DNS of High Karlovitz Number Turbulent Premixed Flames under Engine-Relevant Conditions

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DoD HPC Modernization Program
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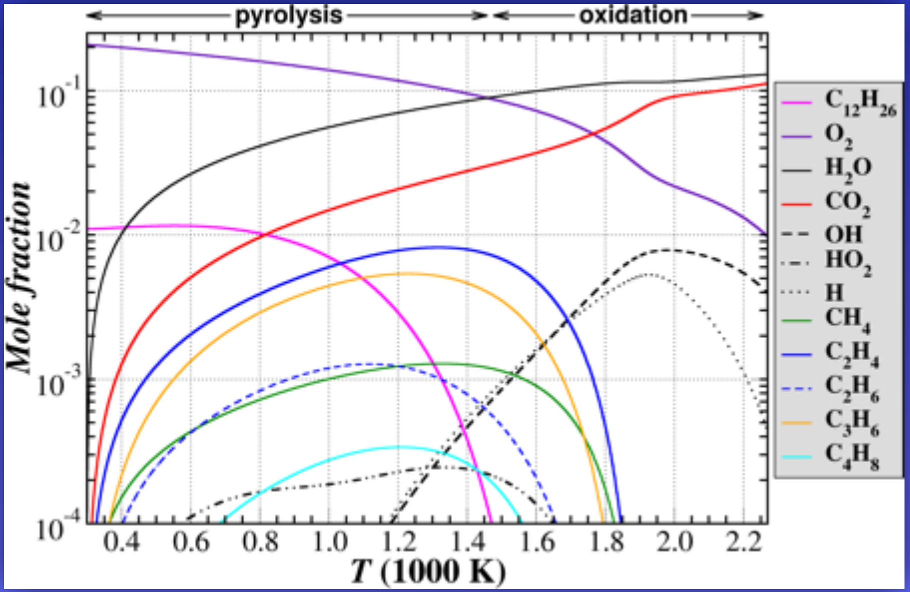
Comparative Study of Hydrocarbon Fuels under Engine-Relevant Conditions

Range of reduced chemical kinetics models

Gao et al. CNF (2016)

- Compact (< 30 species) reaction models for jet fuels and jet fuel surrogates based on the ***HyChem approach*** (Hai Wang, Stanford)
- Stanford (Hai Wang) / University of Connecticut (Tianfeng Lu) mechanisms
  - CH_4 (19 species)
  - n-dodecane (24 species)
  - Cat A2 (29 species)
  - Cat C1 (26 species)
- **Pyrolysis** is approximated by a few semi-global steps
- **Oxidation** is represented by H_2, CO, and C_1-C_4
- **Combination of DRG-based methods and QSSA** to produce extremely compact reaction models



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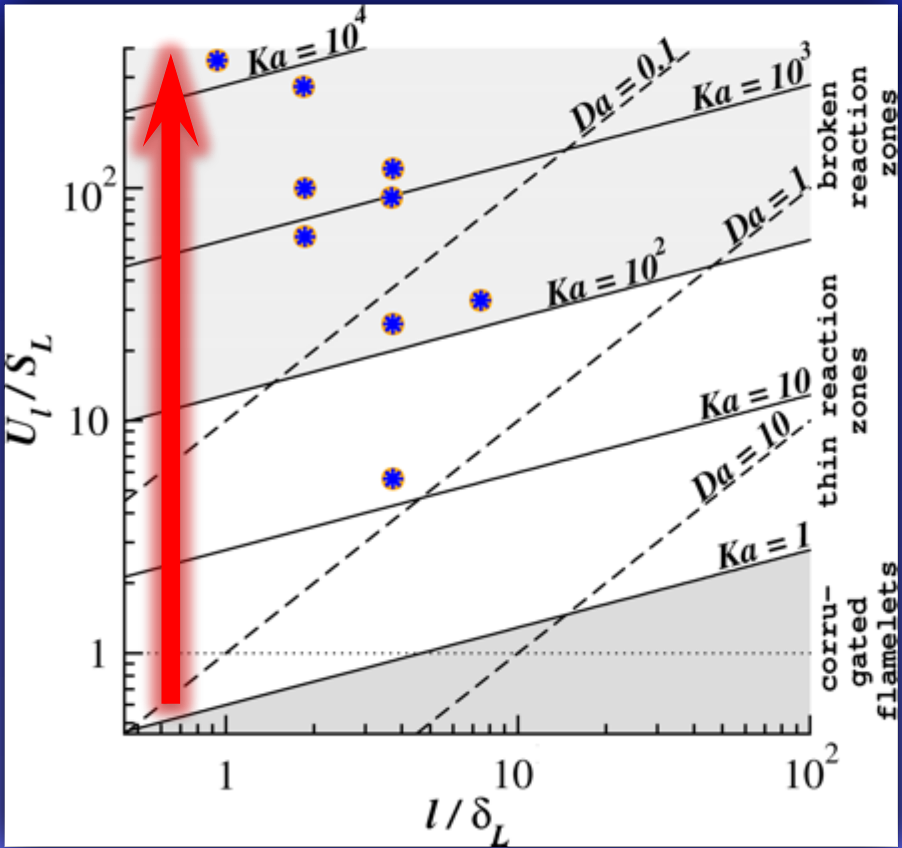
Focus on engine-relevant conditions

- High-pressure (30 bar), lean (ϕ = 0.7) conditions
- Broad range of turbulent intensities:
  - Ka = 10, 10^2, 10^3, 10^4



