Clean Combustion Research Center

Using of H_2O_2/H_2O as the Oxidant: 1-D Flames Study

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Introduction

- Hydrogen peroxide, as a fuel additive to lower CO_2/NO_x emissions in flames have been investigated in the past.
- It has also been used as a rocket propellant, where 70-98% H_2O_2 reacts with a catalyst to produce hot O_2/steam mixtures to generate thrust.
- Hydrogen and ammonia are promising carbon-free energy to achieve zero-net emission in 2050.
- This project is focused on using H_2O_2 as oxygen carrier and using it as an oxidant for fossil based and renewable fuels.
- In this study, we investigate:
  - Stability of H_2/NH_3-H_2O_2/H_2O flame in a counter-flow configuration;
  - The chemical kinetic coupling between H_2/NH_3-H_2O_2 in diffusion flames.

Methodology

- 1-D simulations were conducted using the opposed-flow non-premixed laminar flame solver of CHEMKIN Pro and GRI-Mech 3.0.
- The fuel stream consists of diluted H_2 or pure ammonia.
- The oxidizer is H_2O_2 in H_2O at different fraction.
- The oxidizer temperature was kept above the boiling point of H_2O_2 solution in water. Experimental measurements were carried out using the counter-flow setup shown below.

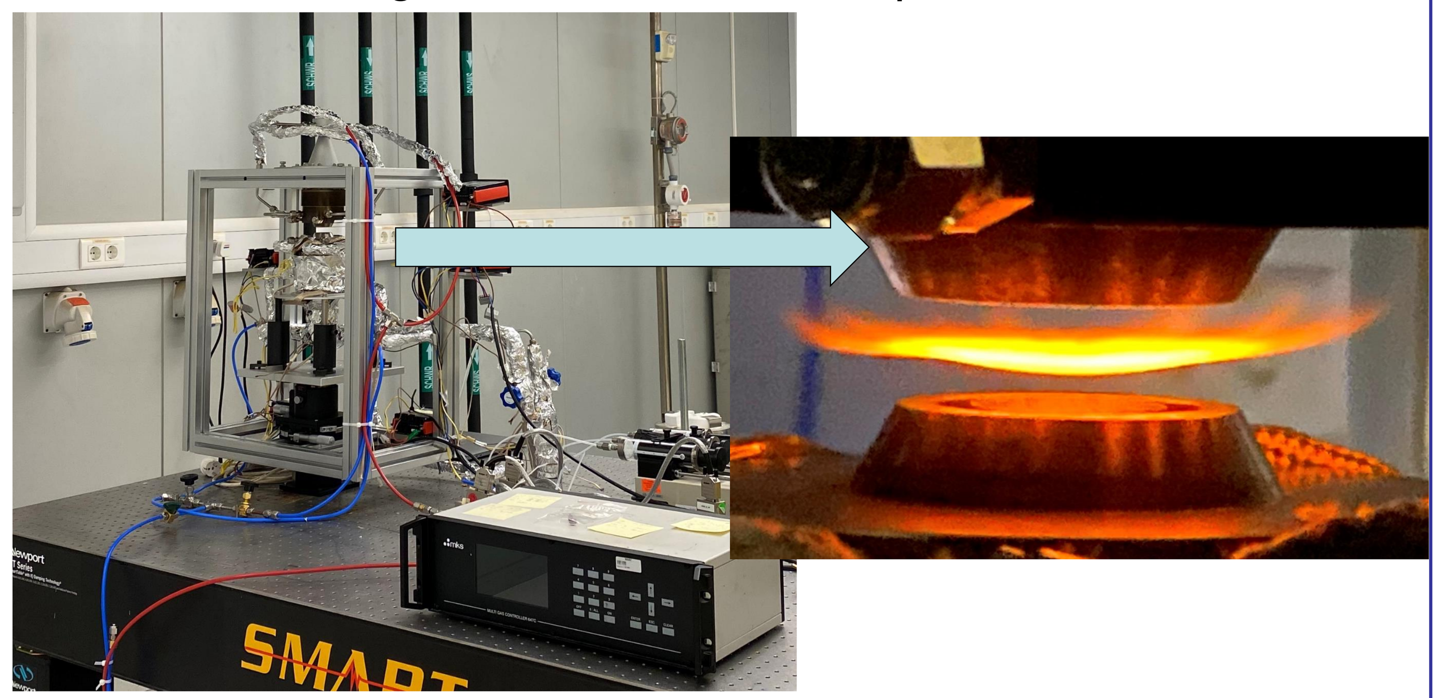

Figure 1. Experimental setup and H_2-O_2/H_2O flame.

