Global diffusion flame extinction strain rate experiments of single large hydrocarbon fuels.

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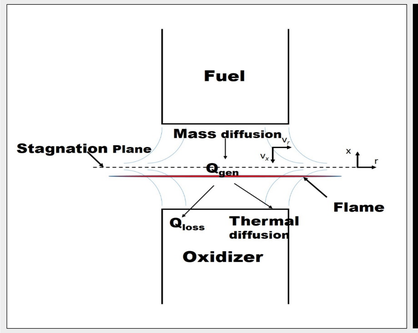
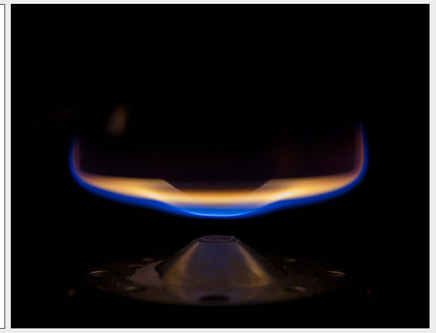
Introduction

- Surrogate fuels are mixtures of simple fuel that can emulate either physical or chemical properties of real fuel.
- Important for future engine development. They are selected to reproduce the chemical kinetics, transport, and physical properties of the real fuel.
- Chemical properties include ignition delay times, flame speeds, extinction limits and soot properties.
- Counterflow flame burners are often used to measure flame extinction.
- Flame extinction occurs when:

Rate of heat lost > Rate of heat produced.



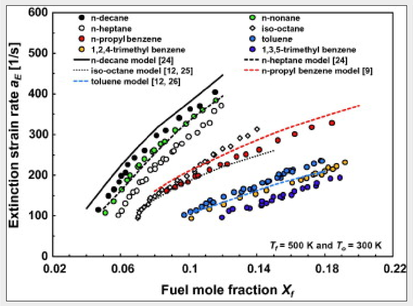
Counterflow flame burner

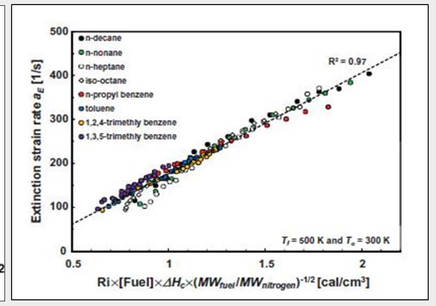


Counterflow flame

Background

- Study based on radical index methodology[1].
- Radical index approach normalizes extinction strain rate of different fuels accounting for differences in
  - Energy
  - Transport
  - Chemical effects





Objective

Predict flame extinction limit of surrogate fuels that would benefit surrogate fuel formulation practices.

Experiment

- The experimental setup consists of a counterflow flame burner with a liquid fuel vaporization system and flow controllers.
- The fuels that are used to study the extinction strain limit are n-heptane, n-decane, and toluene.
- The blended fuel is comprised of equal parts (by volume) of the above three fuels.
- The experiments were conducted at 0.84 atm pressure, the fuel exit temperature was maintained at 500K(±10), and the oxidizer was at 298K.
- The strain rate is calculated by

$$a = \frac{2Uo}{L}\left(1 + \frac{Uf}{Uo}\left(\sqrt{\frac{\rho f}{\rho o}}\right)\right)$$

where, Uo is the velocity of oxidizer, U_f is the velocity of fuel, L is the axial distance, ρ_f is the density of fuel, and ρ_o is the density of oxidizer.

Experimental setup

Numerical computations

- An OPPDIF module of ANSYS CHEMKIN was used to calculate the extinction strain limits.
- For n-heptane, the reduced kinetic mechanism was obtained from Princeton[2].
- For n-decane and toluene, the detailed kinetic mechanisms were obtained from LLNL[3,4] and Metcalfe et al[3,5] respectively, these mechanism were then reduced using CHEMKIN Reaction Workbench

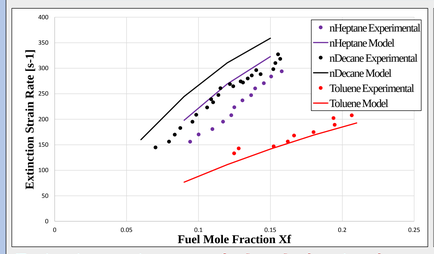
Results

- N-decane showed the maximum extinction strain rate followed by n-heptane and finally toluene. The modeled extinction strain rate for alkanes over predicted the experimental measurements.
- Toluene extinction limit prediction reproduced experiments well.
- The radical index is given by

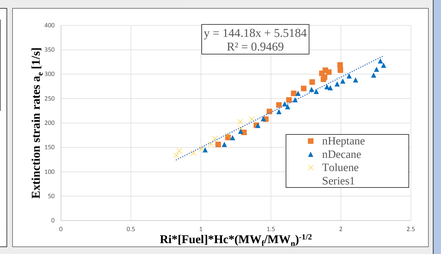
$$Ri = \zeta_{OH,fuel} / \zeta_{OH,n\text{-}alkane}$$

- The Radical index for alkanes is found out to be 0.98-1, and that for toluene is 0.644.
- The correlation obtained from previous study is

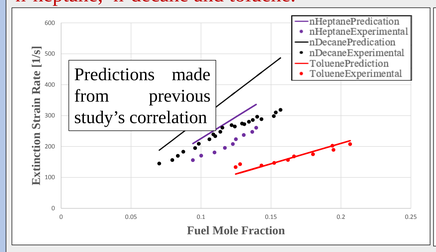
$$a_E = 230 * Ri * [Fuel] * \Delta Hc * \sqrt{\frac{MW_{N2}}{MWf}} - 54$$

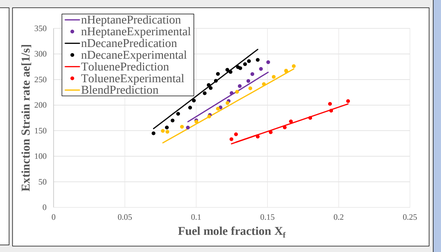


Extinction strain rate vs fuel mole fraction for n-heptane, n-decane and toluene.



Linear trend shown by fuels





Demonstration of predictability with universal correlation for surrogate mixture by accounting for radical index, heat of combustion and average molecular weight using equation from this study.

- The correlation obtained from our study is,

$$a_E = 144.18 * Ri * [Fuel] * \Delta Hc * \sqrt{\frac{MW_{N2}}{MWf}} + 5.5184$$

- Accounting for the Ri, all three fuels collapse to a single linear trend.
- The radical index of the blended fuel is evaluated to be 0.868 by linear summation of the component fuel radical indexes.

Conclusion

- N-alkanes had the highest extinction strain rate, toluene had the least.
- The extinction limits of any blend can be calculated by using the radical index approach.
- By using the correlation obtained from previous study the extinction strain rates for a blended fuel were over predicted.
- This may be because of differences between experiments including the different pressure at which experiments were carried out.

References

1. Hee Won, Sang & Dooley, Stephen & Dryer, Frederick & Ju, Yiguang. (2012).
2. Ju, Yiguang et al. *Proc. Combust. Inst.* 33 (2011): n. pag. Web. doi:10.1016/j.proci.2010.06.110.
3. Sun, Wenting, et al. 157.7 (2010): 1298-1307.