- ✓ 30 calculations in total
- ✓ Domain: 1 billion cells

Flame structure

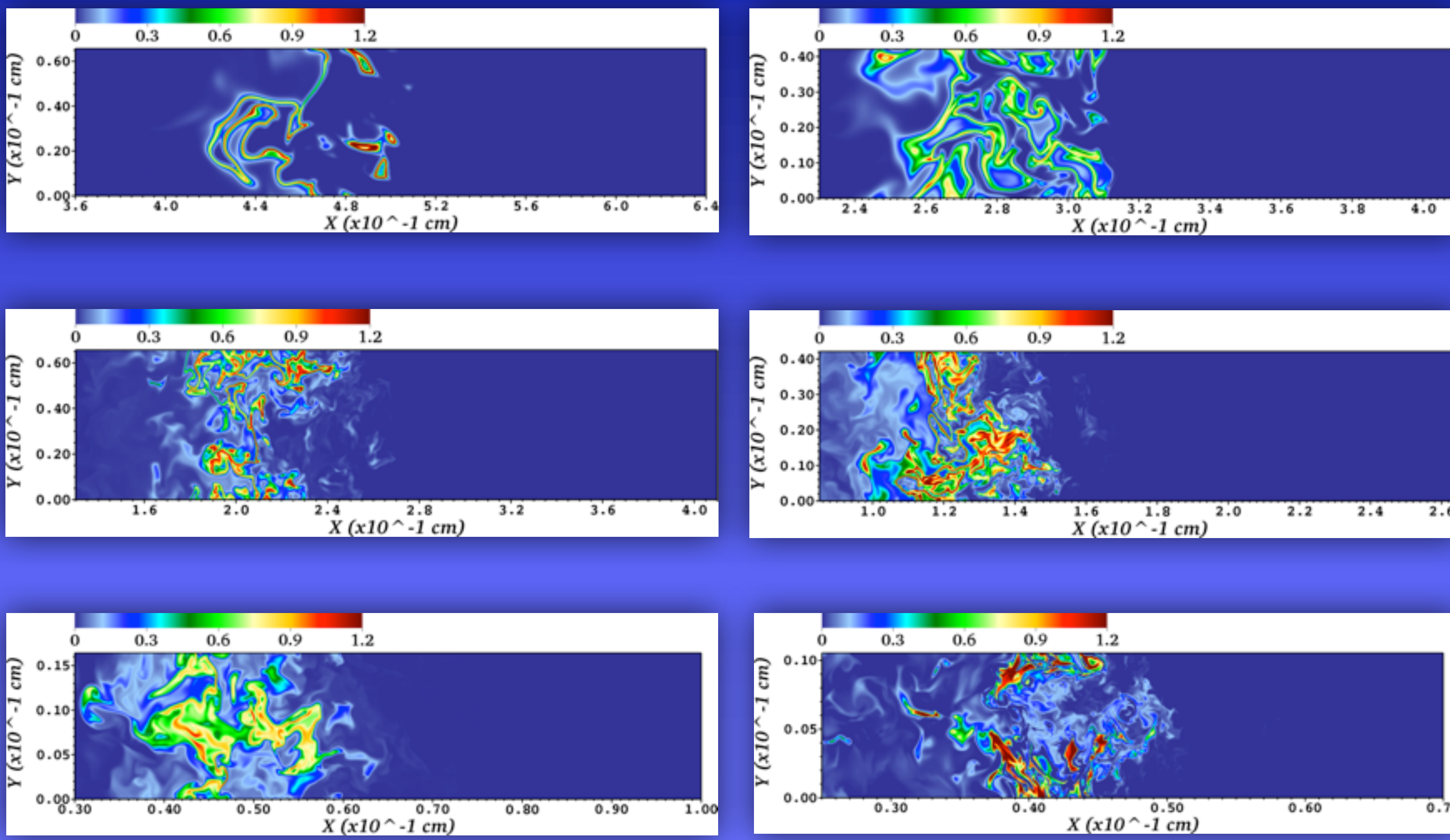
Normalized heat release rate structure

Methane | **Dodecane**

Ka = 100

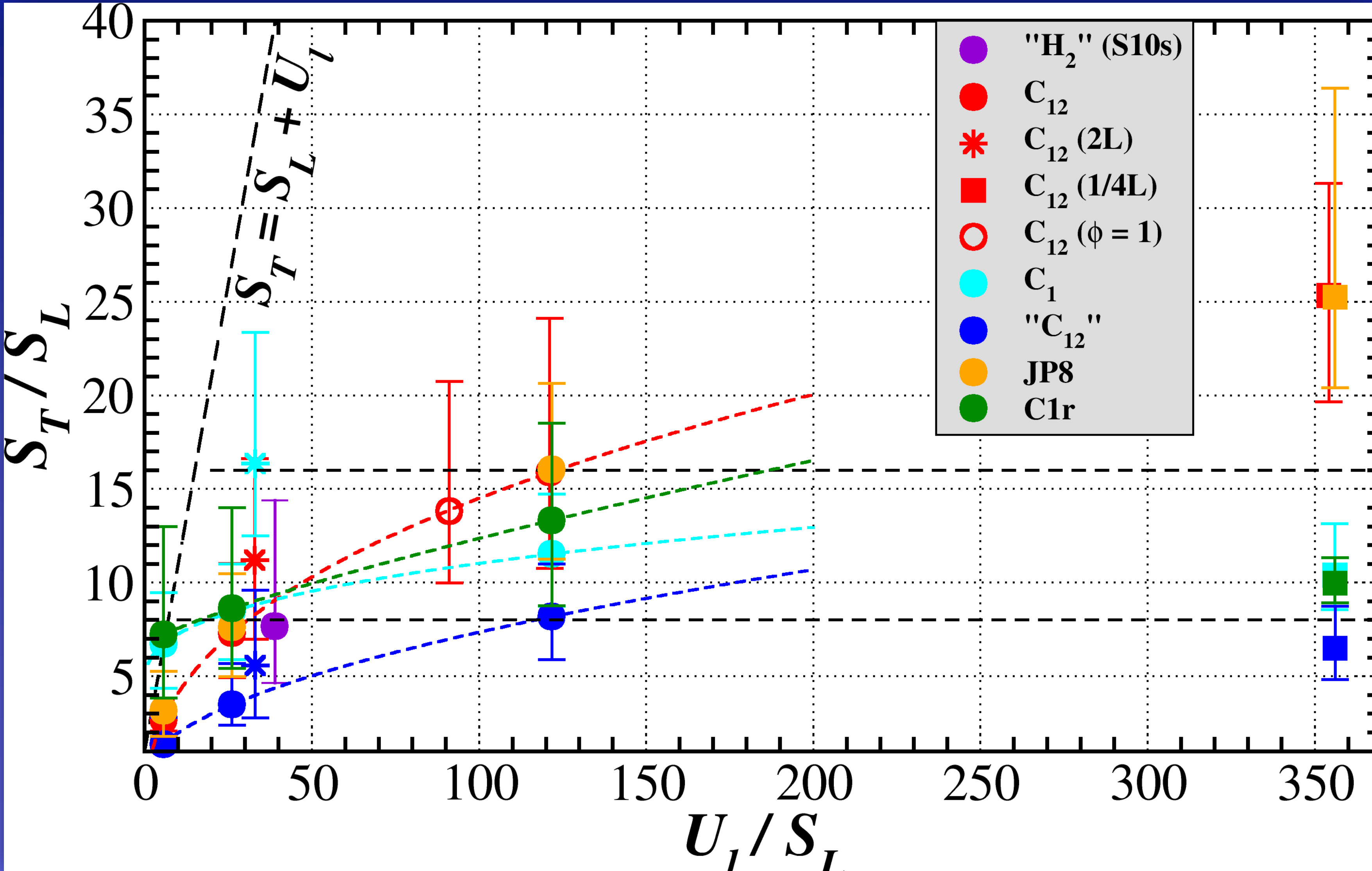
Ka = 1000

Ka = 10,000



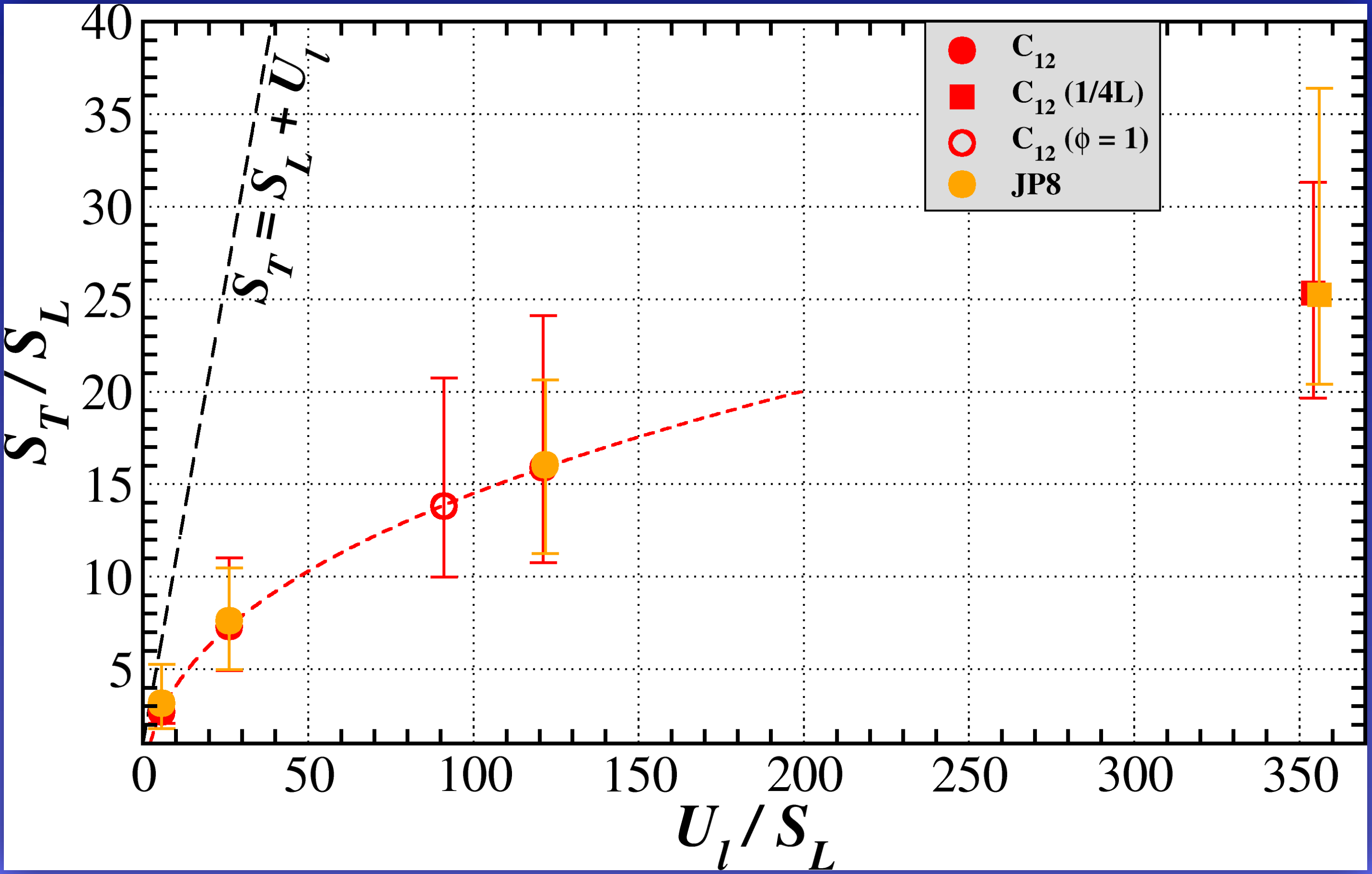
Turbulent flame speed vs. turbulent intensity

