

Comprehensive JP8 Mechanism for Vitiated Flows

K. M. Hall

Chemical Biomolecular Engineering, University of Pennsylvania

X. Fu and K. Brezinsky

Mechanical and Industrial Engineering, University of Illinois at Chicago

With the intent of optimizing the combustion process of complex hydrocarbon liquid fuels such as JP8 in internal combustion jet engines and their afterburners, simpler surrogate hydrocarbon compounds were used in a counterflow diffusion flat flame burner to validate the chemical kinetic modeling process. The combustion products sampled from the flame produced during the burning of the validation fuels methane and n-heptane were analyzed using a Varian CP3800 gas chromatograph. The effects of sampling with a 350 micron outer diameter (OD) fused-silica tube were compared to those of a 3.5 mm quartz probe in order to minimize sampling effect on the flame. Simulations of the sampled species were performed using the OPPDIF package of CHEMKIN with chemistry models provided by UIC. Concentrations of major species (e.g. CO, CH₄, CO₂, O₂) were found to be well simulated with the models, with the best fit occurring for methane and n-heptane, and wider variation occurring with some species in all validation fuels.

Introduction

With the increasing demand for green energy and efficient, environmentally friendly fuels, the combustion of complex hydrocarbon liquid fuels such as JP8 in internal combustion jet engines and their afterburners becomes increasingly important. However, with the benefits that come from burning these fuels come enormous environmental impacts. In addition to the desired energy, combustion products of these fuels include harmful pollutants such as soot, carbon monoxide, unburned hydrocarbons, and others. In order to optimize the combustion process of these fuels for maximum efficiency and minimum negative environmental and health impacts, it is necessary to develop a comprehensive chemical kinetic model of the process.

JP8 is a liquid fuel mixture of various hydrocarbons ranging in size from C₄ to C₁₆, which makes it a prohibitively complex task to accurately and completely model its combustion.¹ Hence, in order to validate the experimental protocols and establish a standard for modeling, simpler surrogate fuels, including m-xylene, n-propylbenzene, decane and n-heptane, are used.

Preliminary combustion models have been developed for m-xylene, n-propylbenzene, and n-heptane and been found to correlate within experimental uncertainty with the predictions generated by the computer simulation.

Materials and Methods

The experimental apparatus is a counterflow diffusion flat flame burner, into which the oxidizer gases are injected from the top and the prevaporized fuel is injected from the bottom with a syringe pump. This type of burner, shown in Figure 1(a)1(b), consists of two oppos-

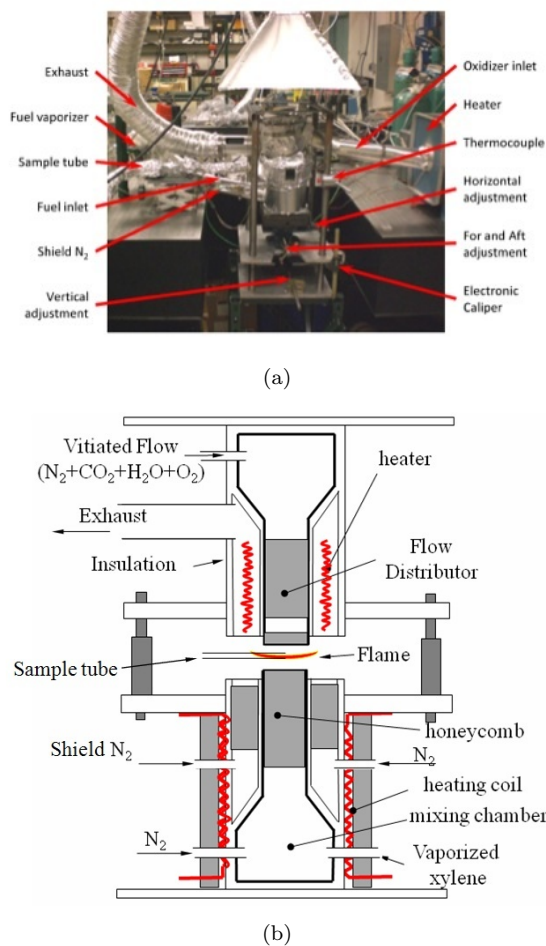


FIG. 1: Methane experimental setup. Counterflow diffusion flame burner.

