Flow Reactor Studies of Synthetic Oxygenated Fuels for Diesel Engines
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Background

Recent studies of the effect of oxygenated fuels on particulate formation under Diesel engine combustion conditions show that:

- Particulate emissions are significantly reduced.
- The emissions reductions depend on both the amount of oxygen in the fuel and the oxygenate structure.
- Using oxygenated fuels to replace or supplement petroleum-based fuels in high-efficiency Diesel engines is a promising technology for reducing greenhouse gas emissions from the transportation sector.

Objectives

- Acquire experimental data to use in refinement, optimization and reduction of detailed reaction mechanisms for oxygenated fuels.
- Assess model fidelity through complementary flow reactor and shock tube experiments.
- Study a set of representative oxygenated fuels with different oxygen functionality (ethers, ketones, esters, aldehydes) in order to access a variety of soot formation pathways.
- Several oxygenated fuels with potential for particulate emission reduction from Diesel engines have been identified, including dimethyl ether, acetone and butanal.

Here, we present initial results from a flow reactor experimental investigation of dimethyl ether (DME) oxidation.

Approach

- The centerline gas temperature and stable species concentrations are measured at ambient pressure and elevated temperature.
- The effect of temperature, pressure, and reactant concentration on reaction timescales, heat release rate and intermediate and product species profiles are determined for rich conditions.
- The measured species and temperature profiles are compared to the model predictions using a detailed reaction mechanism.

Reacting Flow Model

- Mixing-reacting model is based on reactor flow conditions and measured temperature profiles, with boundary-layer correction from centerline velocity measurements.

Results

- Rich DME experiments (Φ = 2) have been conducted at 1 atm with an initial temperature of 1200 K.
- The reactor flow rates, geometry and measured temperature profile are used as input to the mixing-reacting model simulation.

Conclusions

- The measured and predicted time-evolution of species concentrations are in relatively good agreement.
- At longer reaction times, measured carbon balance closes to better than 1%. At early times, only approximately 85% of the carbon can be accounted for due to loss of water-soluble species in the sampling system.

Future work

- High pressure DME experiments
- Experiments at pressures relevant to diesel combustion to investigate the effect of pressure on DME chemistry
- Comparison of DME experimental data with additional DME kinetic mechanisms available in the literature.
- Experiments with DME as an additive to heptane, a common component of diesel surrogates.
- Flow reactor experiments at conditions overlapping with shock tube experiments with representative oxygenates from other functional groups.