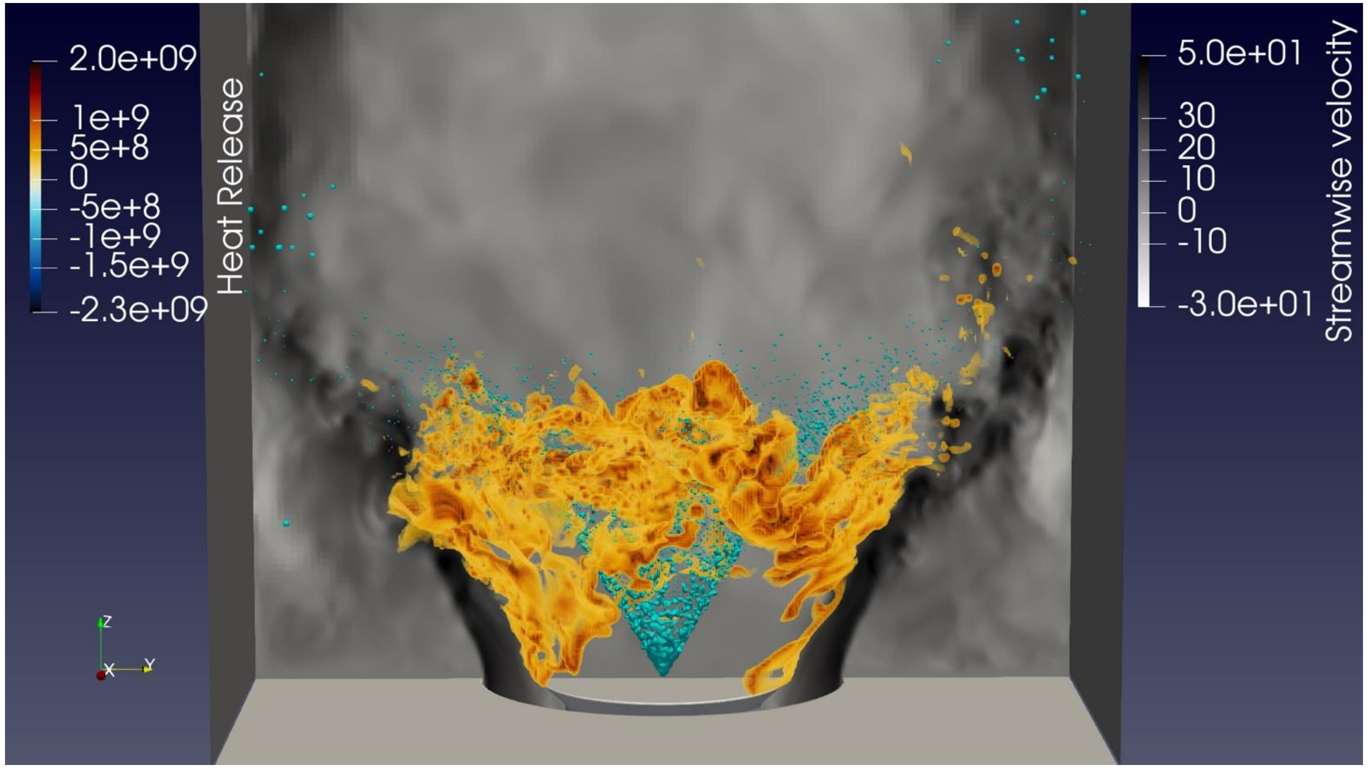
Turbulent Combustion: A Computational Perspective
Part 3. Sustainable Aviation Fuels



High-fidelity simulation of the Cambridge swirl-stabilized spray burner, B. Souza et al. (Combustion and Flame, 2025)

Sponsored by DOE EERE Vehicle Technologies SAF Program

Sandia National Laboratories

Relevance, barriers and objective

Relevance

- Wide range of SAF properties impact mixture preparation, combustion dynamics and emissions
- Predictive and computationally efficient models are required to test alternative fuels using CFD in order to reduce costs related to testing
- High fidelity direct numerical simulation (DNS) can shed light on complex combustion phenomenon and help improve combustion and turbulence models
- Soot emissions require further investigation in realistic configurations using state-of-the-art simulations

Barriers

- Modeling requirements:
  - Correct prediction of multi-phase multi-modal combustion
  - Prediction of soot

Objective

- Accelerate the introduction of SAFs by leveraging DNS to improve turbulent combustion models

Motivation

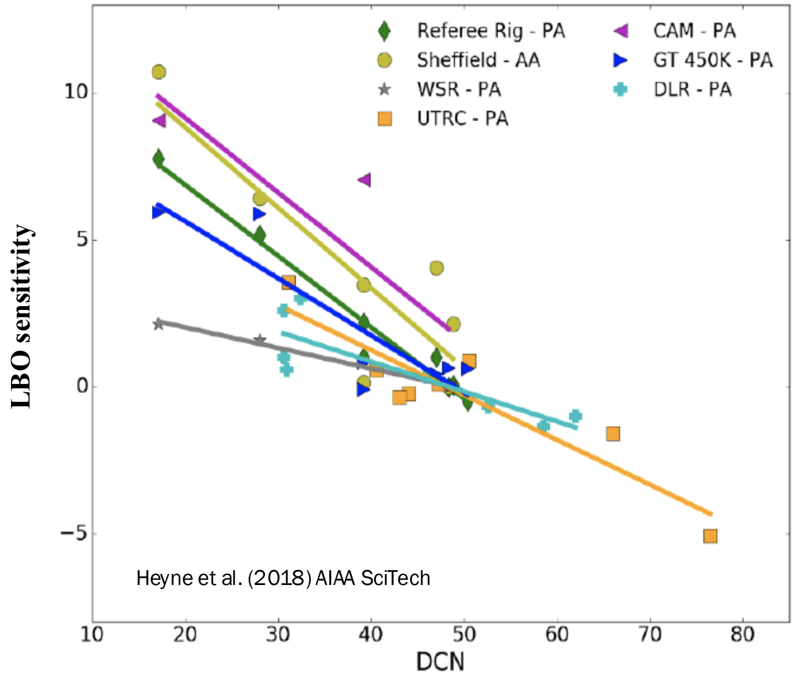
- Testing of SAFs require reliable and computationally efficient models

- Modeling requirements:
  - Multi-modal combustion with lifted flame stabilization
  - Extinction/reignition at adverse conditions
  - Capture multi-component liquid evaporation
  - Soot predictions at high pressure