Global trends



Turbulent flame speed vs. turbulent intensity
Global trends

n-dodecane/air vs. Cat A2/air

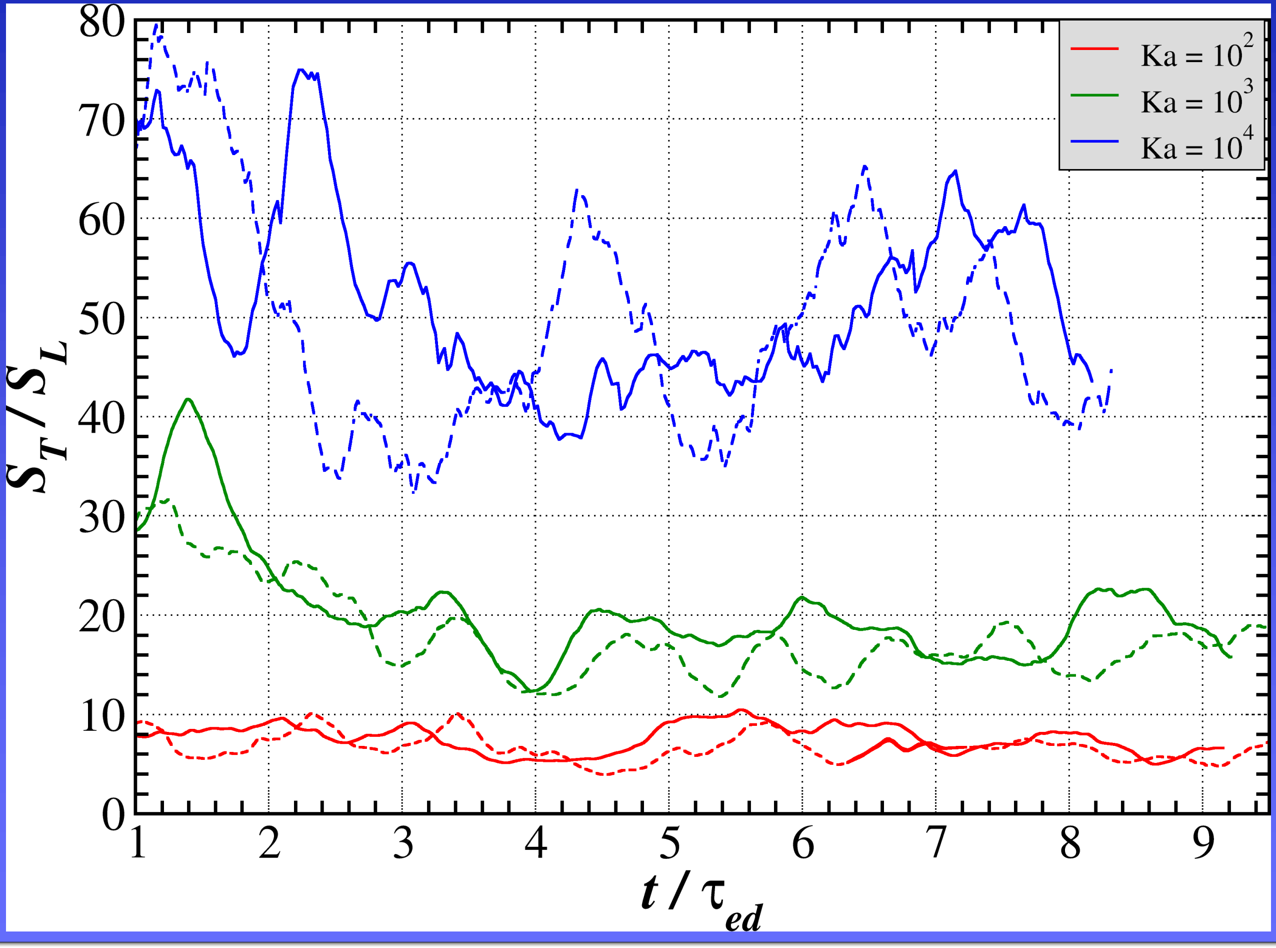


Virtually identical behavior for C_{12} and Cat A2 with reduced kinetics

Turbulent flame speed vs. turbulent intensity

Global trends

Cat A2/air vs. Cat C1/air

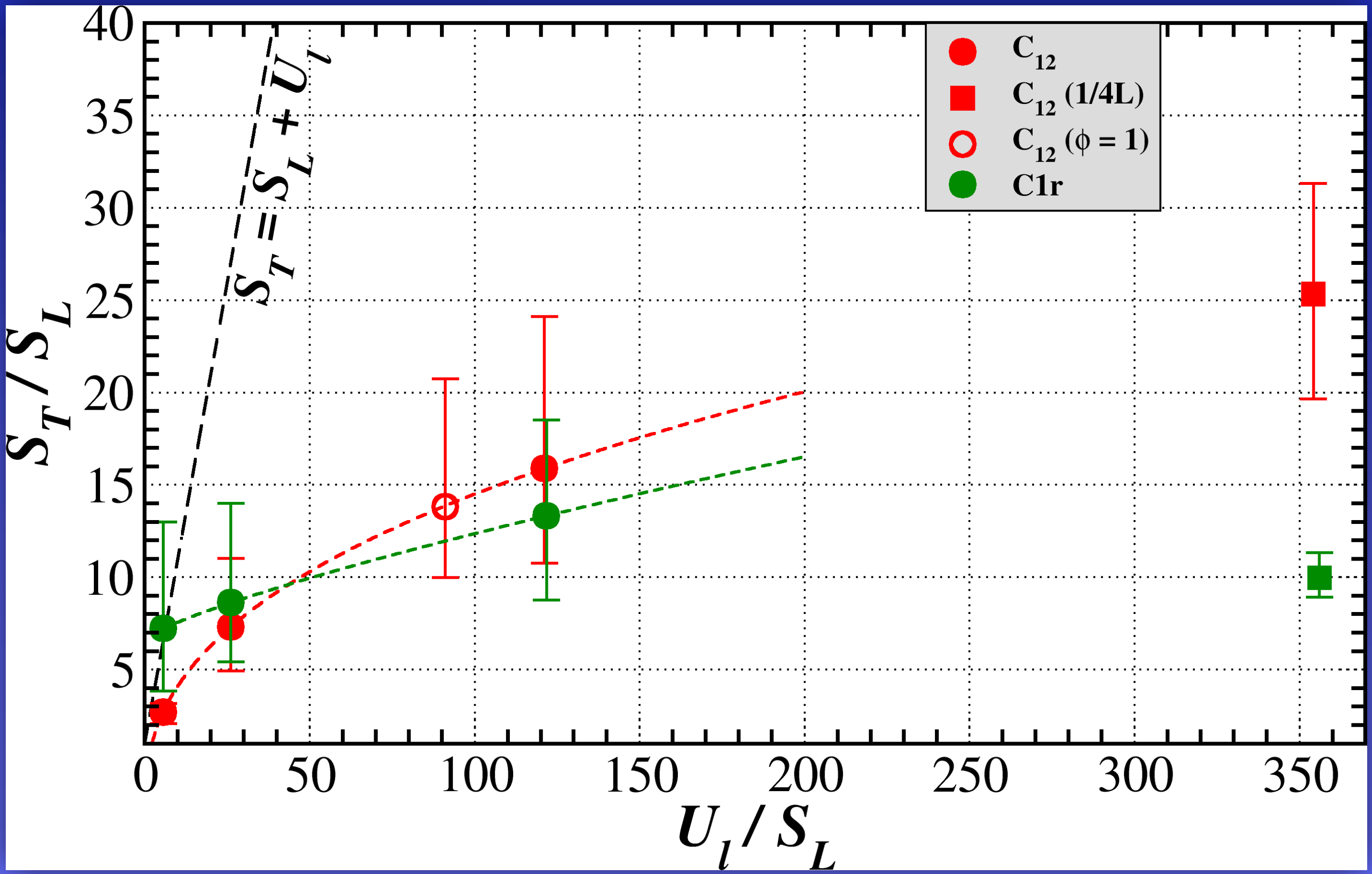


Similarly, virtually identical behavior for Cat A2 and Cat C1 with reduced kinetics

Turbulent flame speed vs. turbulent intensity

Global trends

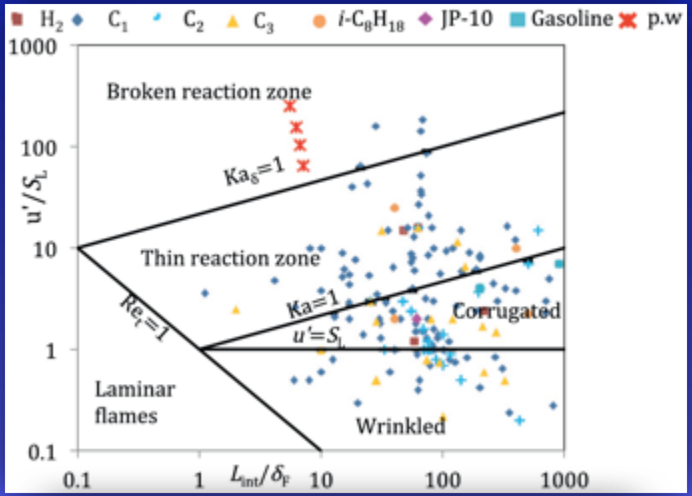
CH_4/air vs. n-dodecane/air

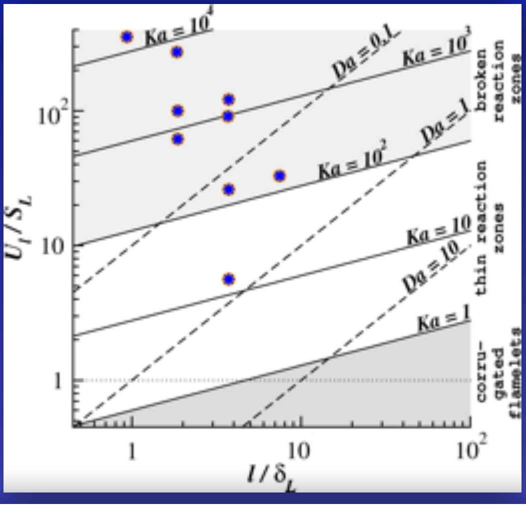


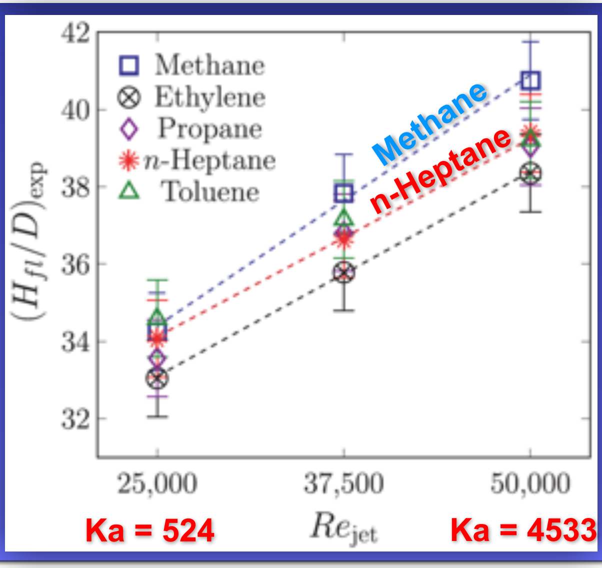
…However, there are differences in global trends between CH_4 and C_{12}

