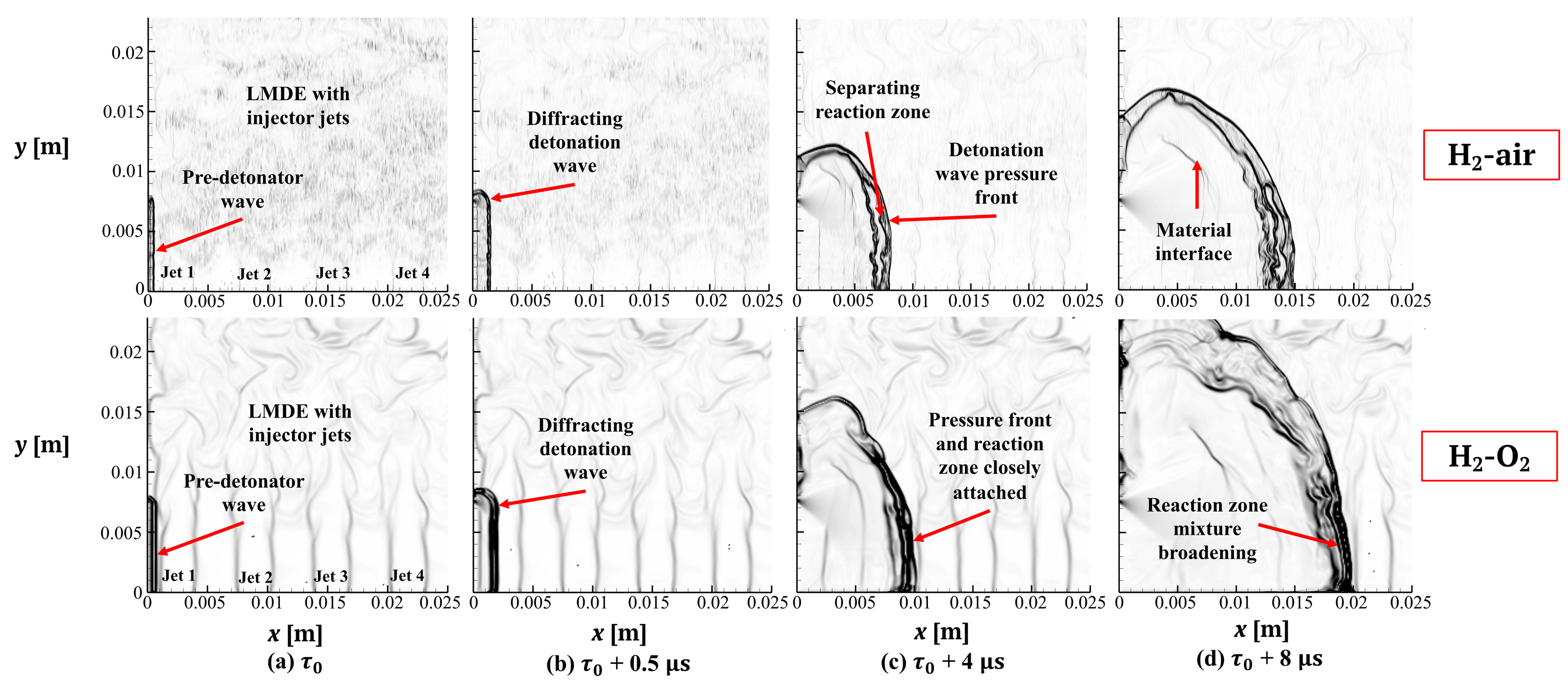

Figure 3: Detonation wave from the pre-detonator inflow entering the LMDE for the (top) H_2-air and (bottom) H_2-O_2 cases.

In the H_2-air case, the wave separates into a leading pressure wave followed by a trailing reaction zone. In the H_2-O_2 case, the shock front is closely attached to the reaction zone. The reaction zone is quite complex and broadens with time. The wave travels faster near the base of the channel due to the lower density of the fuel-oxidizer mixture. The reaction zone is comprised of multiple pressure waves and shock waves, and contains turbulent mixing of post-detonation gases and intermediary species.

Detonation analysis

The relation between pressure and density behind the detonation wave front at various heights above the base of the channel provides insight into the detonation and deflagration processes. Figure 4 displays the Rankine-Hugoniot relation for heights up to 10 injector diameters from the base of the channel. In the H_2-air case, the region approximately 1 injector diameter from the base of the channel results in the strongest detonation. On the other hand, in the H_2-O_2 case, the region approximately 2 injector diameters from the base of the channel results in the highest detonation heat release and pressure, corresponding to those of the triple points. Indeed, as viewed in the numerical schlieren images, the curved detonation wave front can be characterized by the existence of visible triple points.