- Near Blow-off behavior at adverse conditions for hard to ignite SAFs like ATJ (C1) compared to Jet-A

- In the scenario where SAFs are completely different than Jet-A: reliable and more general models are a requirement

- DNS can provide valuable information for understanding flame stabilization near lean blowoff and flamelet model development for mixed regime combustion



Relative LBO rig sensitivity to DCN for different combustors [2]

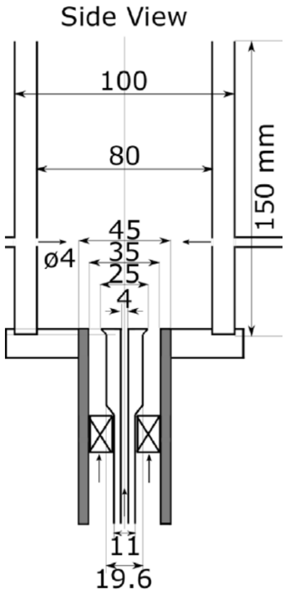
Outline of Part 3: SAF Combustion

- **Flame Stabilization**
- Backscatter

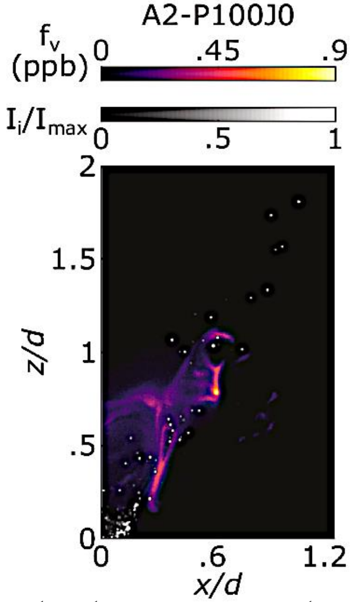
Approach: DNS with complex geometry

Simulation based on Cambridge experiments

Experiment



Schematic of the burner geometry



Instantaneous soot volume fraction and liquid phase measurement

PeleLMeX computational domain

Conditions:

- ○ Bulk velocity as in *El Helou et al (2023) Fuel*: 16 m/s
- ○ Swirl inflow velocity from auxiliary LES simulations
- ○ Zero-mean vel. fluctuation added to inflow velocity:
  - $u' = 0.1U_B$; L_t = half-width of air passage
- ○ T_u = 388 K and P = 1 atm

❖ **Pele: an exascale-ready suite of AMR reactive flow solvers [1]:**

- ○ Low Mach number flows **PeleLMeX**
- ○ Thermo-kinetic library **PelePhysics**
- ○ Multiphysics library **PeleMP**
  - ▪ Spray, soot and radiation

❖ Features:

- Adaptive Mesh Refinement (AMR)
- Support for modern heterogeneous exascale supercomputer
- Embedded boundaries for complex geometries

Targeted fuels

- **Jet-A**: 58 species UIUC chemical mech.
- **C1**: ~60 species UIUC chemical mech.

Soot model: Hybrid Method of Moments (HMOM) [2]

Soot precursor: Naphthalene (A2)

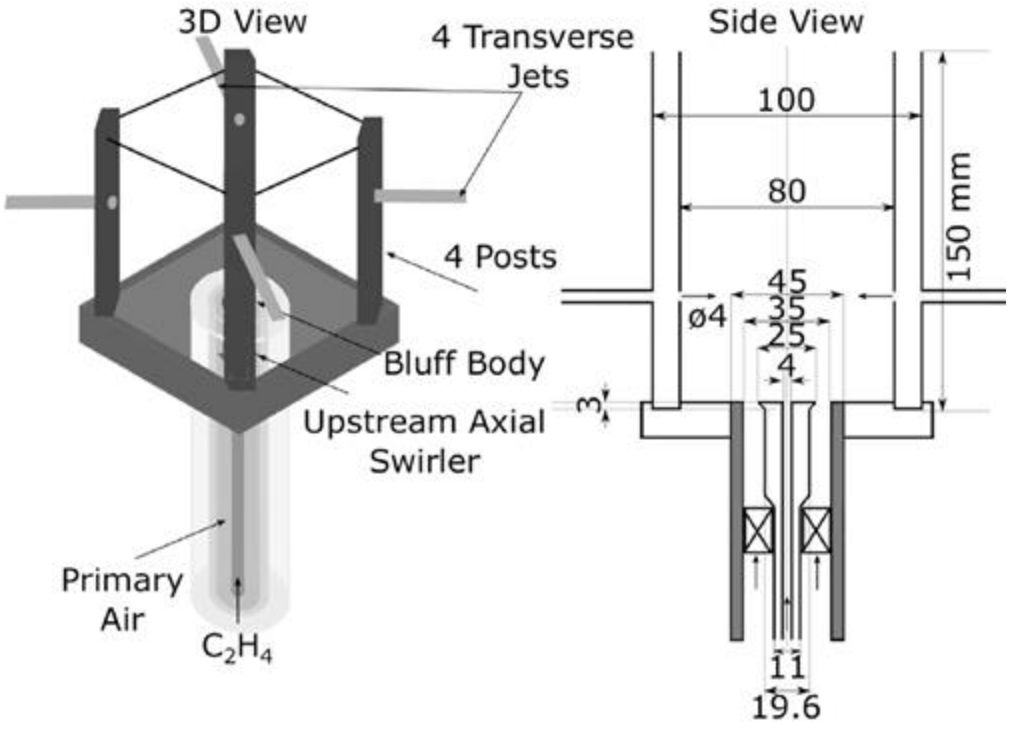
[1] https://amrex-combustion.github.io/

[2] Mueller, M. E., Blanquart, G., and Pitsch, H., 2009, Combustion and Flame, 156

High-fidelity Pele simulation of a lab-scale combustor with sustainable aviation fuels (C1 comparison with Jet-A)

Cambridge swirl-stabilized spray flame

- El Helou et al (2023) *Fuel* https://doi.org/10.1016/j.fuel.2022.125608
- Study soot formation: Jet-A and C5