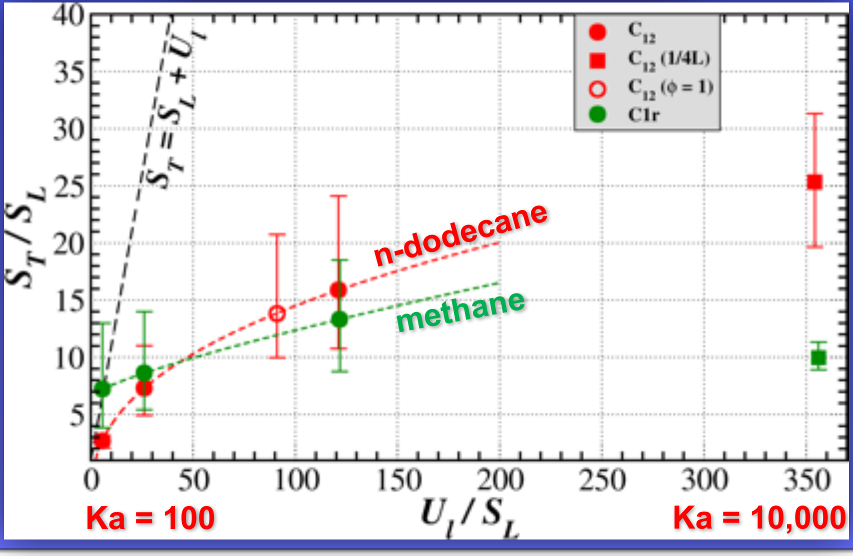
Is there similar evidence present in experiments?

High-speed flames in PPJB, USC/CalTech, Smolke et al. PROCI (2017)





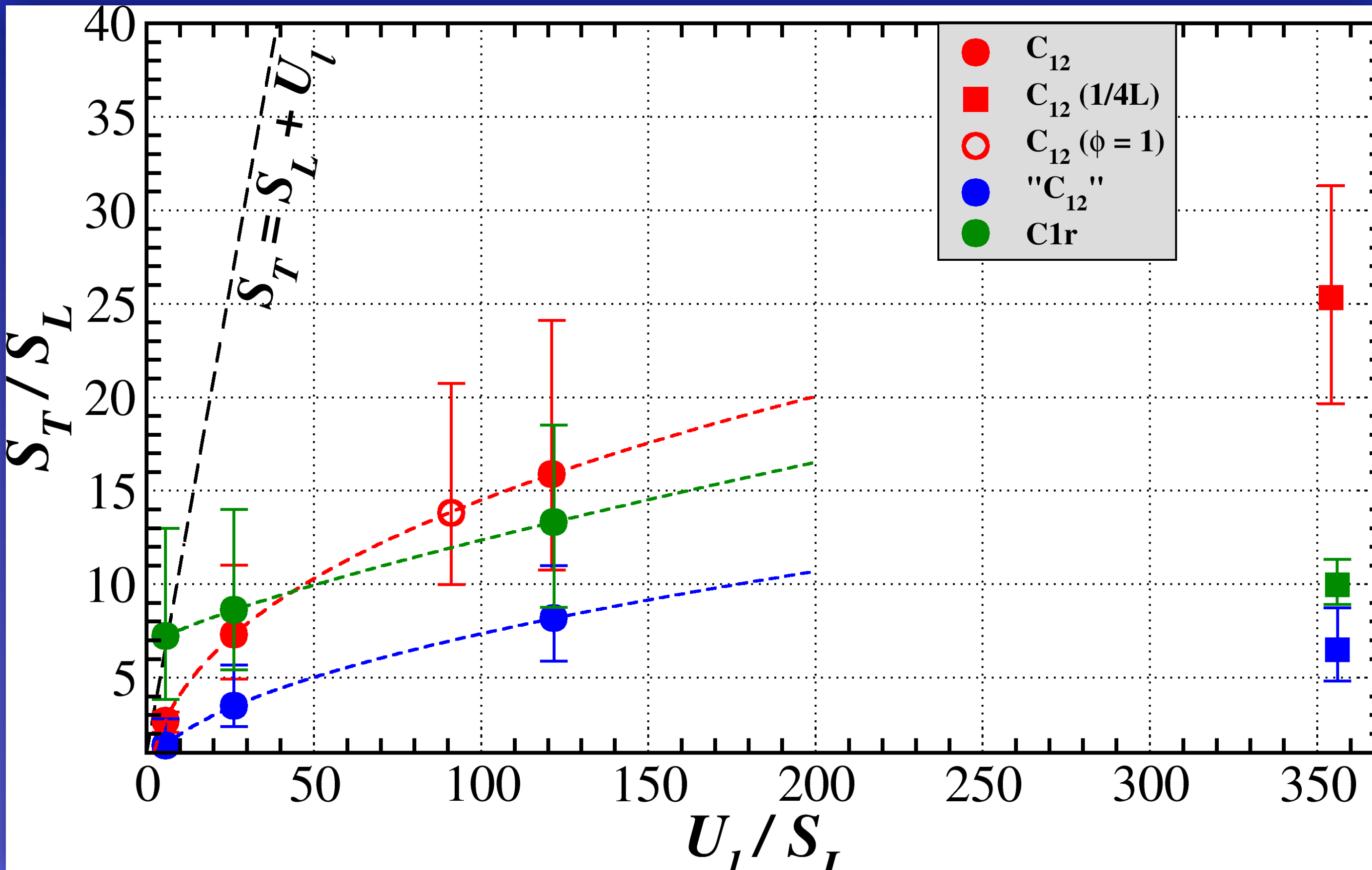




…experimental evidence suggests similar trends for CH_4 and heavier hydrocarbons

Turbulent flame speed vs. turbulent intensity
Global trends

CH_4/air vs. n-dodecane/air vs. single-step kinetics



Single-step kinetics gives reasonable agreement at Ka = 10, but is qualitatively wrong at high intensities

Dependence of the turbulent flame speed on turbulent intensity: global trends

- Observed trends show classical "bending" phenomenon ***for all fuels***

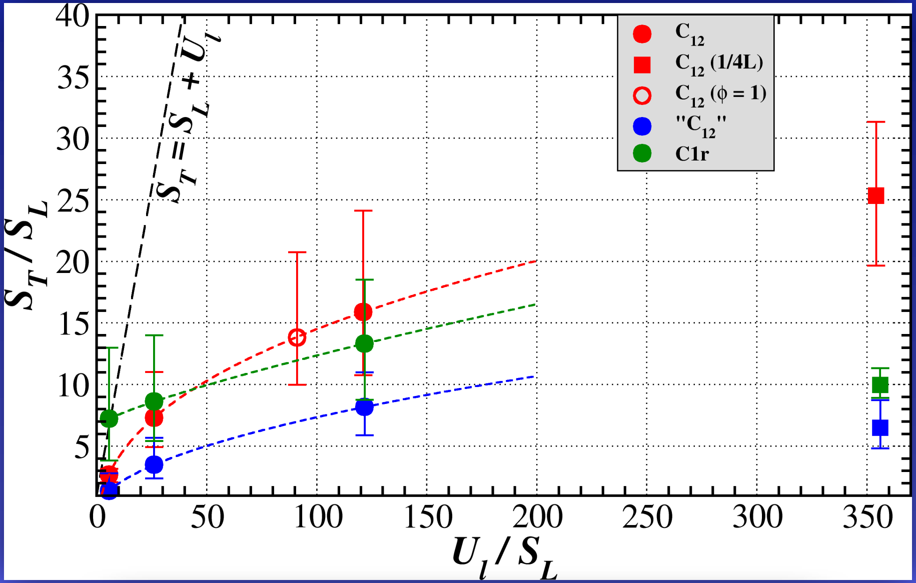
No global extinction

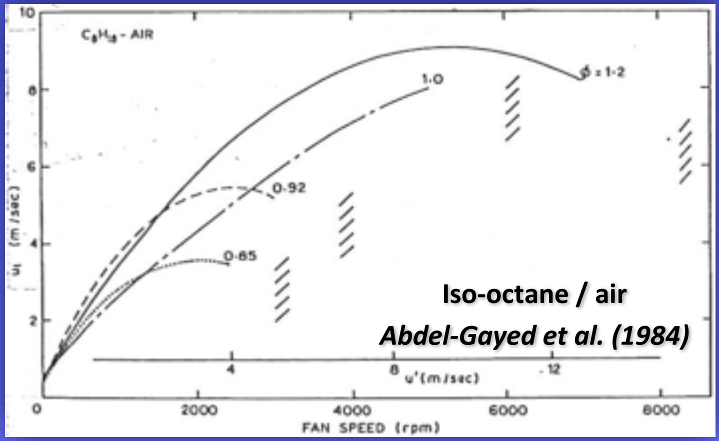
- Pronounced difference between C_1 and C_{12} both at high and low intensities
- Virtually no difference between all heavy hydrocarbons ***at all intensities***

Is this an artifact of a reduced kinetics?