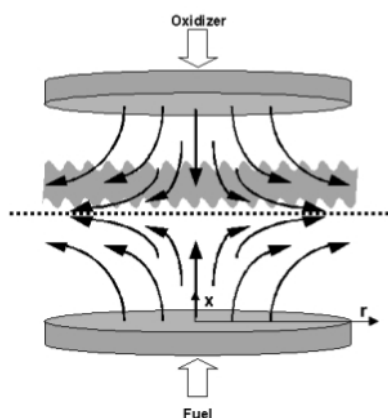


FIG. 2: Geometry of the axisymmetric opposed flow diffusion flame which enables 1D modeling. From OPPDIF Application User Manual.

run opposite to one another and create a flame between the two inlets, simulating the flow of fuel from an afterburner against the oxidizing gases in the atmospheric air.² This setup, as shown in Figure 2, enables the formation of a stable stagnation plane and flat diffusion flame, which greatly simplifies the geometry and enables one-dimensional modeling of the flame structure due to the relatively high strain rate. In order to simulate the conditions of the jet engine afterburner, the fuel is heated to 300°C and the oxidizer gases are heated to 700°C prior to injection. A quartz probe with an outer diameter of 3.5 mm is used to sample the combustion products and attached to a gas chromatograph to measure the mole fractions of different species present in the flame. After a 6-minute equilibration period during which the flame stabilizes, a gas sample is withdrawn and injected into the GC for analysis.

A type K thermocouple is used to measure flame temperature. Because this type of thermocouple cannot withstand the high temperatures of the flame, it is used to measure the temperature of the exit fuel (350 to 360°C) and oxidizer gases (650 to 710°C). Future work includes use of Pt-Pt/13%Rh thermocouples to obtain complete temperature profiles of the flames.

A nitrogen shield is run from bottom to the top of the apparatus to prevent the combustion products from mixing with the environmental air and maintain an accurate sampling of the concentration profile of the components within the burner.

The burner is placed on an adjustable platform, which is moved up and down relative to the stationary sampling probe in order to adjust the distance from the fuel inlet in the burner to the probe. This sampling process is repeated, increasing the distance from the fuel inlet to the probe in 0.5 mm intervals spanning the 1.44 cm total distance from the fuel inlet to oxidizer nozzle in order to create a complete 1D profile of the combustion products

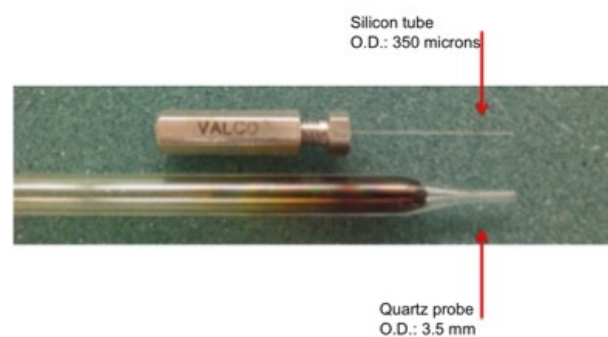


FIG. 3: Sampling devices. Above, fused-silica tube; below, quartz probe.

of each fuel.

The large size of the quartz probe was found to interfere with the flame's flow and introduce additional error into the measurement of species. For the n-heptane flame sampling and later experiments, the probe was replaced with a smaller fused-silica column of outer diameter of 300 microns, retaining the same inner diameter as of the quartz probe, 250 microns. The upcoming experiments include repeating the process using this setup with methane as the fuel. Figure 3 shows the difference in outer diameter of the two sampling devices.