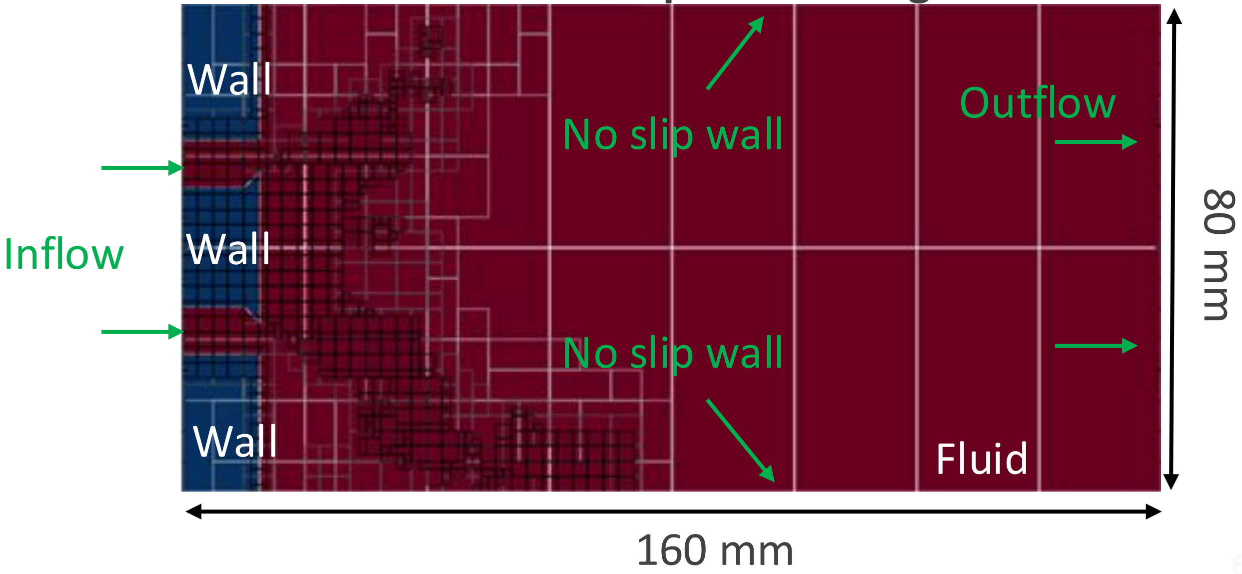


- Embedded boundary treatment
- 4 AMR levels (base + 3 levels): dx = 78 µm. Number of cells: approx. 350M

Targeted fuels

- Jet-A: 48-species UIUC mech (Ryu et al. 2021)
- C1: 57-species UIUC mech (Kim et al. 2021)

PeleLMeX set up with AMR grid

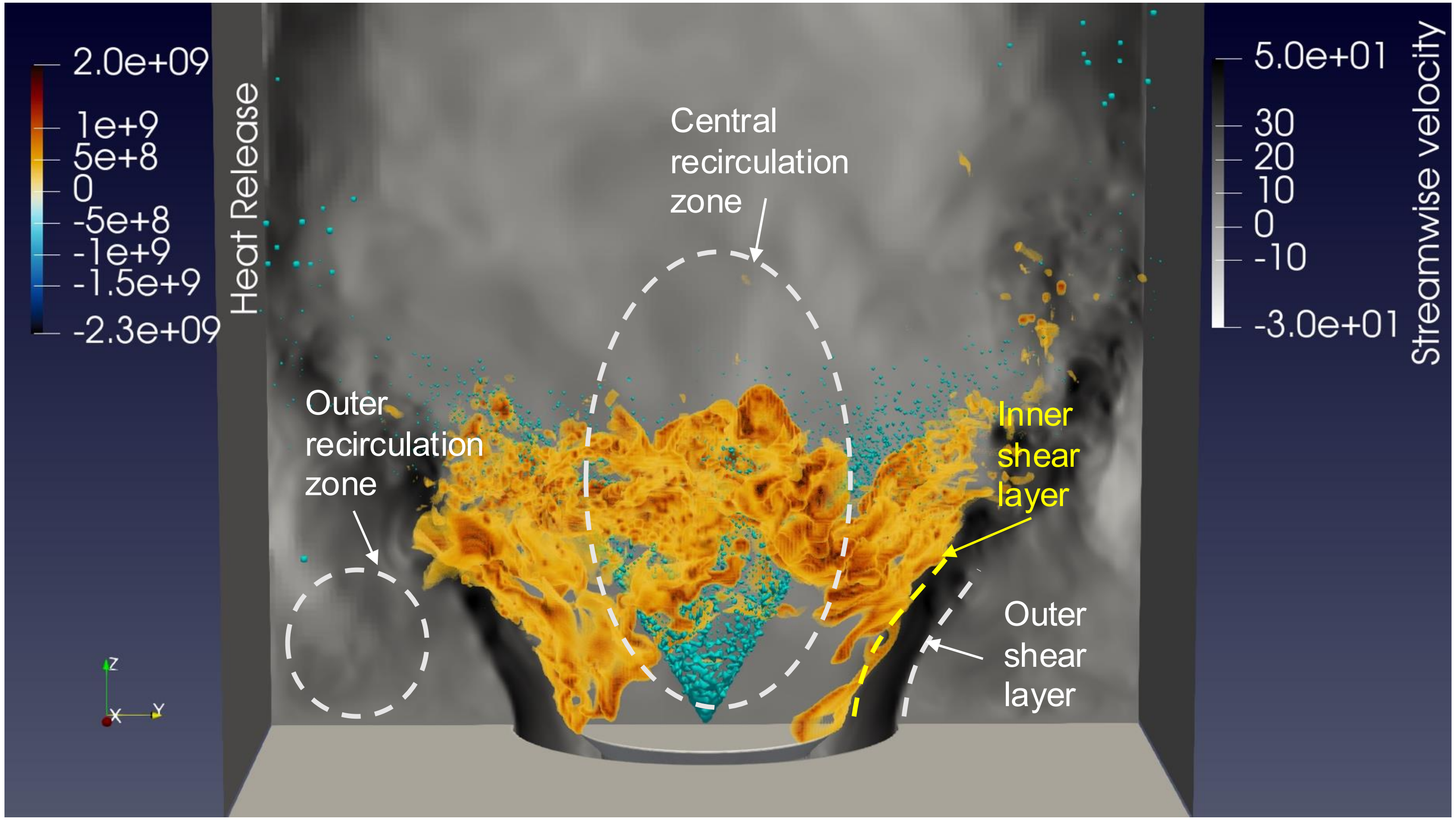


B. Soriano, et al. 2023 (in prep)

DNS of swirl-stabilized spray flame with Alcohol-to-Jet, C1 sustainable aviation fuel (SAF) compared with Jet-A