- At low intensities, the difference between C_1 and C_{12} is due to the thermodiffusive effects (Lewis #)
- At high intensities, however, the laminar flame is disrupted and Le $\rightarrow$ 1 due to turbulence
- Purely coupling of turbulence and chemistry

One possible clue comes from the PSR extinction curves for different mixtures (Tianfeng Lu)



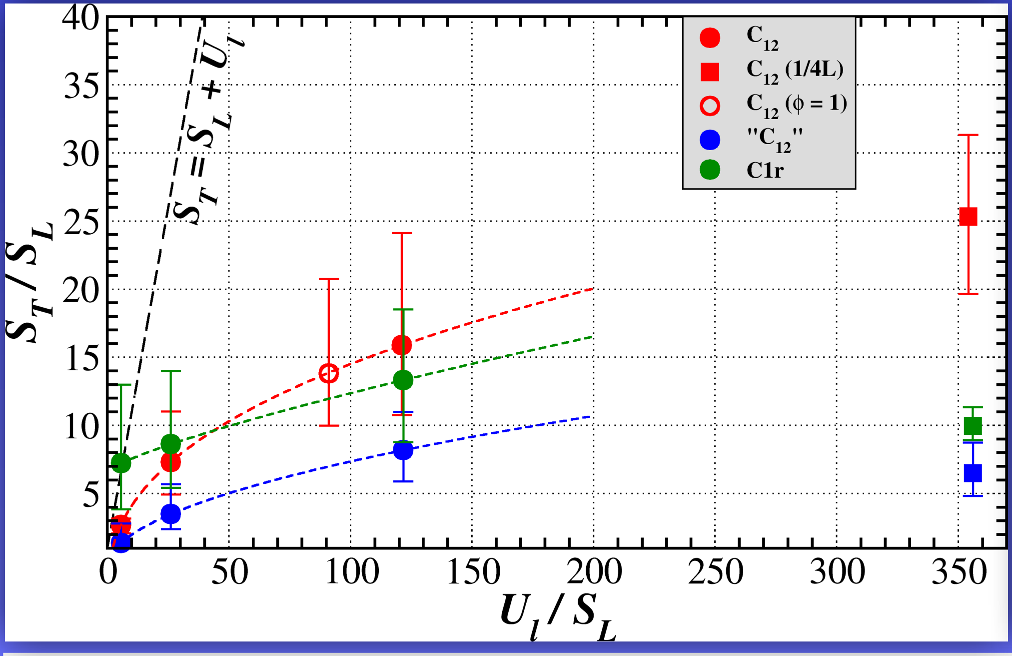


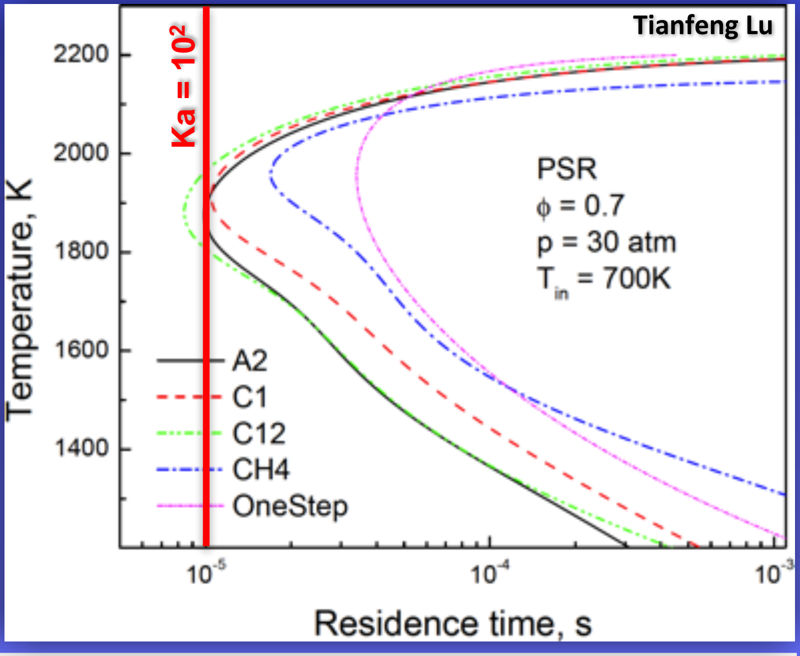
Turbulence-chemistry interaction at high intensities

At high turbulent intensities, burning rate is controlled by the extinction properties of the fuel

- These are controlled by HCO → CO and CO → CO_2
- For heavy hydrocarbons, the range of extinction behaviors is bounded by C_2H_4 and i-C_4H_8, which differ by a factor 2.5 (4 – 10 μs)

This suggests the cause of the similarity in behavior between C12, Cat A2, and Cat C1





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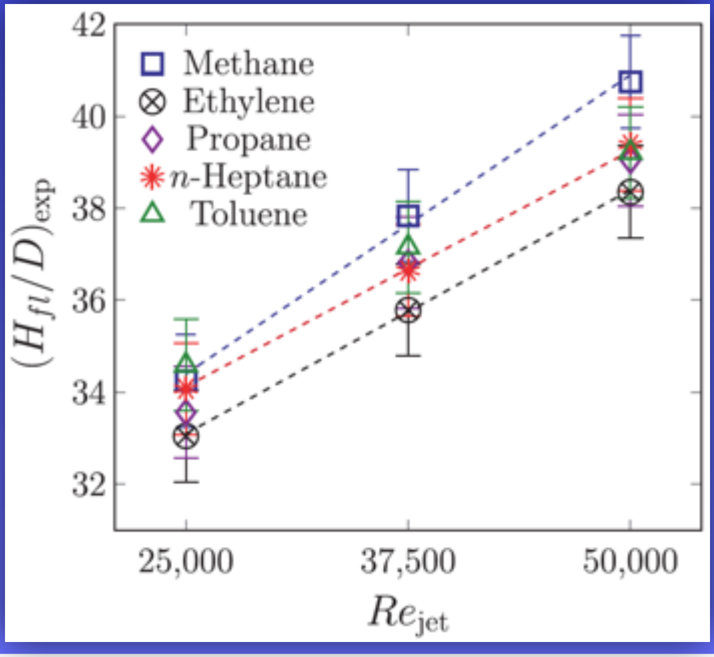
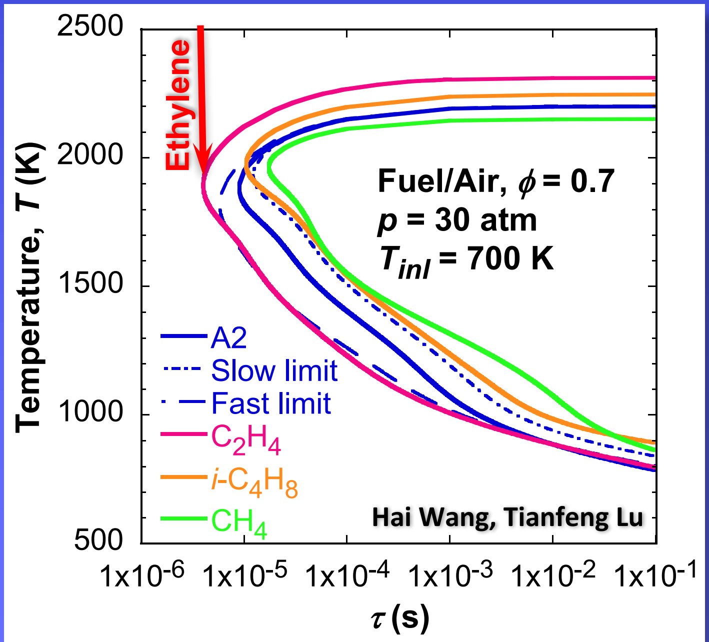
Finally, this picture also would agree with the experimental observation of the ethylene giving the highest turbulent burning speed





