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TRANSIENT NEAR-WALL EMISSION CHARACTERISTICS OF NH₃/H₂/N₂ FLAMES

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Topic: Combustion Fundamental

Introduction

To advance the development of combustion devices that operate on alternative fuels, it is important to clarify near-wall flame behaviour. As the flame and wall mutually interact, the wall acts as a heat and radical sink, with significant implications on pollutant formation, efficiency, and combustor wall durability [1]. However, accurately measuring the propagation of flames toward solid surfaces and characterizing the behaviour of these near-wall quenching flames in a laboratory setting poses considerable challenges [2]. Although studies such as Okafor et al. [3] and Bioche et al. [4] have explored heat loss effects on ammonia-based swirl-burner setups, it is challenging to draw non-configuration specific conclusions about the evolution of near-wall chemistry from these studies. Therefore, the present work explores ammonia/hydrogen/nitrogen flames in a head-on quenching (HOQ) configuration at various wall temperatures and equivalence ratios. This study aims to provide insights near-wall chemistry, especially emissions formation reaction routes and the underlying transport mechanisms of these species.

Materials and Methods

In the present study, laminar premixed flames in a head-on quenching configuration are studied for $\phi = 1.00, 1.06$ and wall temperatures 450K, 600K and 750K. The fuel employed is a premixed blend of ammonia/hydrogen/nitrogen with composition of 0.42/0.44/0.14 (mol. %) at atmospheric pressure and an unburnt mixture temperature which is in equilibrium with the wall. Numerical simulations were conducted using S3D, a Direct Numerical Simulation (DNS) code developed by Sandia National Laboratories [5], with further solver and boundary condition details given by previous flame-wall interaction studies utilising S3D [6,7] and further details on governing equations and equations of state are described by Chen et al. [5]. Reaction chemistry and transport properties are calculated using Cantera 2.6.0. A transport budget analysis is shown by Eq. (1), where the right-hand terms represent convection, diffusion and reaction contributions to species flux, respectively. This definition is taken from Rieth et al. [8] combined with the transport budget calculation of Palulli et al. [9] based on the mixture-averaged diffusion formulation:

$$\frac{\partial Y_\alpha}{\partial t} = \left[-u_j \frac{\partial Y_\alpha}{\partial x_j} \right] + \left[-\frac{1}{\rho} \frac{\partial}{\partial x_j} \left(\rho \frac{W_\alpha}{W_m} D_\alpha \frac{\partial X_\alpha}{\partial x_j} \right) \right] + \left[\frac{W_\alpha \dot{\omega}_\alpha}{\rho} \right] \quad (1)$$

The maximum convective and diffusive flux of various species at each time condition was used for calculation of Peclet numbers, as per Eq. (2):

$$Pe = \frac{|c_\alpha|_{1D,max}}{|D_\alpha|_{1D,max}} = \frac{\left| u_j \frac{\partial Y_\alpha}{\partial x_j} \right|_{1D,max}}{\left| \frac{1}{\rho} \frac{\partial}{\partial x_j} \left(\rho \frac{W_\alpha}{W_m} D_\alpha \frac{\partial X_\alpha}{\partial x_j} \right) \right|_{1D,max}} \quad (2)$$

Results and Discussions

Figure 1 shows the variation of emissions for hot and cold wall temperatures. Results show that higher temperatures encourage NO formation in the flame zone and therefore near-wall emissions. As the unburnt gas is in equilibrium with the wall, higher adiabatic flame temperature and unburnt gas temperature promotes the formation of NO through both Zel'dovich and HNO routes likely due to the acceleration of high temperature of high temperature kinetics providing higher O, OH, H radical production in the flame zone. When the wall temperature is lower, N₂O is not fully consumed at the wall. Meanwhile, higher wall temperatures encourage both production and downstream consumption of N₂O. On the other hand, lower NO₂ is found at higher wall temperatures with most NO₂ emissions found at the cold wall. Since NO is the main production and consumption route for NO₂, it is often seen highly correlated to NO emissions when fuel blends are varied. Although more complex formation routes for NO₂ are known [10], the present study proposes that NO₂ formation is instead more strongly correlated to heat loss than NO concentration due change with temperature in reaction rate of the H + NO₂ => NO + OH consumption reaction, as shown by Fig. 2.