Complex flame behavior

- Diffusion flame
- Local extinction
- Edge flame propagation

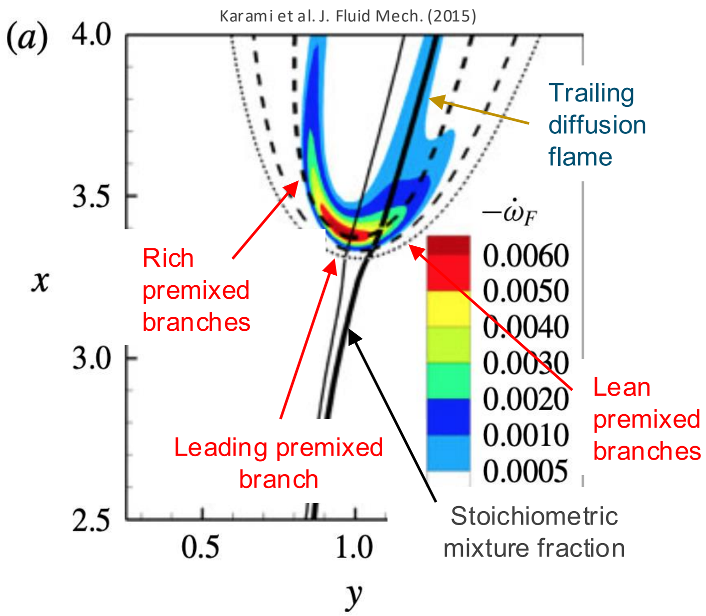


Instantaneous fields for Jet-A flame stabilization

Cambridge Burner (Panthania 2021, 2022; Helou et al. 2023)

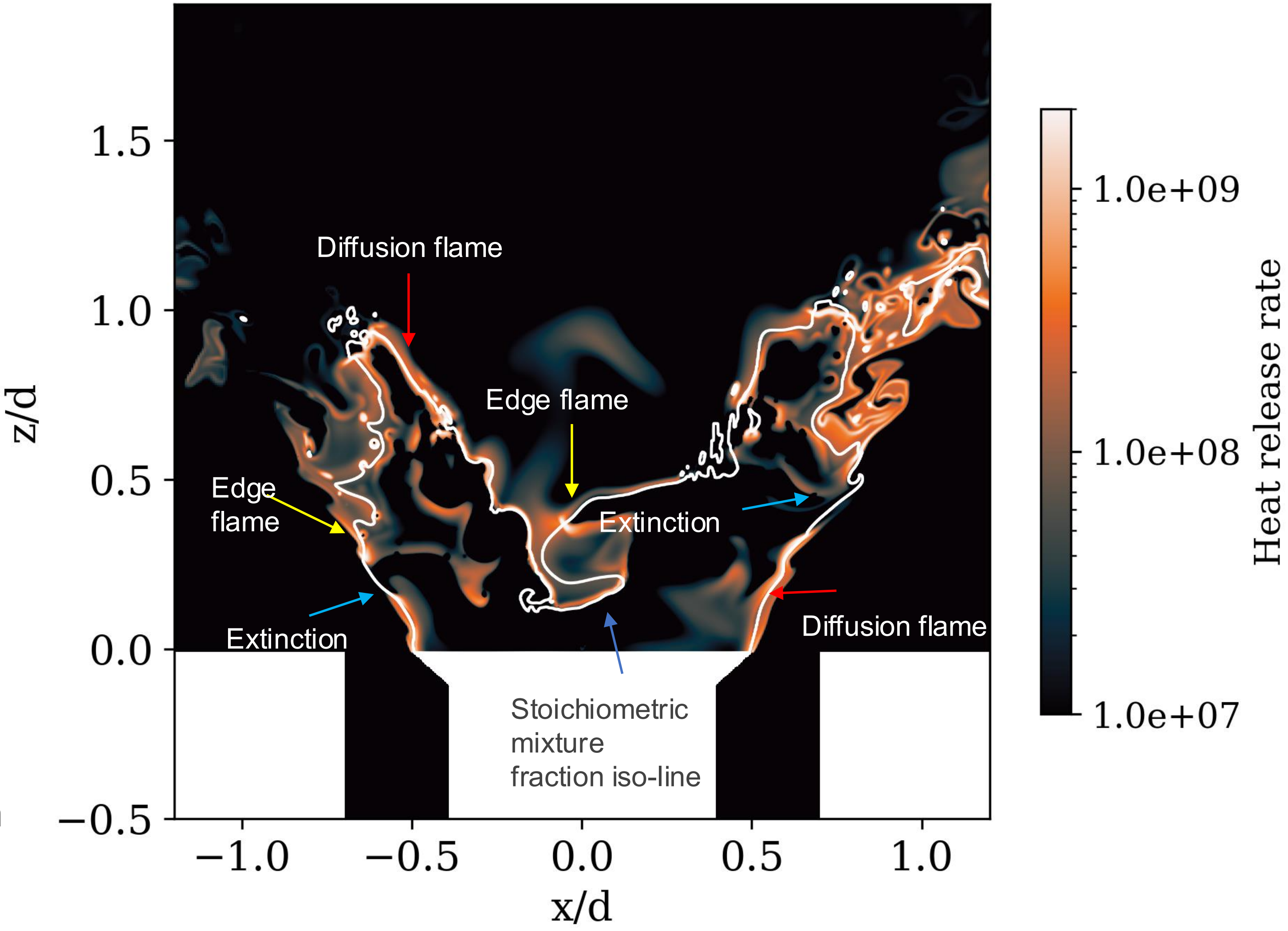
Identification of combustion dynamics

- DNS simulations provide detailed information on combustion dynamics
- Stabilization involves complex flame characteristics
  - Diffusion flame
  - Local extinction
  - Edge flame propagation