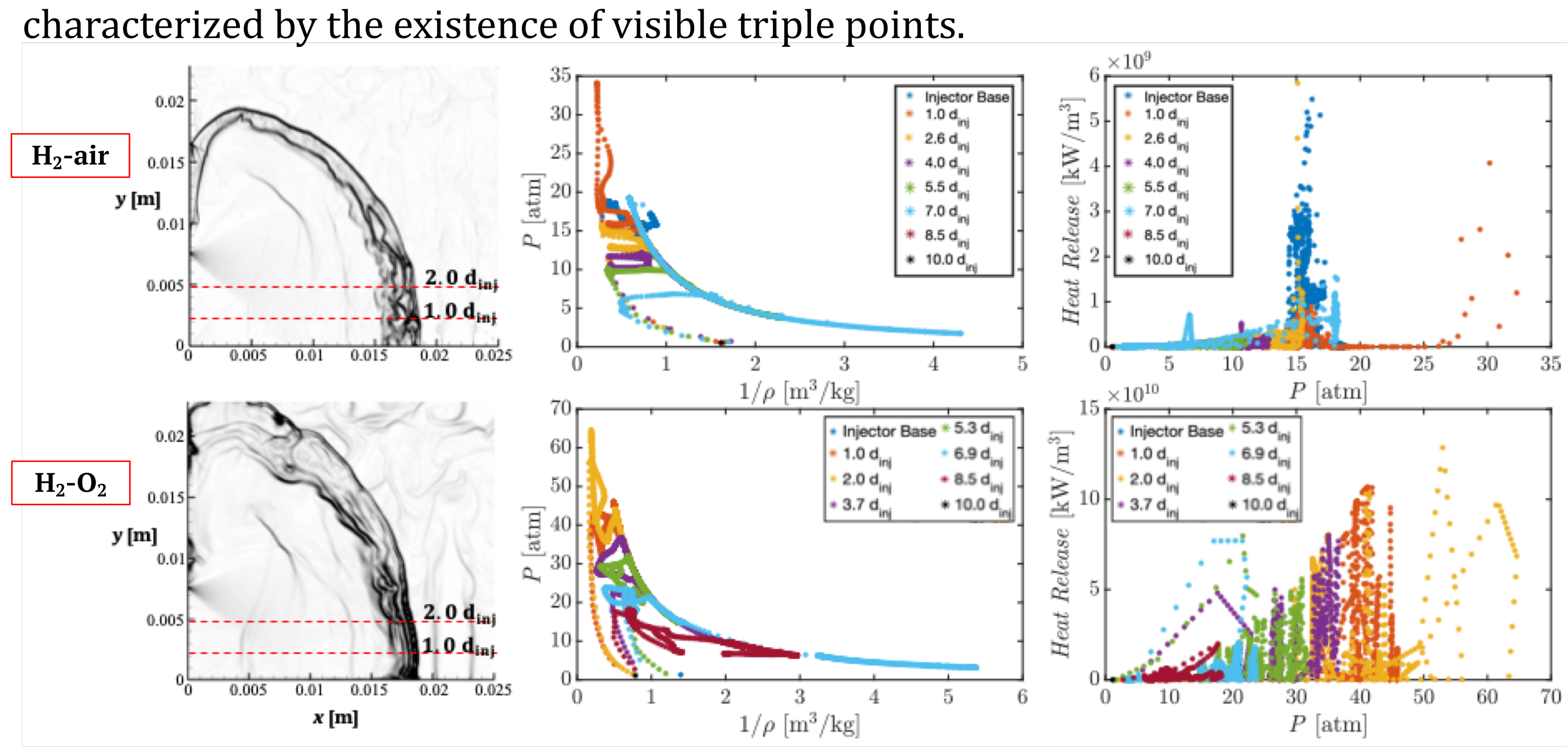

Figure 4: Rankine-Hugoniot and heat released per unit volume and pressure relations as the detonation wave is between the 3rd and 4th injectors for the (top) H_2-air and (bottom) H_2-O_2 cases.