Figure 3 clarifies the contribution and direction of reactive transport relative to the absolute sum of convective, diffusive and reactive transport in time. Figure 3 demonstrates that close to the wall, NO₂ is the only one of the analyzed species that has significant contribution from the reaction flux. While the near-wall production of NO and N₂O is slightly positive, it is significantly slower both at the cold wall and after quenching at t = 0 s. Meanwhile for all species the intermediate-near wall region is dominated by emissions consumption which helps support the trends seen in Fig. 1. This can impact the defining species used for Peclet number definition as the suggested by Fig. 4 where different species show different ratio of convection to diffusion. Mainly, the Peclet trends suggest that the flame front propagates predominantly through convective transport until it reaches a critical point at t = 0 s where the diffusion takes over, leading to the quenching of the flame. Definitions based on fuel species NH₃ and H₂ imply that even after the flame is extinguished, there is still some convective transport occurring, although its impact diminishes over time and diffusion becomes the dominant mode of species transport.

Conclusions

This study informs the underlying trends of near-wall emissions, relevant to practical applications where hot combustion products impinge on a colder combustion wall. Higher wall temperatures encourage the NO production which is transported by diffusion from the flame zone. Meanwhile, higher wall temperatures lead to higher N₂O production and consumption. However, NO₂ production is significantly promoted by the cold wall even after flame quenching. A transport budget analysis and Peclet number trends shed light on mechanisms of flame propagation and quenching for different species.

Figures

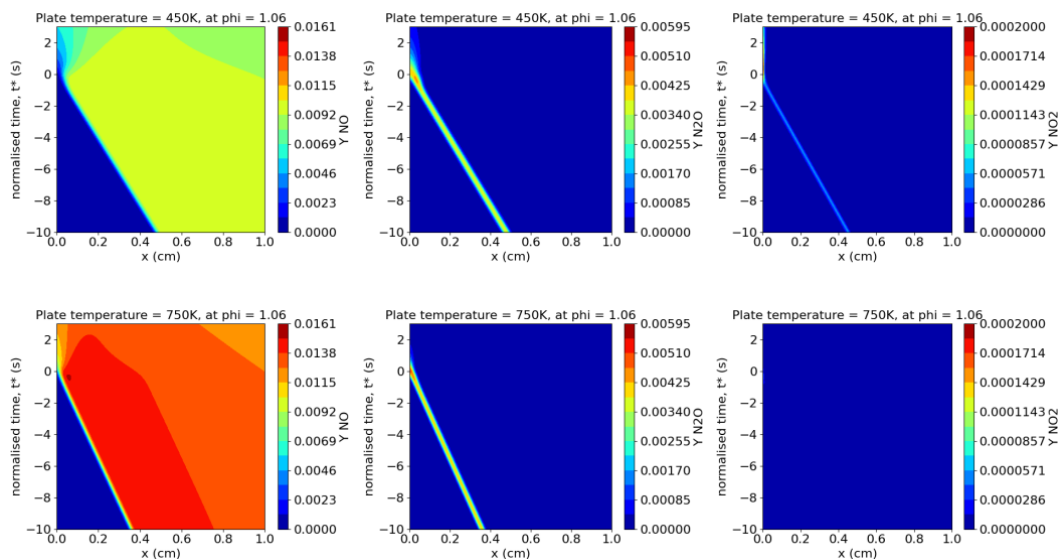


Fig. 1 Temporal evolution of NO, N₂O and NO₂ mass fractions with various wall flame temperatures at $\phi = 1.06$