Flame structure

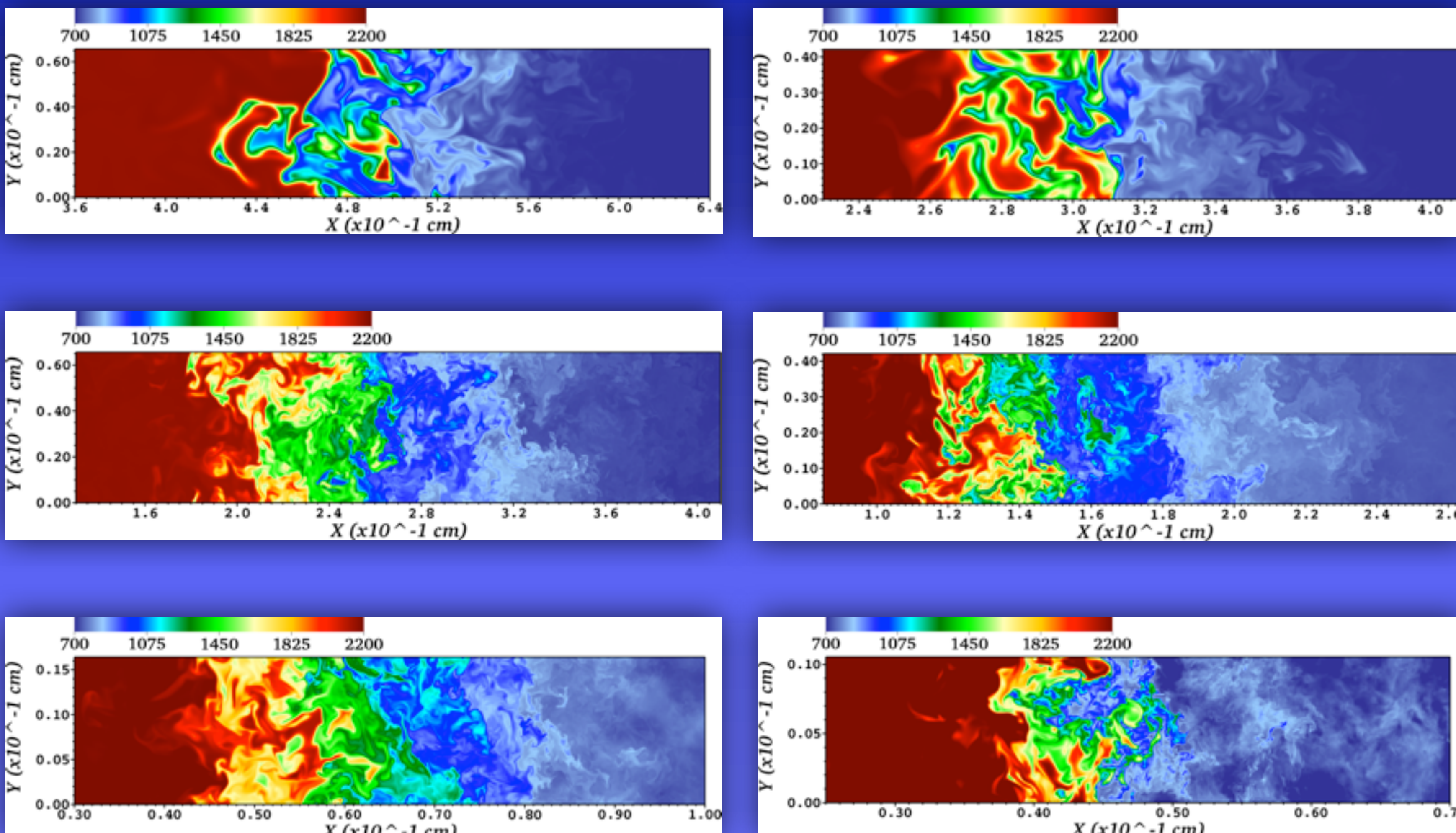
Temperature structure

Methane | Dodecane

Ka = 100

Ka = 1000

Ka = 10,000



Flame structure

Temperature structure

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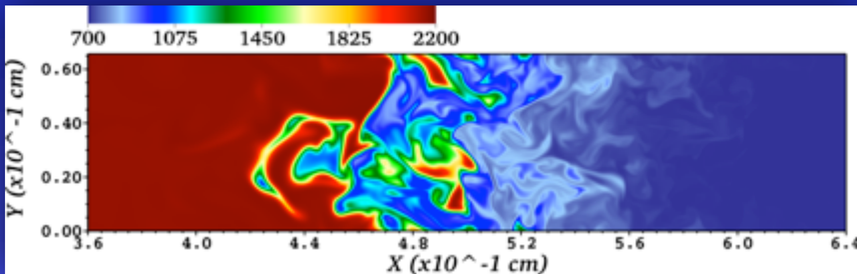
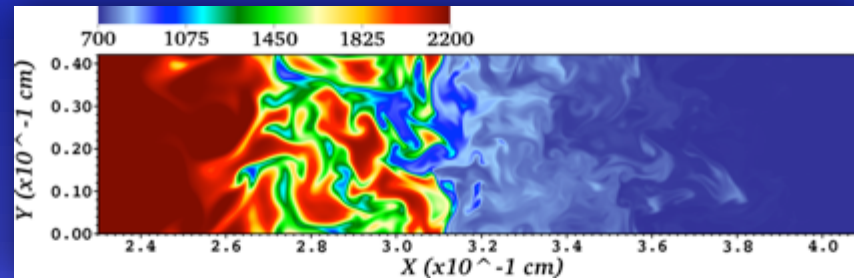
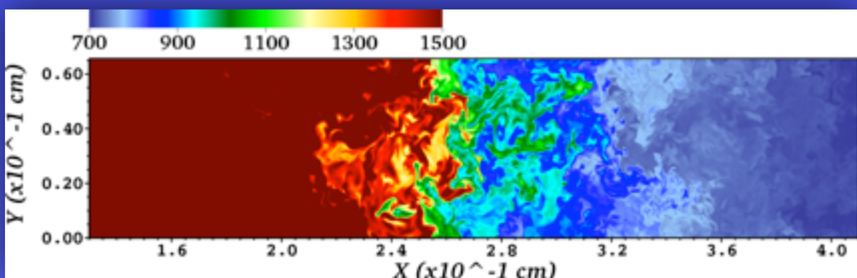
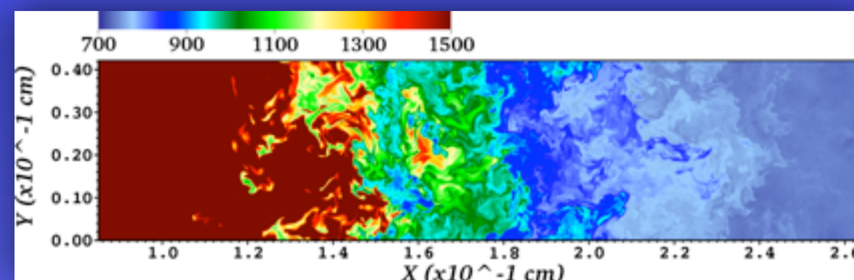