Due to the relatively few species produced during its combustion and the predictability of the concentration profile, methane has been used as a validation fuel to test and optimize the apparatus.

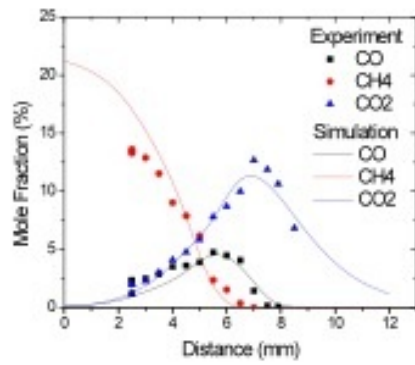
Simulations of methane and n-heptane flames are performed using the OPPDIF package of CHEMKIN with chemistry models provided by UIC, and compared to the data obtained with the flame apparatus. The simulation uses the UIC m-xylene model³ and the GRImech model⁴ for the methane experiments, and Paolo Berta's n-heptane combustion model for the heptane experiments. By entering methane as the only fuel in the UIC model, the simulation is forced to bypass the xylene and larger molecule chemistry in its prediction.

Results and Discussion

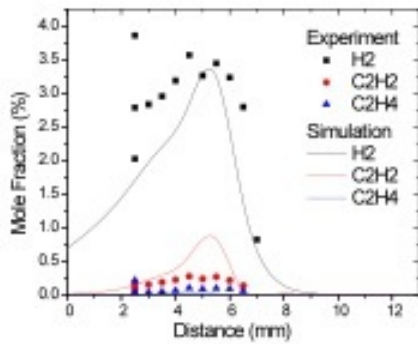
In the methane experiment with the original quartz probe setup, the observed concentrations of CO, CH₄, CO₂, N₂, and O₂ were found to agree highly with the calculated concentrations from CHEMKIN, while other species (H₃, C₂H₂, C₂H₄) showed much larger deviation from the simulation, as shown in Figure 4(a)4(b)4(c).

In a new series of simulations, it was found that the GRI mechanism provides a better fit to the experimental data than the UIC m-xylene model, as shown in Figure 5(a)5(b), due to differences in kinetics and additional chemical species in the models.

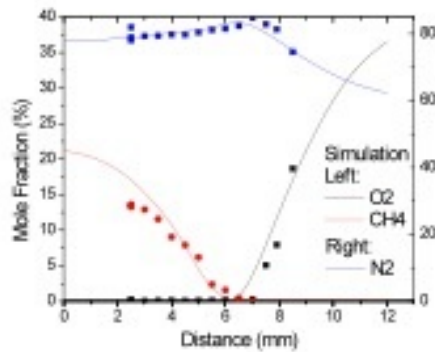
Because the large quartz probe used for sampling was



(a)



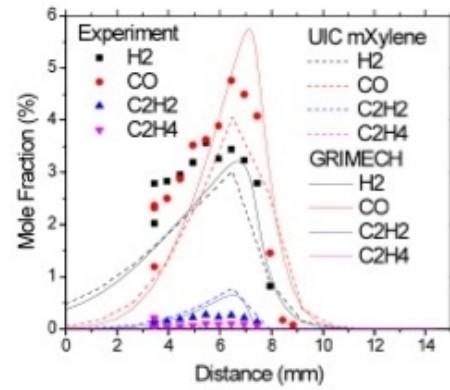
(b)



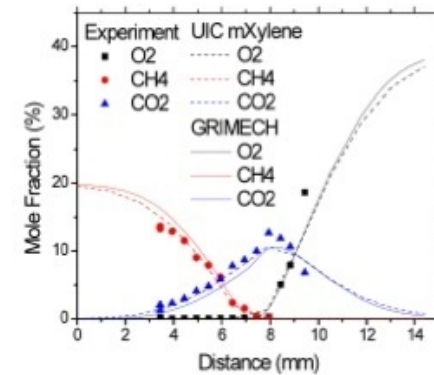
(c)