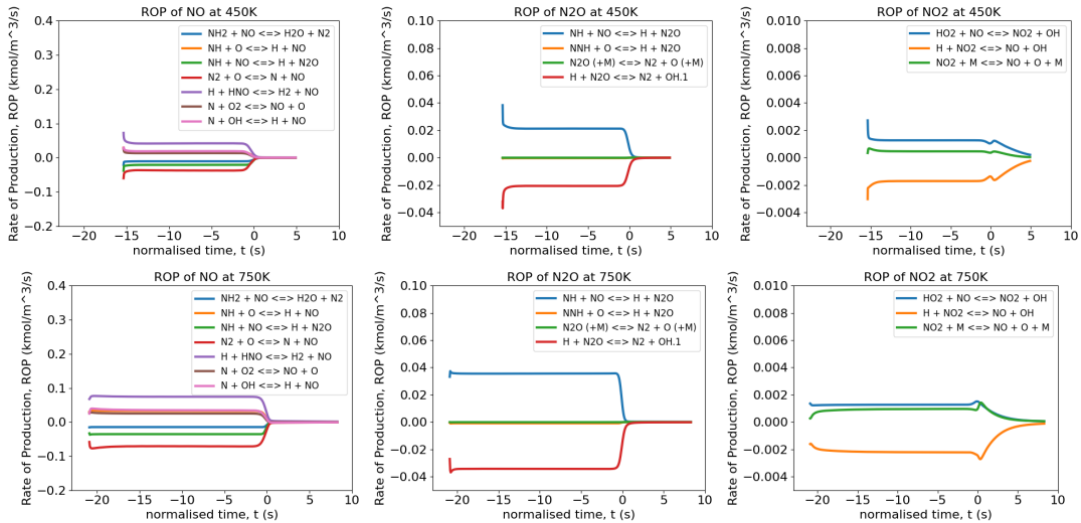


Fig. 2 Spatially integrated ROP temporal plots for the most significant reactions only at $\phi = 1.06$

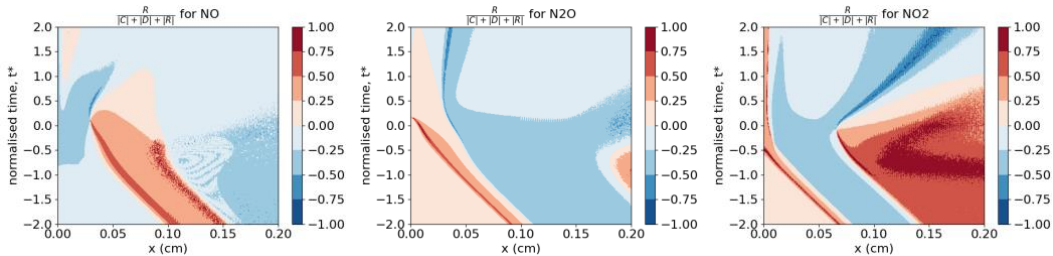


Fig. 3 Near-wall contribution of reaction transport at $\phi = 1.06$ and 450K wall temperature

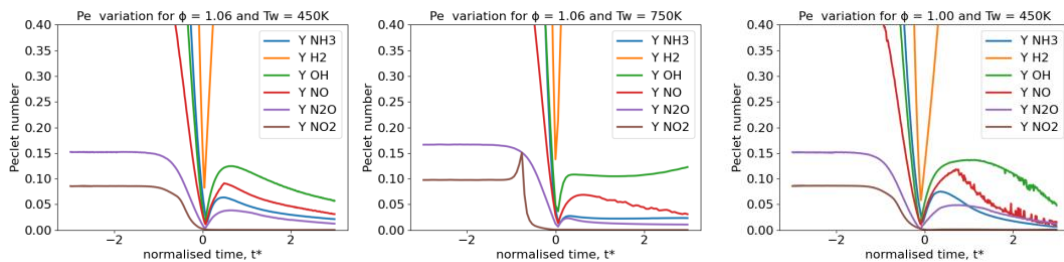


Fig. 4 Peclet number variation at quenching for $\phi = 1.06$ and 450K, 750K wall temperatures

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