THE INFLUENCE OF PLASMA ON DETONATION FOR HYDROGEN/OXYGEN MIXTURES

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Abstract
This study investigates plasma-assisted detonation in hydrogen–oxygen mixtures. A novel two-step modeling approach is proposed, combining ZDPlasKin for simulating plasma kinetic effects with the ZND model for shock wave analysis. Key detonation parameters, including temperature and Chapman–Jouguet (CJ) conditions, are correlated with pressure, reduced electric field (E/N), and equivalence ratio (Φ). The results provide new insights into the role of plasma discharges in detonation enhancement.

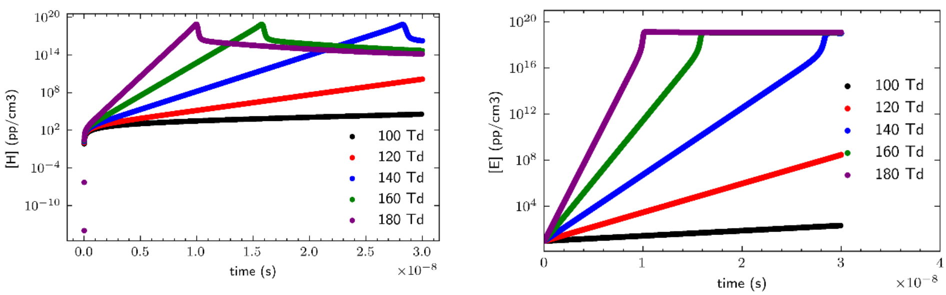
Introduction
Combustion can occur in various regimes, including laminar flames, deflagrations, and detonations. The structure of a stable detonation wave is typically described by the Zeldovich–von Neumann–Döring (ZND) model, which features a leading shock followed by a reaction zone. The minimum possible detonation velocity in this model is the Chapman–Jouguet (CJ) speed. This study explores plasma-assisted detonation in H_2 mixtures, a topic still largely underexplored in the literature, particularly from a numerical perspective. Hydrogen, a clean and sustainable energy carrier, holds promise as a fossil fuel alternative. This work provides a comprehensive analysis of the influence of plasma discharges across various equivalence ratios and reduced electric fields. Additionally, simulations were conducted using the Shock and Detonation Toolbox to correlate temperature, CJ parameters, and cell size with plasma-induced effects, aiming to clarify kinetic impacts and their dependence on mixture composition.

Methodology
A dual-step modeling approach is proposed for assessing the kinetic effects of plasma on the deflagration-to-detonation transition (DDT). In the first step, a plasma discharge simulation is carried out using the ZDPlasKin toolbox to determine the final composition of the gas mixture after the discharge. This composition is then used as the input for the ZND model to perform detonation analysis. A nanosecond discharge of 30 ns is applied at an initial temperature of 503 K, with the reduced

electric field (E/N) varying between 100 and 180 Td, pressure ranging from 1 to 7 bar, and equivalence ratio (Φ) between 0.2 and 1. The H_2 reaction mechanism employed is that developed by Mao et al.[1], who investigated the influence of nanosecond pulsed plasma discharges on ignition delay times. Detonation simulations are performed using the Shock & Detonation Toolbox [2], which relies on the Cantera software suite and incorporates detailed chemical kinetics and thermodynamic data. The ZND model is used to solve for Chapman–Jouguet (CJ) conditions and to describe the thermodynamic state of the mixture throughout the detonation wave.

