

Experimental and Numerical Studies of Primary Reference Fuels Oxidation: Flow Reactor Experiments and Model Comparison

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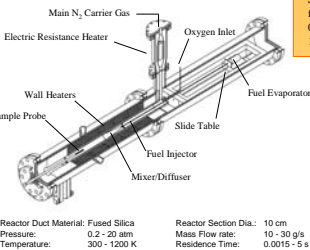
Motivation

- The chemical kinetics of Primary Reference Fuels (PRFs) are frequently used to represent complex combustion chemistry behavior (autoignition, oxidation rate, heat release rate, and chemical species evolution) for gasoline blends.
- The predictive nature of all kinetic mechanisms depends strongly on the experimental observations used in their validation.
- Additional high pressure PRF oxidation data that include species measurements offer an opportunity to compare and improve model performance.
- Large-dimensional, validated detailed kinetic mechanisms represent a means of understanding complex kinetic behavior and of embodying the experimental data base.

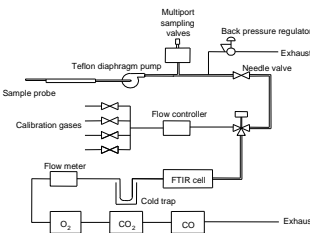
Outline of the Present Study

- Provide new experimental data on PRF oxidation at high-pressure conditions.
- Compare predictions using the detailed PRF mechanism of Curran et al. (1998, 2004) and new experimental results.
- Apply numerical flux, sensitivity and other analysis methods to further advance mechanistic understanding.

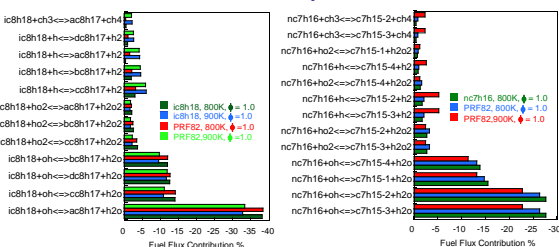
Princeton Variable Pressure Flow Reactor (VPFR)