Results

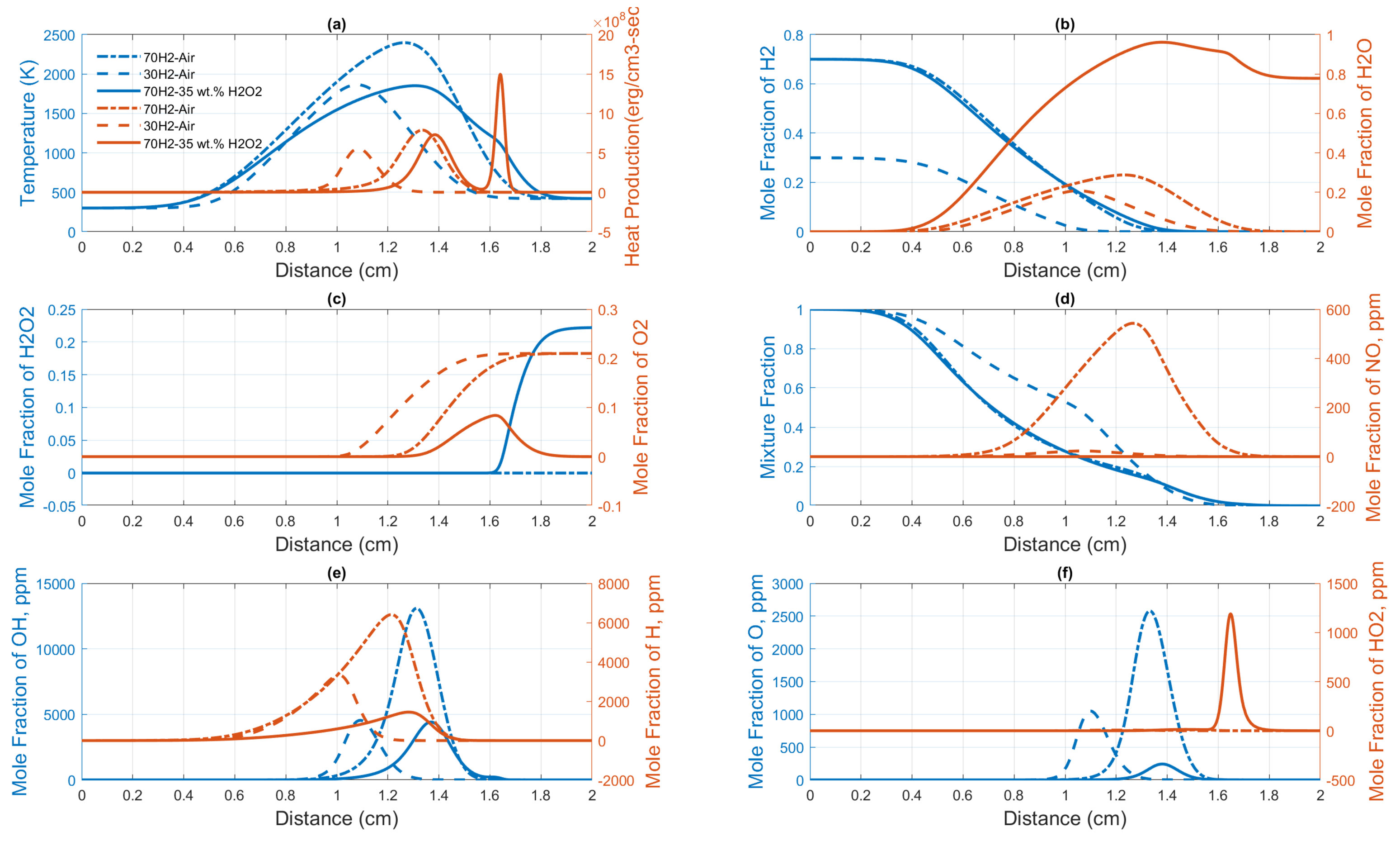

Figure 2. Axial profiles of computed Temperature, heat release, and species for diluted hydrogen-air vs. diluted hydrogen-35wt.% H_2O_2. The strain rate is kept constant at 45 1/s. OH, H, and O of 35wt.% H_2O_2 are lower than 30 H_2-air even flame temperatures are approximately the same.