FIG. 4: Species of UIC m-xylene model methane flame simulation and experiment comparison. Dots: experiment data, lines: simulation data Condition CH_4 0.4 L/min, N_2 (fuel side) 1.6 L/min, O_2 0.7 L/min, N_2 1 L/min

found to affect the flow in the flame, it was replaced by much smaller, less-invasive fused-silica tubing. However the smaller tubing of the less invasive probe cannot withstand the high temperatures of this experiment, and has been observed to melt when exposed to the high-temperature flame of the hotter-burning fuels for a long



(a)



(b)

FIG. 5: Comparison of UIC m-xylene model, GRIMECH model and experiment. Condition CH_4 0.4 L/min, N_2 (fuel side) 1.6 L/min, O_2 0.7 L/min, N_2 1 L/min.

period. In order to correct for this, the equilibration period in the flame was altered to allow the flame to burn for 4 minutes rather than 6 prior to insertion, and then allow the tube to spend 2 minutes in the flame before sampling.

The use of this tubing showed much promise for precision in species measurement in the n-heptane combustion, and reduced the experimental limits of precise and accurate measurement of the species in an actual afterburner. As predicted, the OPPSMOKE modified OPPDIF simulation, using n-heptane combustion chemistry provided by Paolo Berta,¹ shows excellent agreement with the n-heptane experimental data, as shown in Figures 6(a) and 6(b).

Although some discrepancies still exist between the simulation and experimental data, the fused-silica tube setup shows great promise for increasingly accurate and consistent experimental measurements that will provide confidence in the validation of these and future models for combustion.

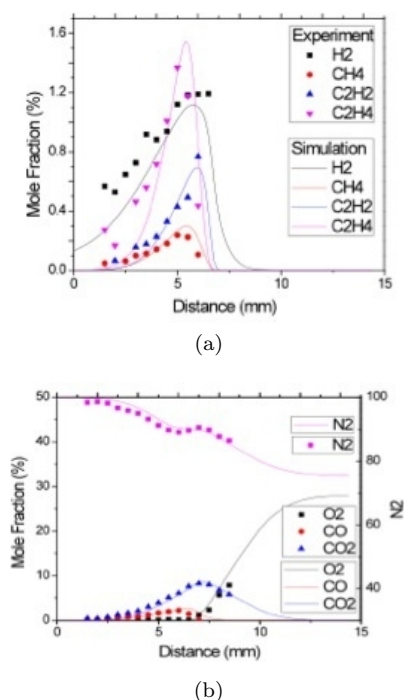


FIG. 6: Species of n-heptane flame simulation and experiment.

Future Work

In order to truly validate these models, the methane and heptane experiments must be repeated to provide proof of repeatability and consistency of data. Sampling of the methane flame should be done using the new probe setup, in order to quantify the comparison in accuracy between the quartz and fused-silica probes and verify the heptane results. Other hydrocarbon fuels should also be simulated and sampled for further validation, as well as simple surrogate mixtures such as a methane/heptane mixture.

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- ² R. Seiser, L. Truett, D. Trees, and K. Seshadri, Proceedings of the Combustion Institute **27**, 649 (1998).
- ³ R. Sivaramakrishnan, L. et al, and B. et al., uIC mMXYLENE model: Includes Sivaramakrishnan's Toluene oxidation model with updated pyrolysis steps, m-Xylene thermochemistry from Dagaut's m-Xylene model, methylcyclopentadiene reactions from Lifshitz et al, updated cyclopentadiene reactions from Burcat et al.
- ⁴ G. P. Smith, D. M. Golden, M. Frenklach, N. W. Moriarty, B. Eiteneer, M. Goldenberg, C. T. Bowman, R. K. Hanson, S. Song, W. C. G. Jr., et al., Tech. Rep., University of California, Berkeley, http://www.me.berkeley.edu/gri_mech/ (2010).