Edge flame example

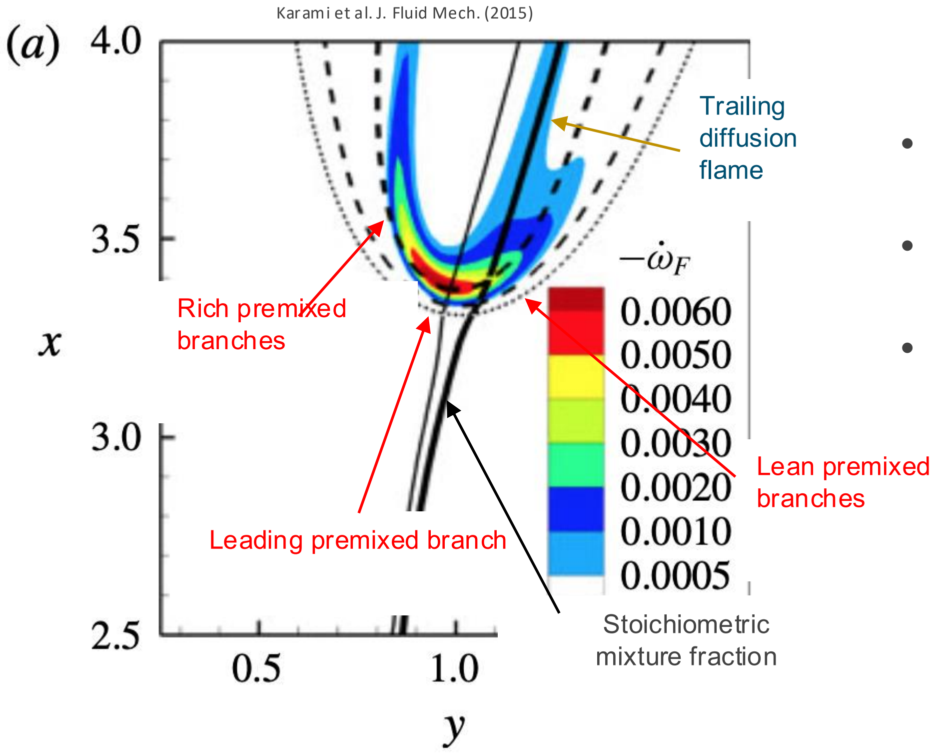
- Iso-contours for products reaction rate
- Lean/rich and leading premixed branches
- Trailing diffusion flame



Instantaneous heat release rate for Jet-A with different flame features identified. Stoichiometric mixture fraction iso-line in white

Triple Flame Structure and Propagation

Kioni et al. 1993



- Iso-contours for products reaction rate
- Lean/rich and leading premixed branches
- Trailing diffusion flame

$$S_d / S_L = \sqrt{\frac{\rho_u}{\rho_b}}$$

density ratio

triple flame speed at stoichiometric mixture fraction

laminar flame speed

Ruetsch et al. 1995

Quantification of ignition/deflagration for Jet-A and C1

Damköhler number can be used to quantify deflagration fronts

$$Da = \frac{\dot{\omega}_k}{|-\nabla(\rho Y_k V_k)|}$$

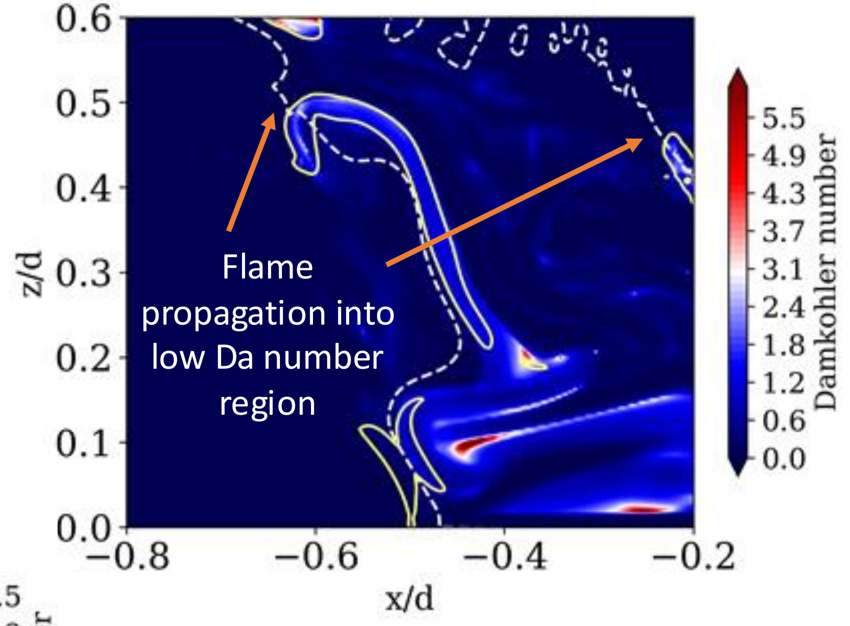
$$Y_c \equiv Y_{CO_2} + Y_{CO}$$

Damköhler number is typically around 3[1]