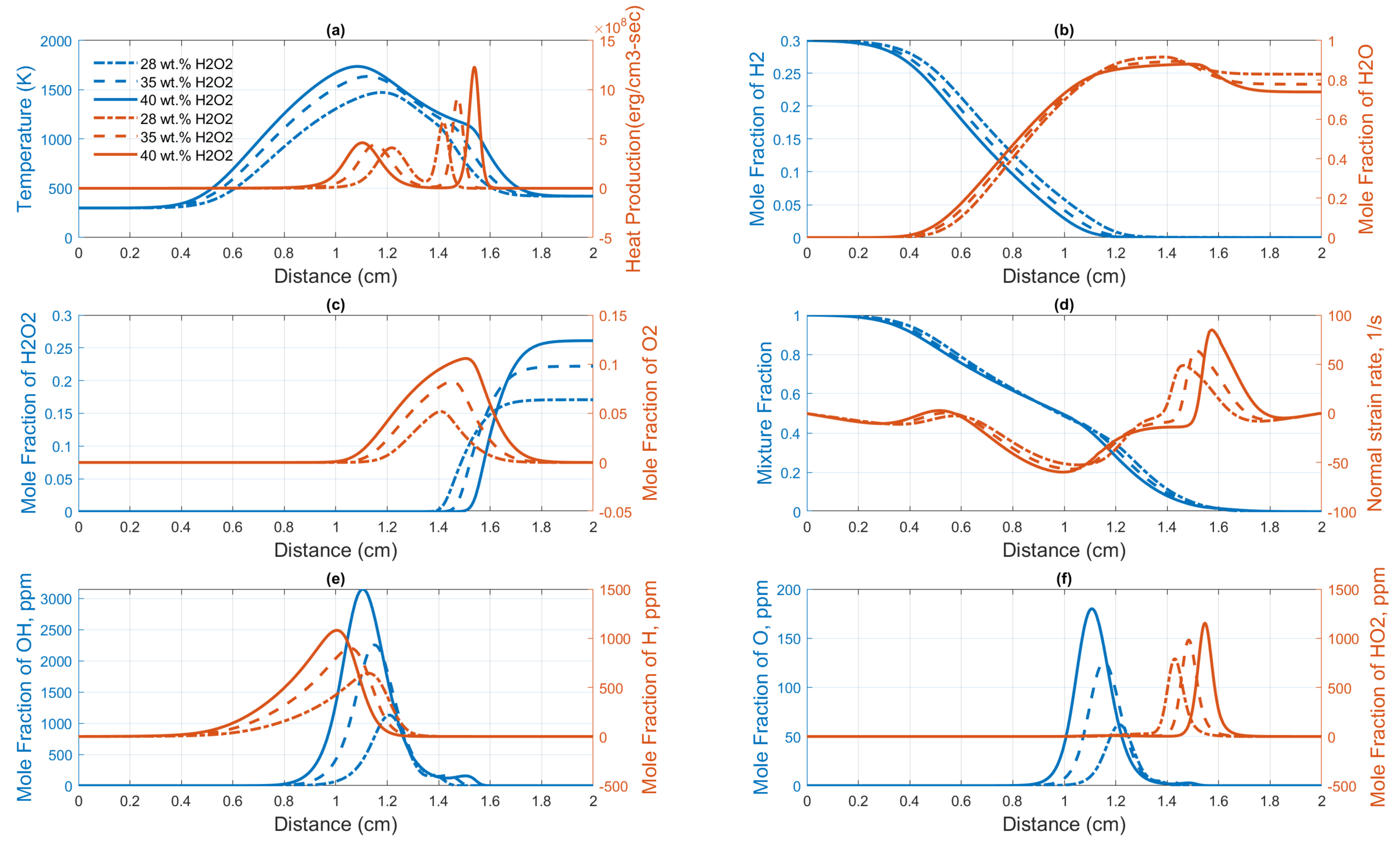

Figure 3. Axial profiles of computed temperature, heat release, and species for diluted hydrogen-H_2O_2 with different concentrations. The strain rate is kept constant at 45 1/s. They are proportionally related to the concentration of H_2O_2.