Similarly, in the heat released per unit volume and pressure relation, the distributions feature a local maxima in both cases at a pressure corresponding to the von Neumann spike pressures of approximately 16 atm and 42 atm for the H_2-air and H_2-O_2 cases, respectively. Figure 5 reveals the detailed species behavior and pressure profile at the shock front. In comparison to the ideal 1D detonation process, the 3D LMDE reaction zone is highly complex and contains post detonation gases captured in between the pressure and shock waves seen in the numerical schlieren images. The peak pressures in the 3D cases are higher than the ideal cases due to the collision of triple points propagating along the shock front.

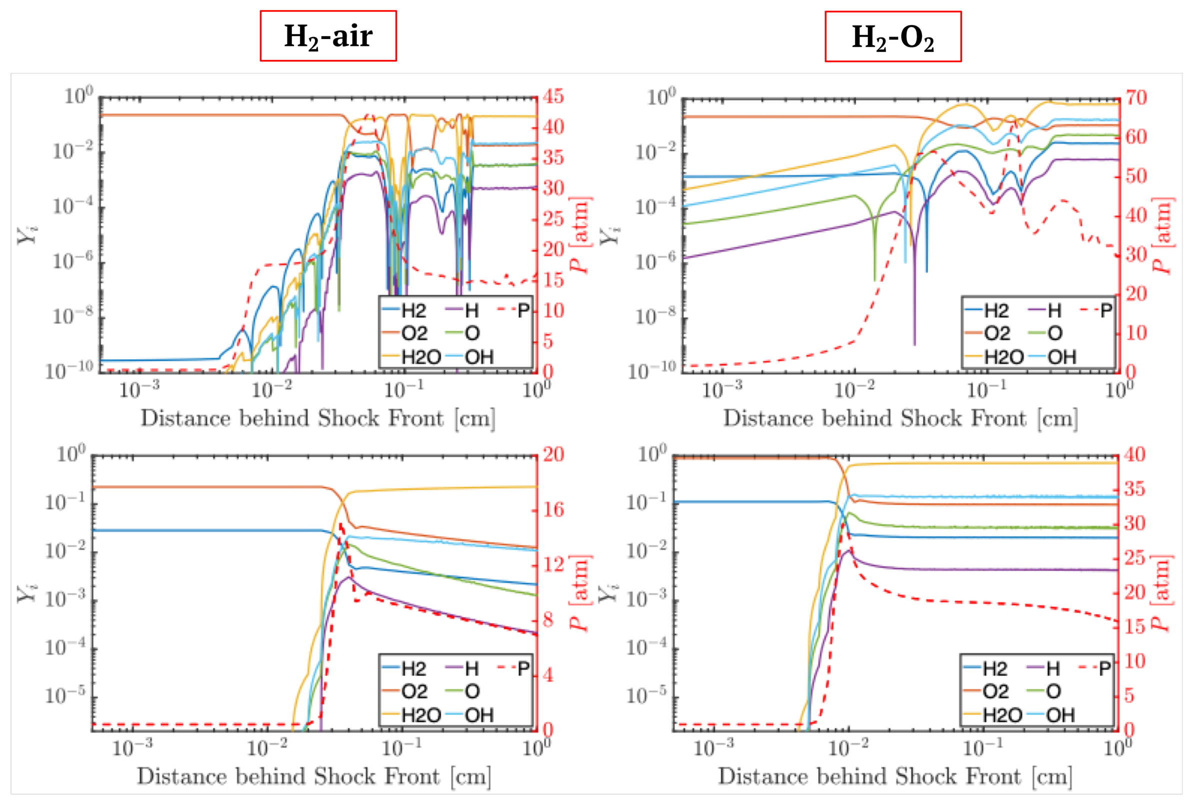

Figure 5: Detailed species behavior at the shock front for (top row) the 3D LMDE detonation cases and (bottom row) the 1D ideal detonation cases for the (left) H_2-air and (right) H_2-O_2 cases.

Conclusion & acknowledgements

Direct numerical simulations were performed to provide a fundamental understanding of the complex detonation wave structure and reaction zone in a linearized RDE. There exist key differences in the shock structure and propagation of the detonation wave for the H_2-air and H_2-O_2 cases. The high energy H_2-O_2 case results in higher peak pressures and heat release in comparison to the H_2-air case. The reaction zone and shock front are more closely attached in the H_2-O_2 case and a larger region of the shock front experiences strong detonation. The research is based on work supported by the DOE/NETL University Turbine Systems Research under Grant No. DE-FE0025315 and Grant No. DE-FE0023983. The authors would like to thank NASA High-End Computing Capability (HECC) for the generous allocation of computational resources.