Da > 3 => ignition

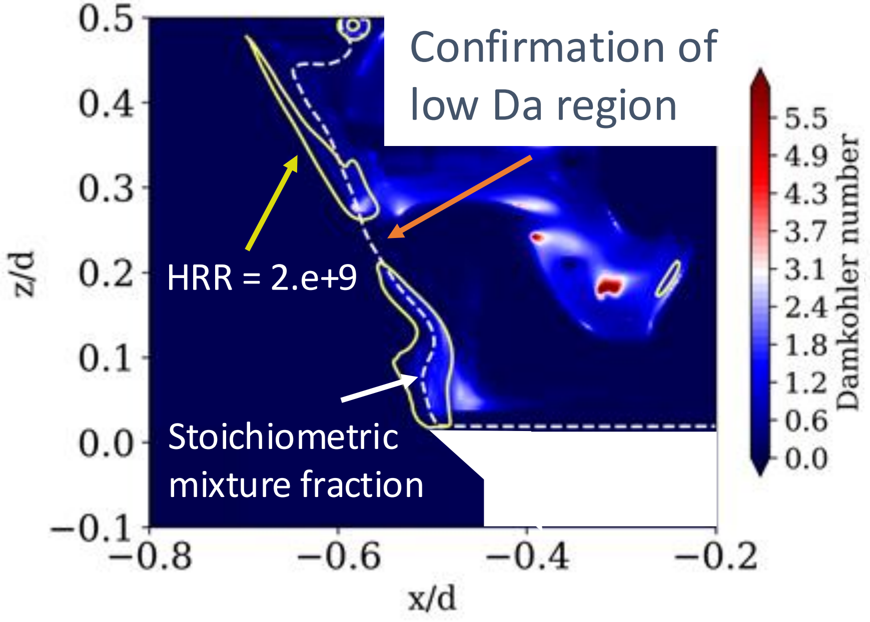
Da < 3 => diffusion limit

C1

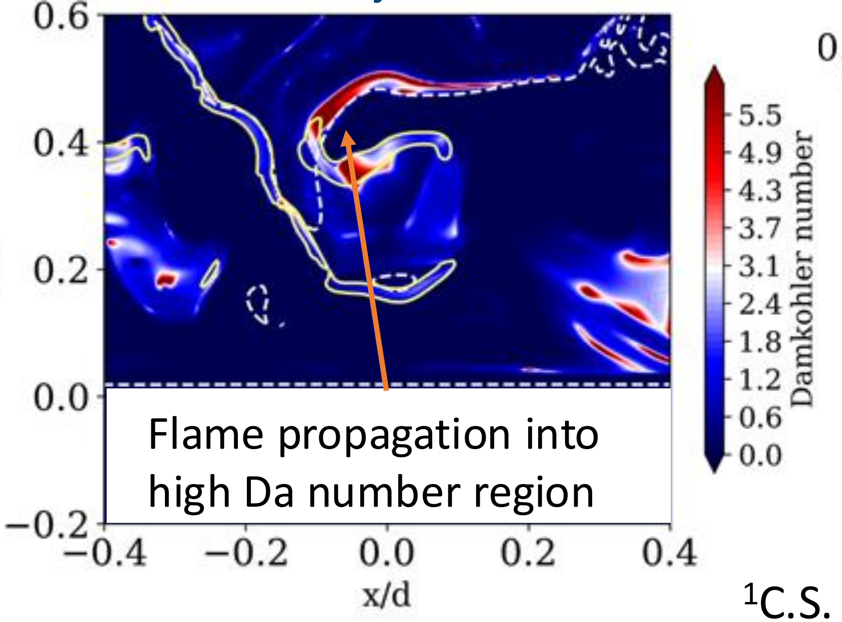


Jet-A

Inner shear layer



Central recirculation near fuel injection



- Deflagration and ignition fronts coexist!
- Ignition effects more pronounced for Jet-A

[1]C.S. Yoo et al. PROCI 34 (2013) 2985–2993

Quantification of combustion modes for Jet A and C1

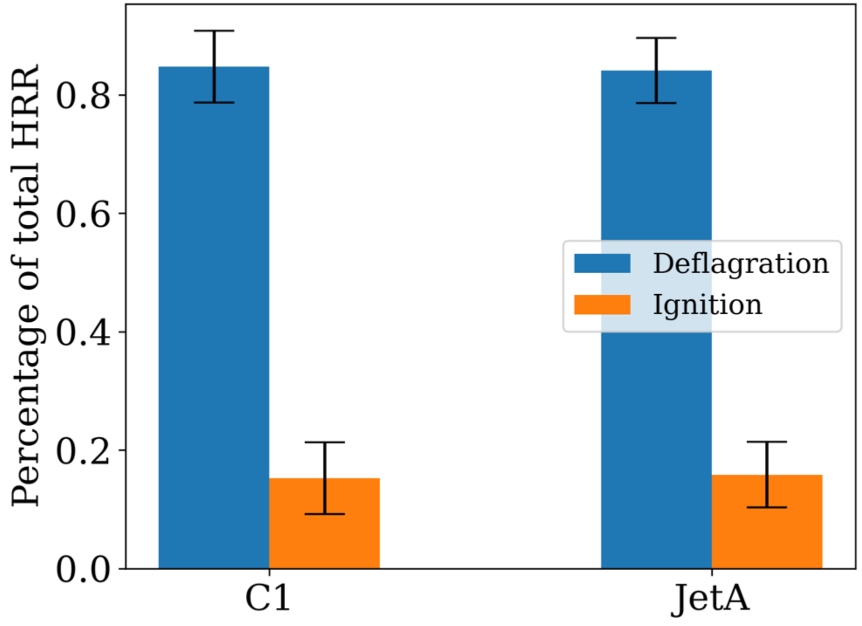
Damköhler number can be used to quantify deflagration fronts

$$Da = \frac{\dot{\omega}_k}{|-\nabla(\rho Y_k V_k)|}$$

Damköhler number is typically around 3[1]

$$Y_c \equiv Y_{CO_2} + Y_{CO}$$

Da > 3 => ignition
Da < 3 => deflagration



[1]C.S. Yoo et al. PROCI 34 (2013) 2985–2993

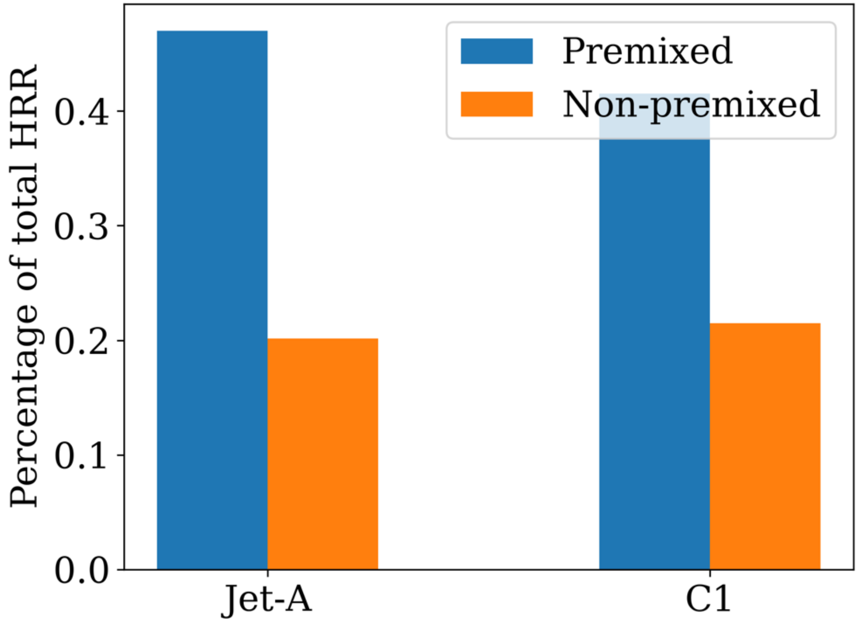
Contribution of premixed and diffusion flames to the total HRR

Normalized flame index (NFI):