Results

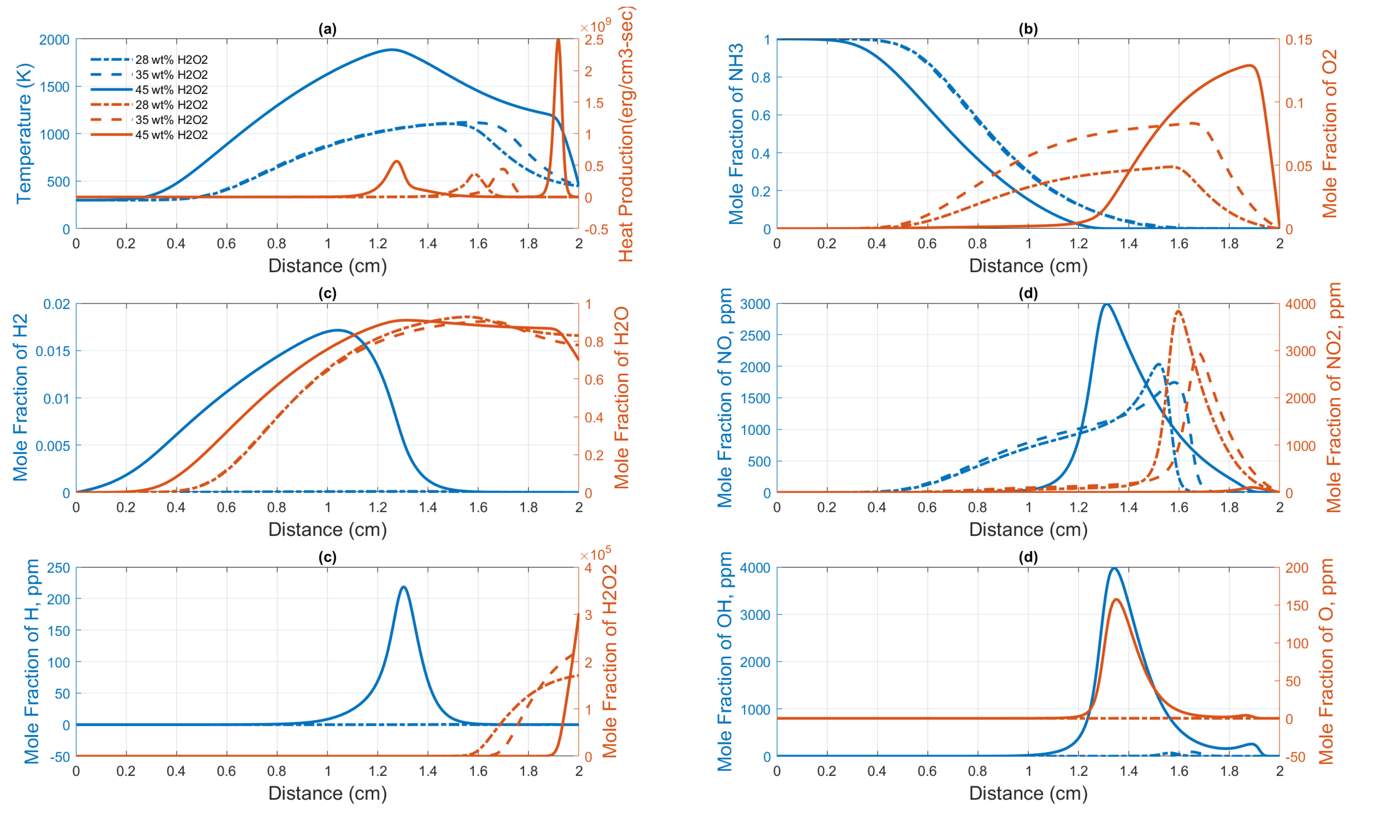

Figure 4. Axial profiles of computed temperature, heat release, and species for pure NH_3-H_2O_2 with different concentrations. The strain rate is kept constant at 20 1/s. High temperature(~1900 K) and intermediate temperature(1100 K) flames are observed.