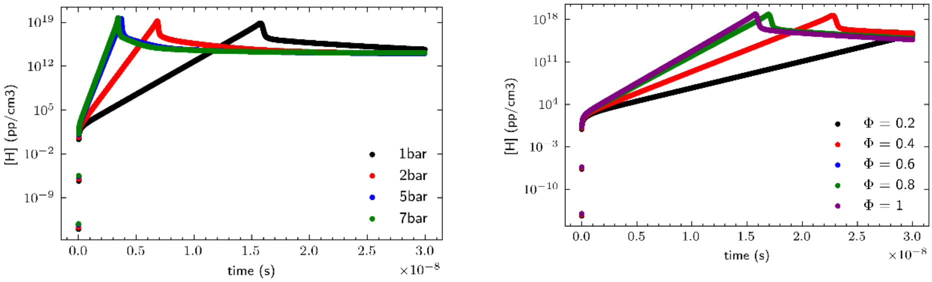
Results

H and e-densities are used to show the effect of plasma. As shown in Figure 1, the discharge behavior varies significantly with the reduced electric field (E/N). For values below 120 Td, the discharge does not exceed the breakdown threshold and fails to ionize the mixture. At 120 Td, partial ionization occurs, with the electron density beginning to rise noticeably. From 140 Td onwards, the plasma fully ionizes the mixture, with electron densities reaching levels sufficient to consider the gas fully ionized. As the discharge intensity increases, the peak electron concentration is reached earlier in time, shifting from approximately 1.5×10^{-8} s to around 1×10^{-8} s. At pressures between 5 and 7 bar, the variation in timing becomes negligible, with peak values occurring at approximately 4×10^{-9} s. Variations in equivalence ratio Φ significantly affect the post-discharge concentration of atomic hydrogen, highlighting the importance of fuel–oxidizer composition in determining plasma reactivity. Figure 2 shows that at Φ = 1 and reduced electric field E/N=160 Td, increasing the pressure from 1 to 7 bar leads to higher peak H concentrations and a faster decay, indicating enhanced dissociation and recombination dynamics with increasing pressure. At fixed pressure (1 bar) and E/N=160 Td, as Φ increases, the H-atom production becomes more intense, with higher peak concentrations and earlier maxima, reflecting the greater availability of hydrogen and more efficient radical chain-branching under fuel-rich conditions.



a) b)

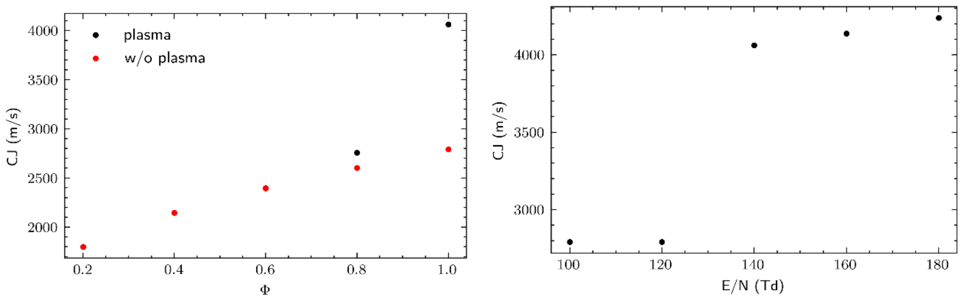
Figure 1 Time evolution of a) H, b) electrons concentration at different E/N values for H_2/O_2 , Φ = 1, p = 1 bar.



a) b)

Figure 2 Time evolution of H a) different pressure values at Φ = 1 and E/N = 160 Td, and b) different Φ values for H_2/O_2, at E/N = 160 Td and p=1 bar.

Figure 3 illustrates the variation of the CJ detonation velocity under different plasma conditions for a stoichiometric H_2/O_2 mixture at 1 bar. The presence of plasma significantly increases the CJ velocity across all Φ values, especially at $\Phi = 1$, where the enhancement is most pronounced. The CJ velocity increases with higher reduced electric field values.



a) b)

Figure 3 CJ for different a) Φ with E/N = 140 Td b) E/N with Φ=1. Conditions are H_2/O_2 , p = 1 bar, E/N = 140 Td.

[1] X. Mao, Q. Chen, A. C. Rousso, T. Y. Chen, and Y. Ju, ‘Effects of controlled non-equilibrium excitation on H2/O2/He ignition using a hybrid repetitive nanosecond and DC discharge’, *Combustion and Flame*, vol. 206, pp. 522–535, Aug. 2019, doi: 10.1016/j.combustflame.2019.05.027.

[2] ‘Explosion Dynamics Laboratory’. Accessed: May 05, 2024. [Online]. Available: https://shepherd.caltech.edu/EDL/PublicResources/sdt/

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