Carbon Mitigation from the Perspective of Combustion -- Fundamentals, Fuel Characteristics, Engine Performance, and Safety

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Outline
- Progress & publications
- Flamefront instabilities
- Dimethly ether (DME) as a diesel fuel
  - Ignition of DME
  - Chemistry reduction for DME
Instabilities in flame propagation, relevant for: transition to turbulence and detonation, engine knock, explosion hazard


Ignition, flame propagation, and chemistry of dimethyl ether (DME)

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Equivalence ratio: 0.60
Mixing ratio: 0.50.

Instability aggravated with increasing pressure, hence promoting knocking in engines
Increasing propane addition

- Equivalence ratio: 0.80
- Pressure: 5 atm
- Flamefront instability diminished or suppressed with propane addition
Dimethly Ether (DME) As A Diesel Fuel

- Chemical formula: CH$_3$OCH$_3$
- An oxygenated hydrocarbon; low C:H ratio; no C-C bonds; cetane no.: 55-60.
- Diesel engine testing: reduced emissions of CO, NO$_x$, formaldehyde, particulates, and UHC.
- As methanol ignition improver
Ignition of DME

- Counterflow experimental determination of ignition temperature

- Computational simulation using most recent DME oxidation mechanism; agrees with experiment
Chemistry Reduction for DME

- Detailed mechanism consists of 78 species and 398 elementary reactions; too large for computational simulation of engine processes.

- By using graph theory, detailed mechanism reduced to a skeletal mechanism consisting of 49 species and 251 elementary reactions.

- By using computational singular perturbation, skeletal mechanism further reduced to a short mechanism consisting of 28 species and 33 lumped reactions.
Both skeletal and short mechanisms mimic the detailed mechanism.

- Computer algorithms developed for automatic and comprehensive mechanism reduction.
- Potential application of computer algorithms to atmospheric chemistry.