WPI Aerospace Engineering Dept

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Dissertation Committee:

Prof. Jagannath Jayachandran, Aerospace Engineering Department, WPI (Advisor)

DH, Prof. Nikolaos Gatsonis, Aerospace Engineering Department, WPI

Prof. David Olinger, Aerospace Engineering Department, WPI

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PhD Dissertation Defense Presentation

An investigation of the reactivity, stability, and dynamics of slowly propagating flames fueled by sustainable fuels and working fluids/refrigerants

With the increasing threat of global warming, the motivation to explore environmentally friendly alternatives to traditional carbon-based fuels and working fluids has grown substantially. In response to the Paris Agreement on climate change, Ammonia (NH3) has received renewed interest as a zero-carbon fuel for energy production and as a safe and efficient energy carrier for hydrogen. In addition, Hydrofluorocarbons (HFC) have received greater attention as a viable low global warming potential alternative to traditional refrigerant and fire-suppressant compounds in order to realize emission reduction targets mandated by the Kyoto Protocol.

Quantifying the flammability and explosive characteristics of NH3 and low-GWP HFCs are key to establishing safety metrics for their storage, transport, and utilization. Upon mixing with air, these compounds can sustain flames that are slowly propagating (relative to hydrocarbon-fueled flames) and are thus greatly affected by radiation heat loss and buoyancy-induced flow. These effects make it challenging to accurately interpret experimental measurements performed to derive the laminar flame speed, a key metric used to quantify flammability. Therefore, radiation heat loss and buoyancy-induced flow effects must be accounted for when measuring laminar flame speeds for slowly propagating NH3/air and low-GWP HFC/air mixtures. This defense presentation will discuss results from numerical simulations that investigate the effects of radiation heat loss on slowly propagating HFC/air and NH3/air flames. Direct numerical simulations (DNS) of spherically expanding flames (SEF) revealed that the radiation-induced flow needs to be considered when interpreting data from SEF experiments. To this end, a new reduced-order model was developed to estimate the burned gas inward flow velocities in SEF experiments. The model was validated against results from DNS of SEFs, showing that the model accurately predicts the inward flow velocity for these mildly flammable mixtures over a range of conditions and performs significantly better compared to existing analytical models.

Recent studies have shown that the explosion risk of mildly flammable HFCs and NH3 can be exacerbated under certain conditions. Despite having very low laminar flame speeds, experiments investigating explosion risk of these compounds depicted large overpressures (a metric for explosion risk) typically corresponding to more reactive flames. After developing the hypothesis that the gravity-driven Rayleigh Taylor (RT) instability could result in flame destabilization, self-turbulization, and hence increased explosion risk, a numerical investigation was undertaken to investigate the effect of the RT instability on slowly propagating HFC/air and NH3/air flames. Dispersion relations, which characterize the range of unstable wavelengths and their growth rates during early stages of instability growth, are derived from DNS of RT-unstable HFC/air and NH3/air flames. Additionally, DNS are performed to study the long-term evolution of instability growth in such flames and to quantify the extent of flame wrinkling and flame acceleration. Results showed that RT-unstable flames can propagate 6-7 times the laminar flame speed, and may propagate much faster at larger scales. Additionally, the derived instability growth rates and flame speed enhancement factors suggest that the RT instability dominates the overall instability growth and flame acceleration in these types of flames, relative to the other intrinsic flame instabilities.

In summary, this defense presentation will highlight the challenges of studying slowly propagating flames and how novel approaches were utilized to improve and advance our understanding of the reactivity and dynamics of these exotic flames, paving a path for developing strategies for safe storage and utilization of these environmentally-friendly fuels and working fluids.