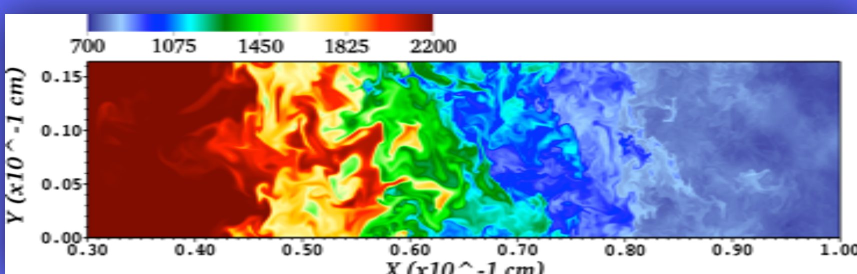
Preheat zone structure at Ka = 1000

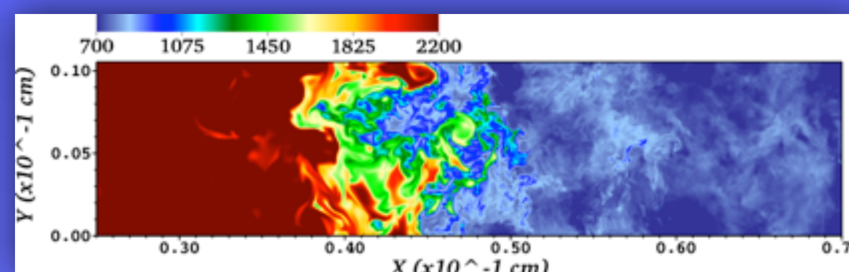
Ka = 1000





Ka = 10,000



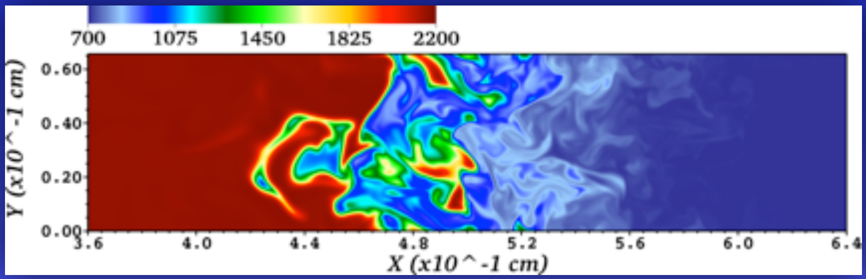


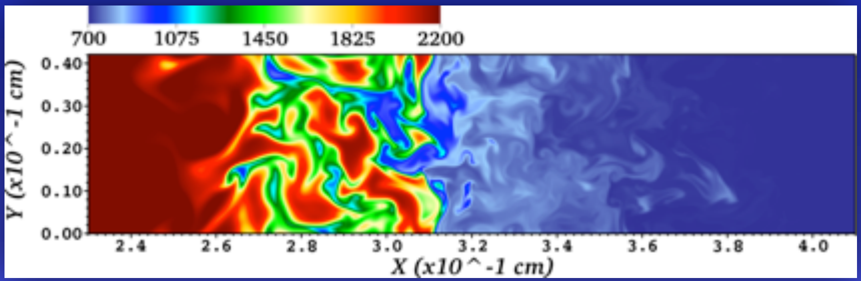
Flame structure

Temperature structure

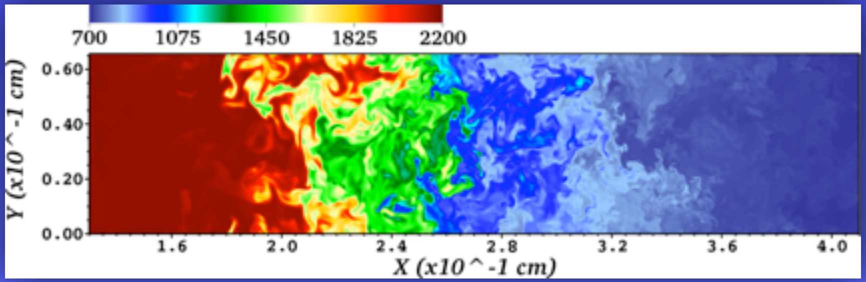
Methane | Dodecane

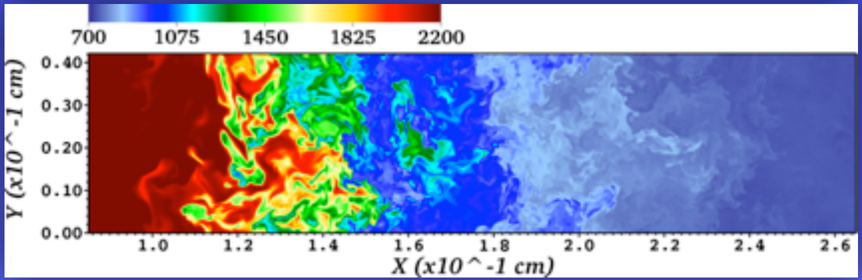
Ka = 100





Ka = 1000





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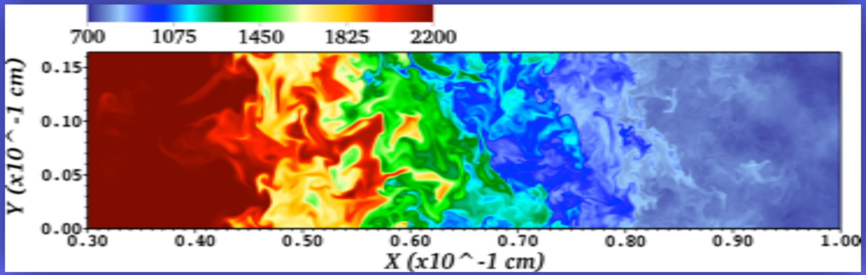
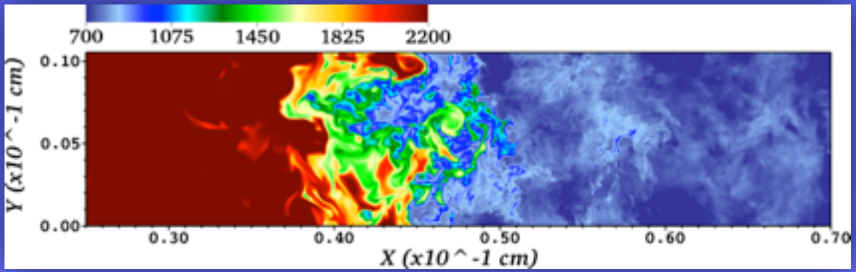