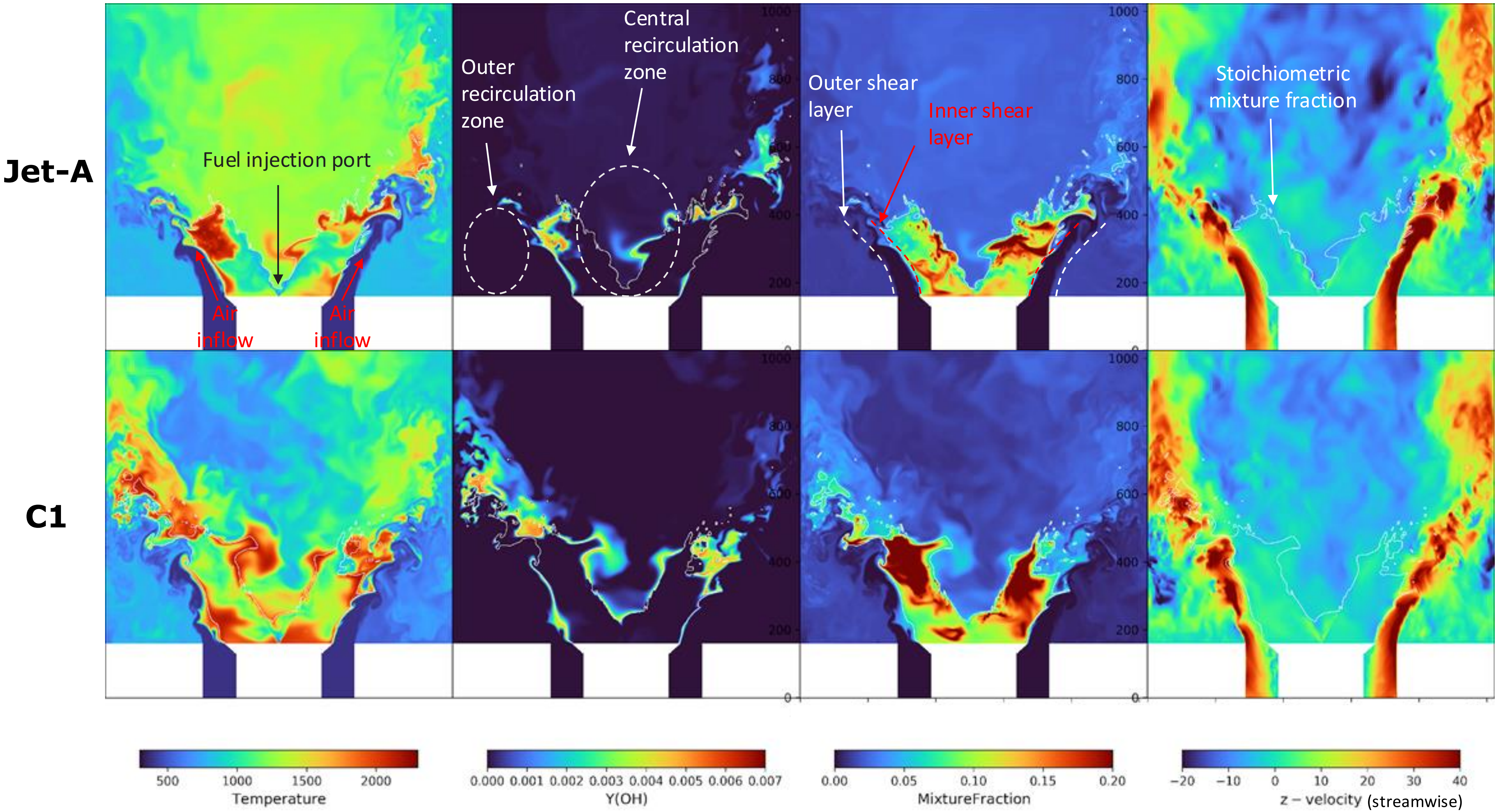
$$NFI = \frac{\nabla Y_F \nabla Y_{O2}}{|\nabla Y_F \nabla Y_{O2}|}$$

$NFI \approx 1$: premixed
$NFI \approx -1$: non-premixed

Y_F = C2H4



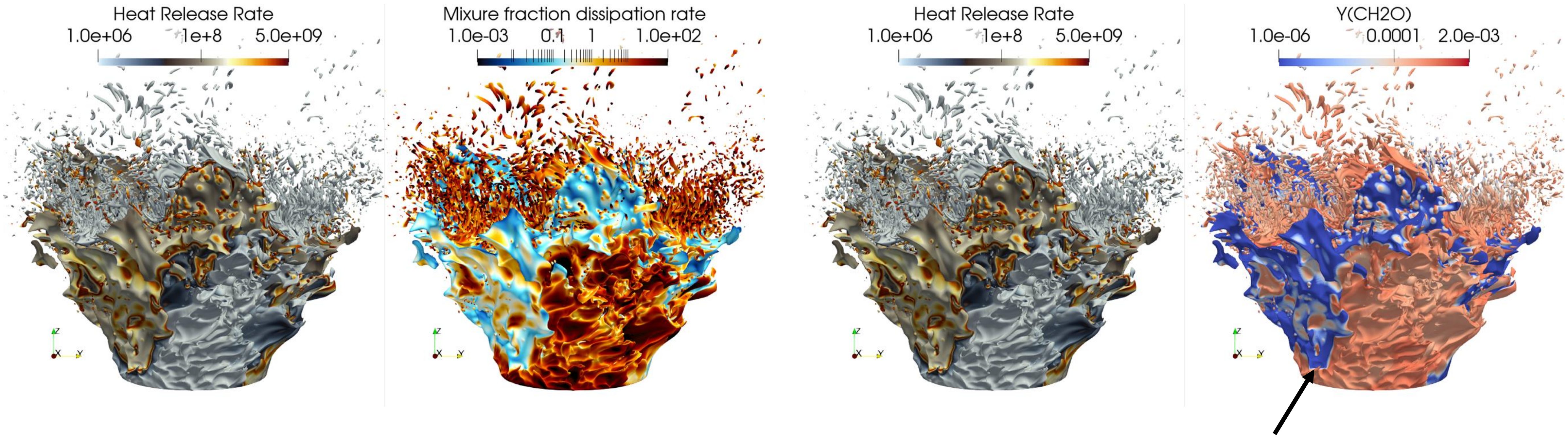
Instantaneous flame behavior for Jet-A and C1



Flame stabilization dynamics: extinction/re-ignition in Jet-A

- Extinction regions show a high mixture fraction dissipation rate

- Edge flame propagation occurs into regions of partially reacted fuel: large CH2O upstream the edge flame



