

Microscopic simulation and analysis of reactive shock wave in a H_2/O_2 fuel mixture

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Abstract:

Non-equilibrium reactive molecular dynamics simulations and data analysis are performed to investigate the shock-induced chemical reactions of a H_2/O_2 mixture in a multiphase fuel mixture. In the simulation, a stoichiometric fuel mixture at 1 atm and 500 K is rapidly compressed by a moving interface of an inert condensed-phase substance. Species distribution near the shock region is quantified and dominant molecular motions induced by the shock wave are analyzed through principal component analysis. Results show rich molecular dynamics and their effects on chemical reactions within and near the shock, implying the potential importance of sub-continuum scale fluid dynamics in high-speed hydrogen combustion.

Keywords: Multiphase reacting flows, Shock wave, Hydrogen combustion, Reactive molecular dynamics

Introduction:

High-speed hydrogen combustion plays a crucial role in a wide range of energy, aviation, and propulsion systems. Detailed understanding of the shock-induced chemical reactions of multiphase fuel mixtures is essential and microscopic dynamics at the scale of shock-thickness remain elusive. In this study, we use non-equilibrium reactive molecular dynamics (MD) simulations to analyze the process of shock-induced reactions in a stoichiometric H_2/O_2 gaseous mixture near a moving interface of inert solid. We quantify the spatial distributions of the pressure and chemical species across the shock wave. The coherent motions of individual molecules after the shock passage are analyzed through the principal component analysis (PCA) of molecular velocities. Results indicate the existence of significant sub-continuum fluctuations in the process of shock-induced combustion.

Methodology:

Reactive MD simulations employing the ReaxFF potential [1] were conducted to track the motion of molecules of reactants, radicals and products. The rectangular computational domain, measuring $0.025 \times 0.025 \times 20 \mu\text{m}^3$ in x - y - z Cartesian coordinates, was initially filled with gaseous H_2 and O_2 molecules at a stoichiometric condition, at $P_0 = 1$ atm and 500 K with zero mean velocity. The inert interface of a condensed-phase substance is initially placed at the $-z$ domain boundary and moves along the z -axis at $c_p = 1685.05 \text{ m.s}^{-1}$ to collide with molecules to generate a shock wave, with the continuum-scale shock speed of 2238.47 m.s^{-1} and the Mach number of 3.22. The evolution of atomic distributions was tracked over a 5 ns after the shock formation. PCA for Lagrangian data, adapted from [2], was applied to the z - molecular velocities to extract the stream-wise coherent motions of molecules after the arrival of the shock wave, later denoted as PC1.

Results:

Figure 1 provides a visualization of molecules projected on the xz -plane at $t = 2.5$ ns. The shock wave is observed as the thin region of transition from high to low molecular densities.

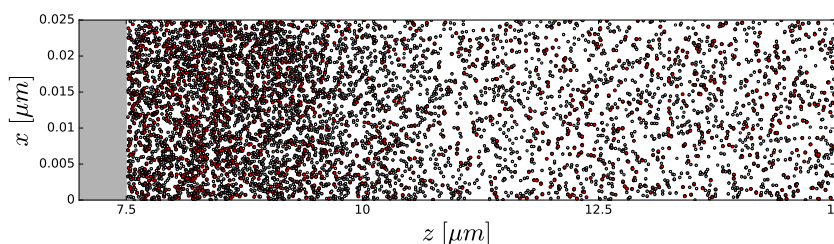


Figure 1: Molecules projected on the xz -plane at 2.5 ns. The shaded area represents the inert surface.

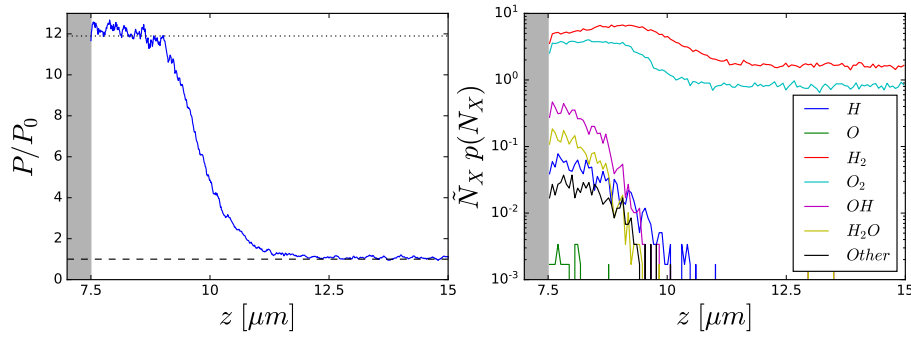


Figure 2: (Left) Pressure normalized by P_0 and (Right) distribution of chemical species along the z -coordinate, where \tilde{N}_X indicates the total atoms per species.

Figure 2(left) shows the corresponding pressure profile normalized by P_0 , illustrating the increase in pressure compressed by the interface. The post-shock pressure agrees with the prediction of the Rankine-Hugoniot (R-H) condition (thin dotted line). The transitions observed in our simulations are gradual unlike continuum theory. Figure 2(right) shows the distribution of chemical species along the z -coordinate, indicating the presence of products in the shock- and post-shock regions.

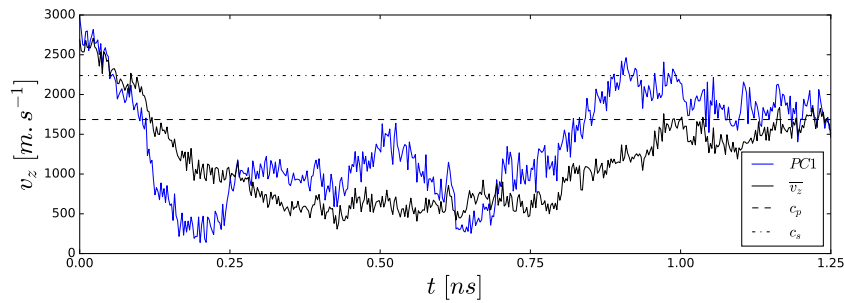


Figure 3: Evolution of the z - mean molecular velocity, \bar{v}_z and PC1, after the arrival of the shock wave.

Figure 3 shows the evolution of the z - mean velocity of molecules (\bar{v}_z) and the first principal component (PC1), after the shock arrival. Both the mean and PC1 present a sharp decrease from near the R-H theoretical shock speed c_s to approximately 600 m.s^{-1} during the initial 0.25 ns. The mean slowly recovers its value to the post-shock velocity c_p at around 1.0 ns. Interestingly, PC1 oscillates around the mean, presumably due to coherent mode of collisions. These results indicate not only significant deviations from continuum theory that predicts instantaneous transitions but also rich sub-continuum dynamics excited by shock waves.

Conclusion:

This study utilized reactive molecular dynamics simulations to investigate the impact of a shock wave on the reaction dynamics of an H_2/O_2 mixture and analyzed the coherent dynamics of molecules through PCA. The results revealed significant deviations from continuum theory, thereby emphasizing the need for sub-continuum scale analysis to accurately predict the dynamics of hydrogen fuel mixtures in high-speed combustion systems. Further investigation will be made on quantifying chemical reactions.

Acknowledgments:

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References

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