Flow Reactor Sampling System



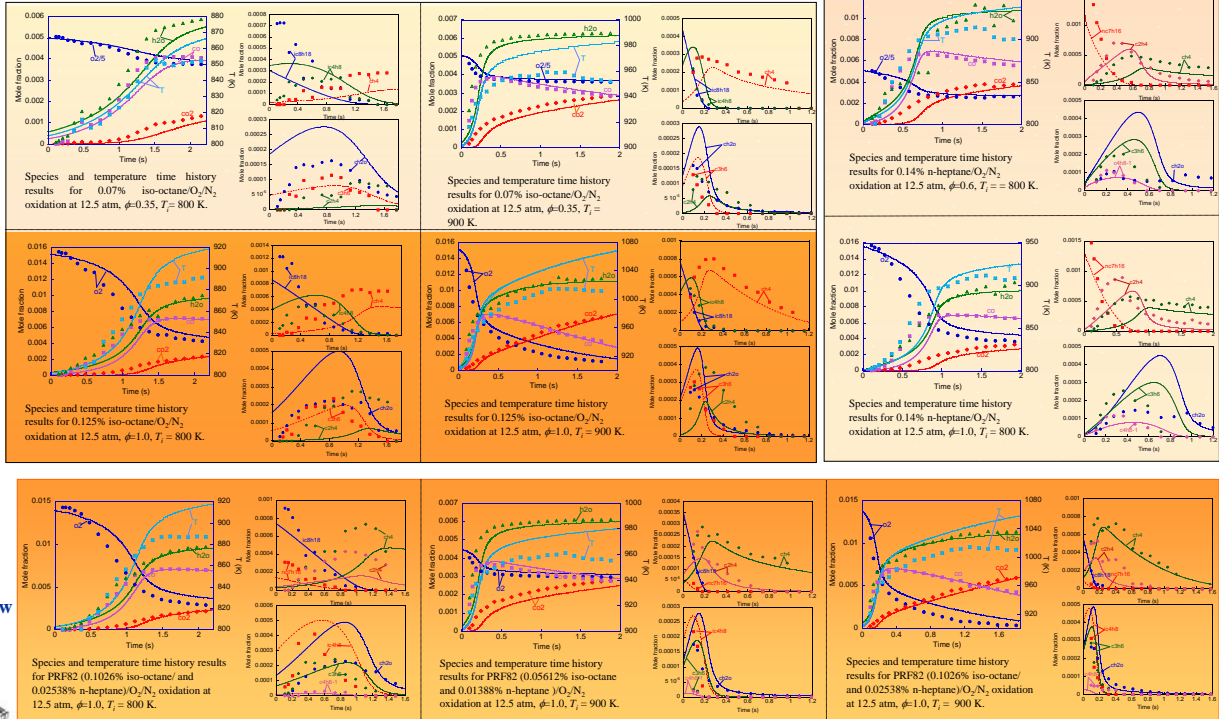
Flux Analysis



- The overall integrated OH abstraction rates are about 90% of the fuel destruction predicted in all calculations.
- The abstraction reactions by h and ho2 also made significant contributions.

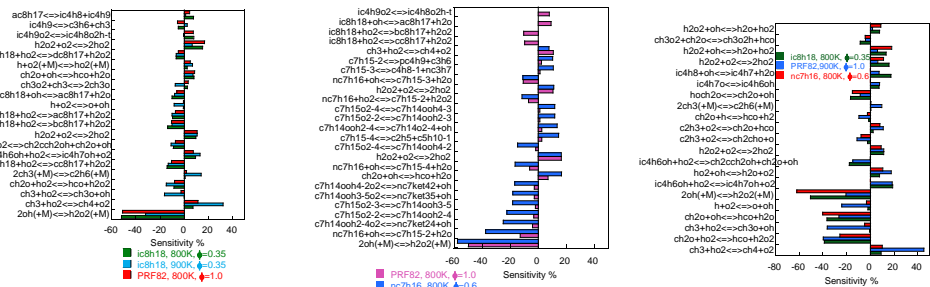
VPFR Oxidation Data vs. Model Prediction

Symbols: present flow reactor experiment; lines: Curran et al. (1998) mechanism



Sensitivity Analysis

Sensitivity analysis of Curran et al. (1998, 2004) mechanism at specified initial conditions for iso-octane, n-heptane, and ch2o.



- 2oh(+M) = h2o2(+M) is the most important reaction affecting the rate of fuel consumption and ch2o profile.
- The termination reactions of ho2 radicals, ho2+ch3 = ch4 + o2 and 2ho2 = h2o2 + o2, are the most influential reactions controlling iso-octane consumption; the latter reaction is also important in controlling n-heptane consumption, while the former affects ch2o concentration.

Summary

- New high-pressure flow reactor PRF oxidation experiments were performed in a VPFR (800-900K and 12.5atm) and the time history of stable species are reported.
- The data have been used to validate a detailed chemical kinetic mechanism of PRF oxidation (Curran et al. 1998, 2004).
- The model predicts reasonably well the heat release rate and major species profiles (e.g., co, co2 and h2o), especially at higher temperatures where the system is controlled by co oxidation. The model generally predicts a slower rate of initial fuel and oxygen consumption as compared to the experimental results. Significant differences between the experimental data and the model predictions are observed for minor species, such as ch2o, i-c4h8, and c2h4. Further model development is necessary to resolve the observed discrepancies.
- Flux and sensitivity analyses of the model have been performed at selected conditions to facilitate further mechanism development and improvement.

Acknowledgements

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- A minimized mechanism which closely replicates all predictions of the original detailed Curran et al. (1998, 2004) mechanism has been also generated in our lab. The model can also be used for 1-D flame speed calculations. It is available for download at <http://www.princeton.edu/~combust>
- A further improved PRF model capable of reproducing the present VPFR data, flame speed data obtained at Princeton, and other available literature data (inclusive of ignition delays) has also been produced. The new model will be released in the near future.