Flame structure

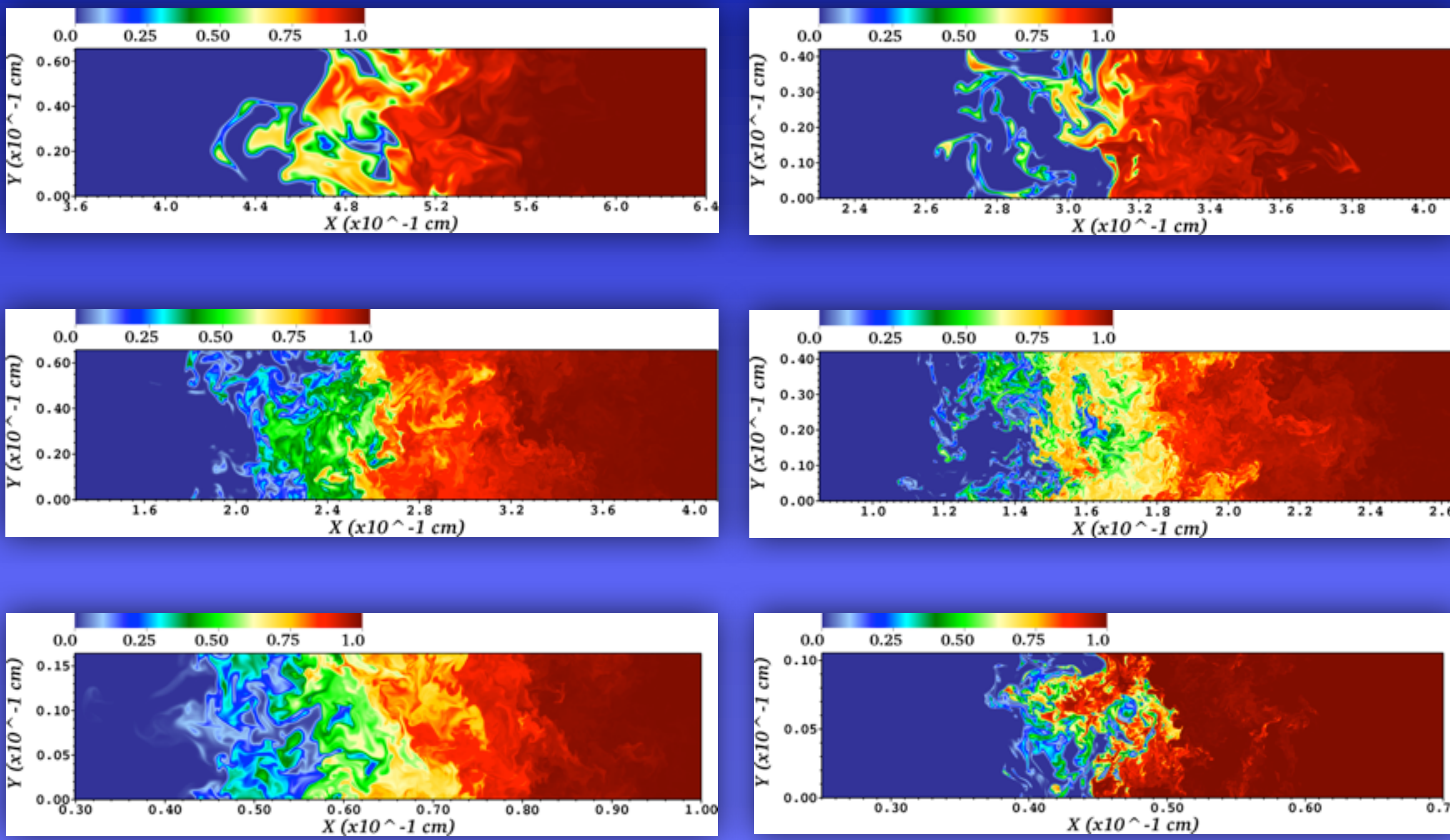
Normalized fuel mass fraction structure

Methane | **Dodecane**

Ka = 100

Ka = 1000

Ka = 10,000

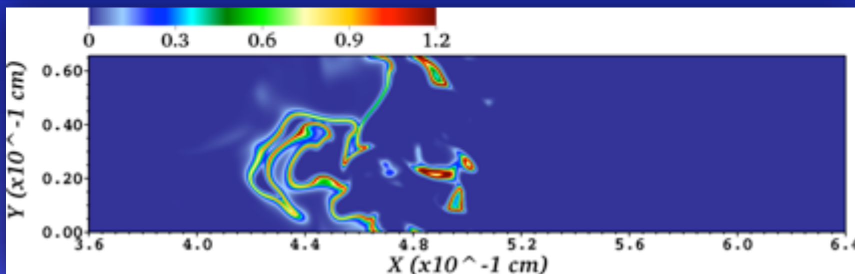


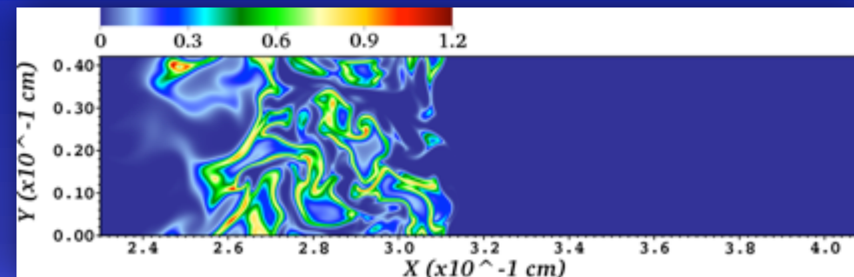
Flame structure

Normalized heat release rate structure

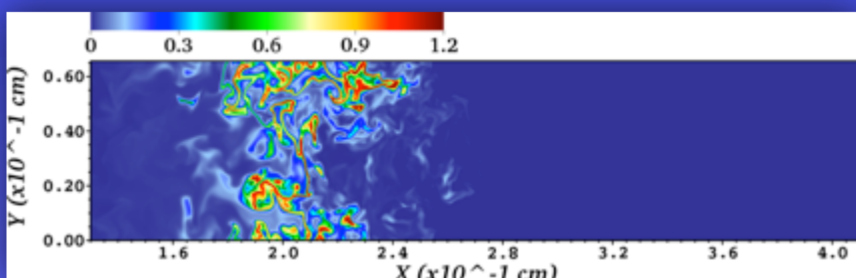
Methane | **Dodecane**

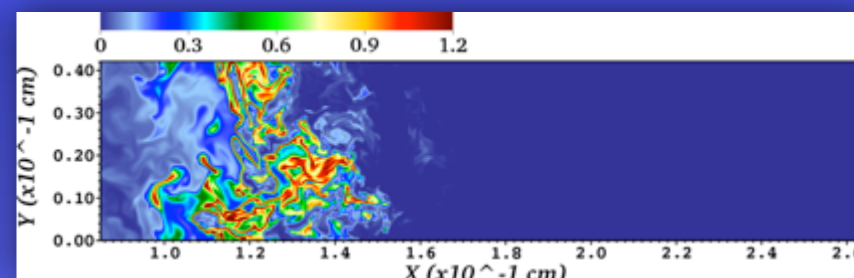
Ka = 100





Ka = 1000





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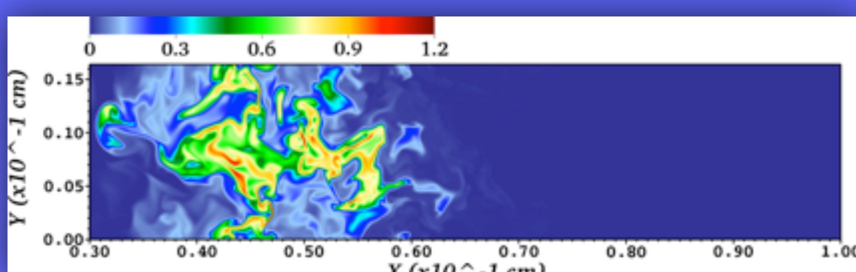
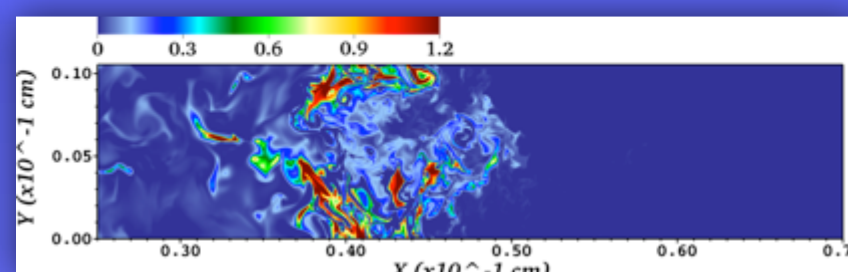


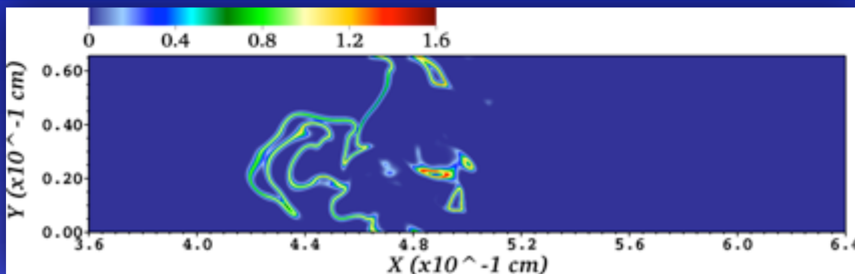


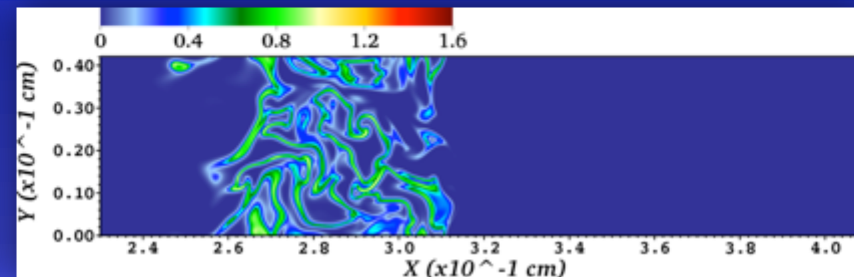
Flame structure

Normalized OH × CH_2O structure

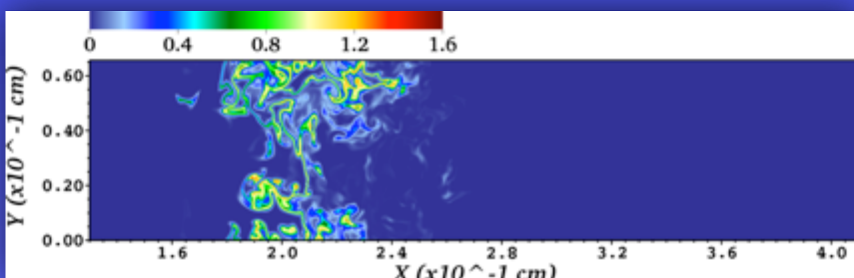
Methane | **Dodecane**

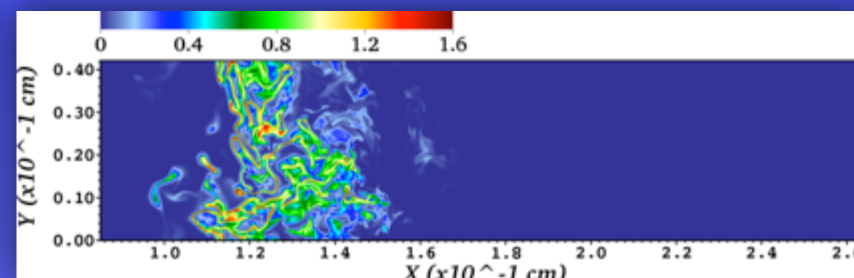
Ka = 100





Ka = 1000





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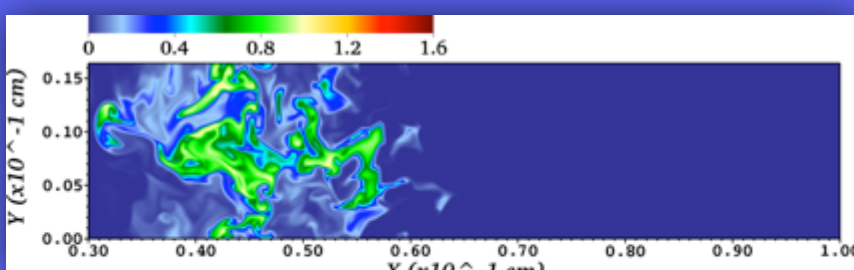
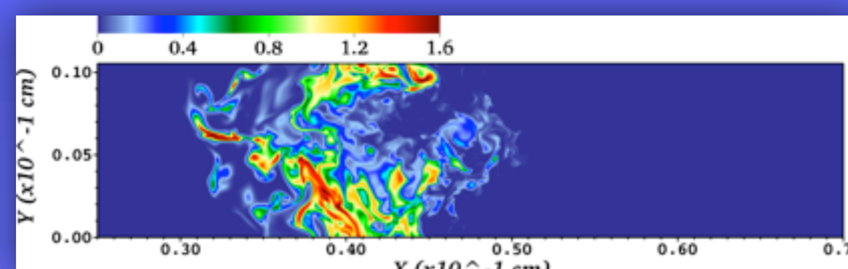


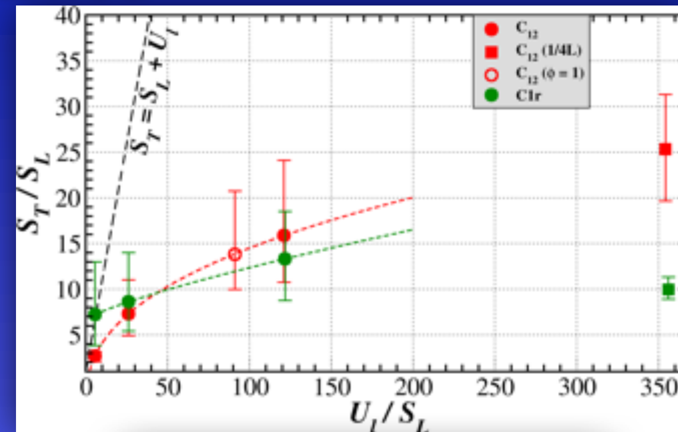


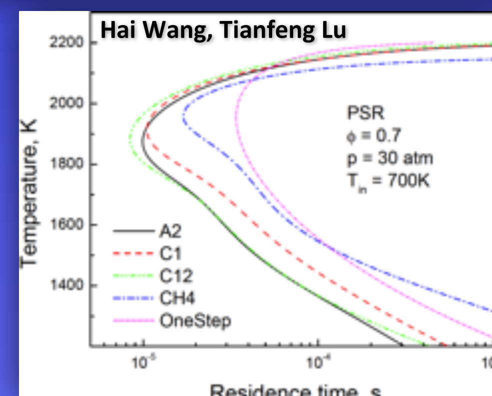
OH x CH_2O is not a reliable marker of heat release rate at high turbulent intensities

Comparative study of hydrocarbon fuels
... a few lessons learned

- Virtually identical behavior for heavy hydrocarbons, C_{12}, Cat A2 and C1, for ***all*** intensities
- Similar behavior for lean and stoichiometric C_{12}
- Virtually identical behavior for CH_4 with two different reduced models
- "Bending" of $S_T(U_l)$ observed for all fuels and models, ***including single-step***
- **... however, qualitatively different trends in S_T between CH_4 and C_{12} with *U'* (or Re / Ka)**
- Tentative evidence suggests this could be related to the differences in extinction behavior

Conclusive experimental confirmation is needed





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