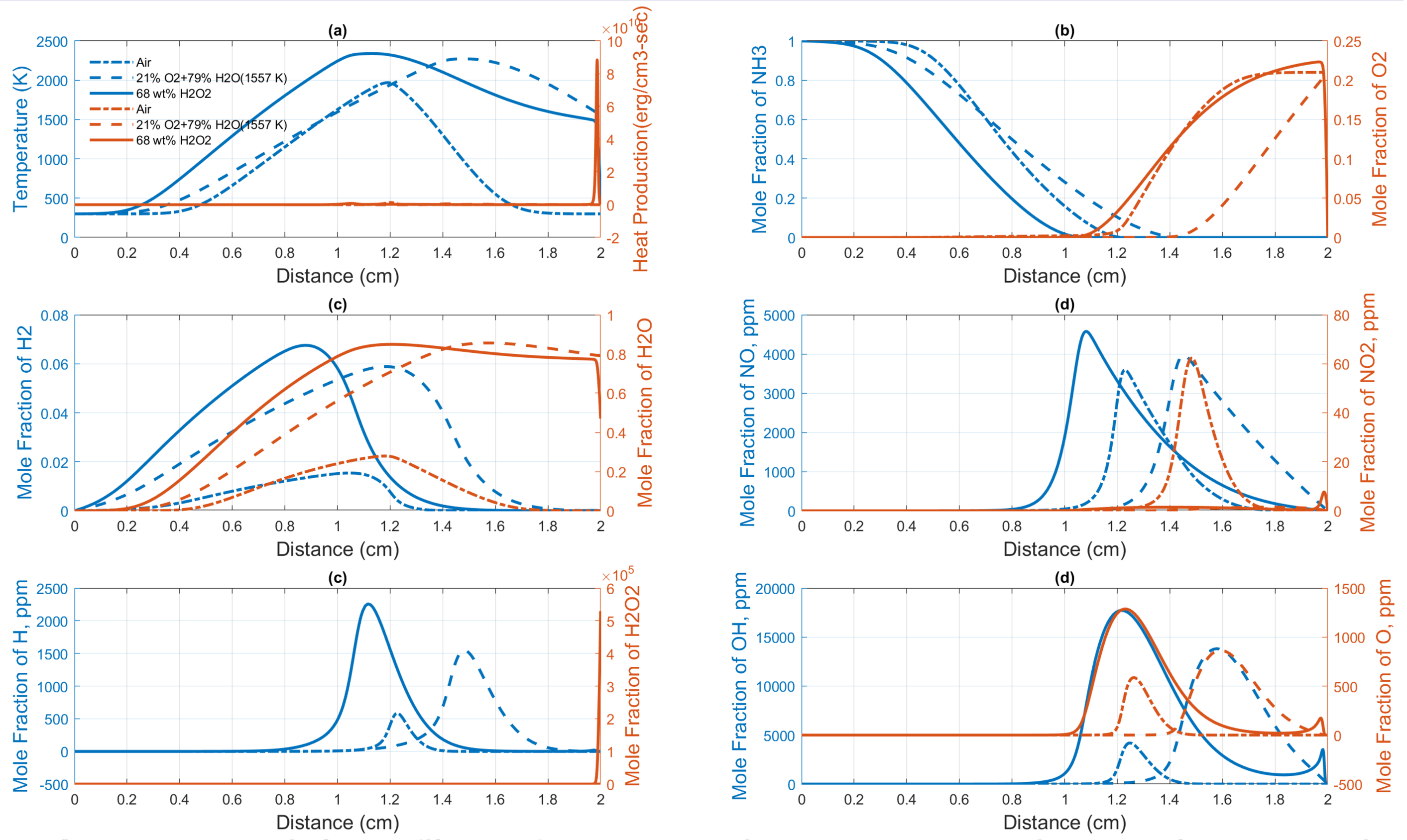

Figure 5. Axial profiles of computed temperature, heat release and species for pure NH_3-air/O_2 steam/H_2O_2 steam. The strain rate is kept constant at 20 1/s. Steam can be a great choice to decrease NO and NO_2.

Summary

- A 1-D laminar non-premixed flame model was used to investigate the flame's structure using H_2O_2/H_2O as the oxidant.
- The effect of hydrogen peroxide concentration, fuel type, and steam on the flame structure was investigated through parametric studies.
- It was found that ammonia flames exhibit a bi-modal flame temperature, one at ~1100 K and the second at ~1900 K. The flame temperature depends mostly on the concentration of HP in water.
- Hydrogen can be highly diluted to avoid thermal NOx when combusting with air.
- Hydrogen-H_2O_2/H_2O flame always has double-peak heat release.

Ongoing Work

- Experiments are expected to validate those flame structures and the dissociation effects of hydrogen peroxide.
- Different compositions of $H_2/NH_3/N_2$ can be used in the fuel side to emulate ammonia cracking.
- Gas analyzer or gas chromatography will be used to detect the important species and steam effect on emission.
- Extinction strain rates' measurement.