Flame propagation into partially reacted mixture

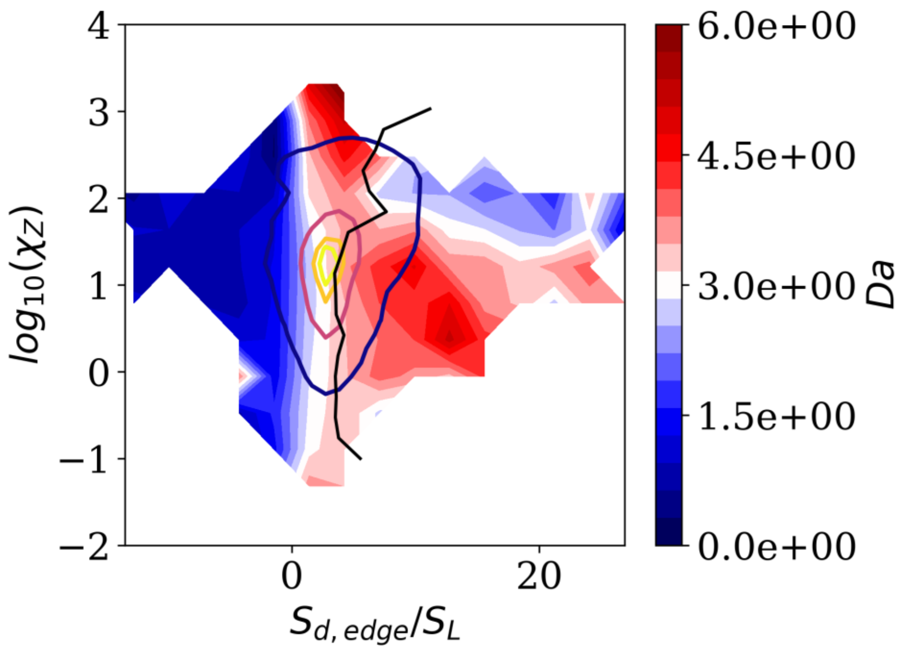
Edge flame speed ($S_{d,\,edge}$) correlation with scalar dissipation rate

$$S_d = \frac{1}{\rho|\nabla c|}\frac{D\rho c}{Dt} \qquad S_Z = \frac{1}{\rho|\nabla Z|}\left(-\frac{\partial}{\partial x_i}\left(D_Z\frac{\partial Z}{\partial x_i}\right)\right)$$

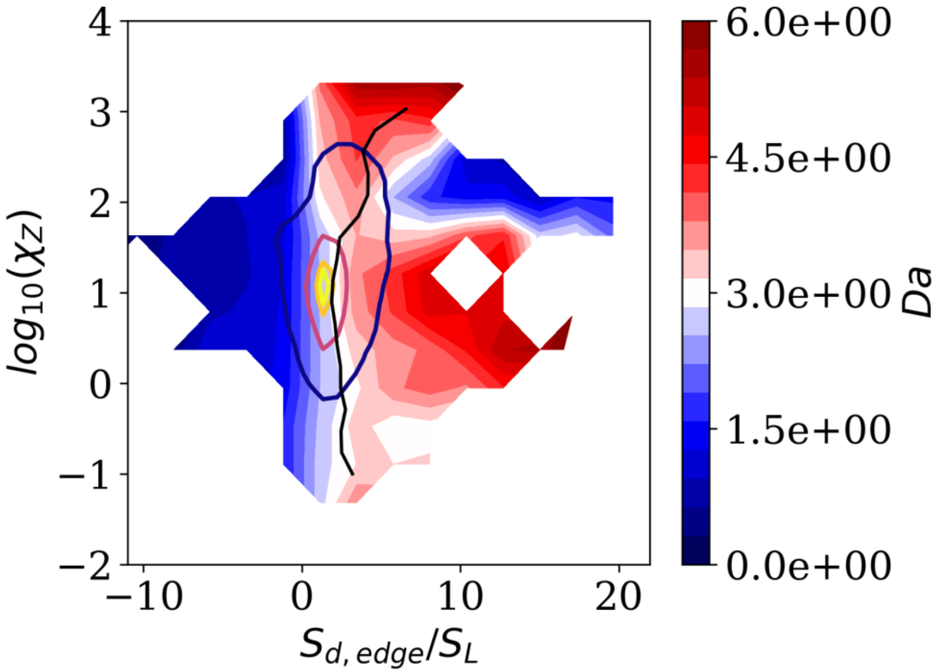
$$S_{d,edge} = \frac{S_d - kS_Z}{\sqrt{1-k^2}}$$

where k is the inner product of normal vectors of progress variable and mixture fraction isosurfaces

Jet-A



C1



- Edge flame speed, $\boldsymbol{S_{d,edge}}$, as a function of scalar dissipation rate, colored by local Damkohler number (Da)
- Da number denotes flame propagation mode: Da > 3 ignition; Da < 3 deflagration
- Large $S_{d\ edge}$ occurs at moderate dissipation as observed in literature

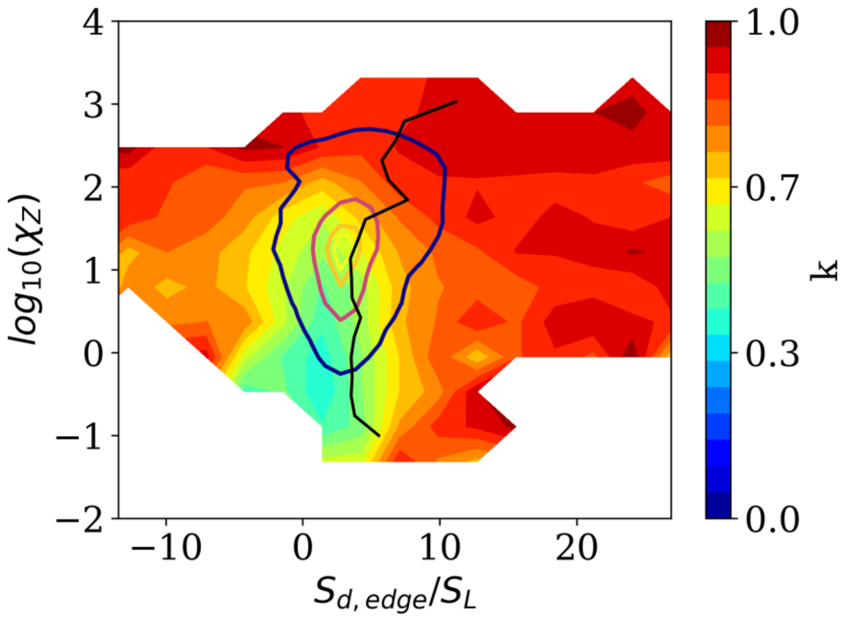
Conditional alignment (k) of stoichiometric mixture fraction and progress variable isosurfaces

$$S_d = \frac{1}{\rho|\nabla c|}\frac{D\rho c}{Dt} \qquad S_Z = \frac{1}{\rho|\nabla Z|}\left(-\frac{\partial}{\partial x_i}\left(D_Z\frac{\partial Z}{\partial x_i}\right)\right)$$

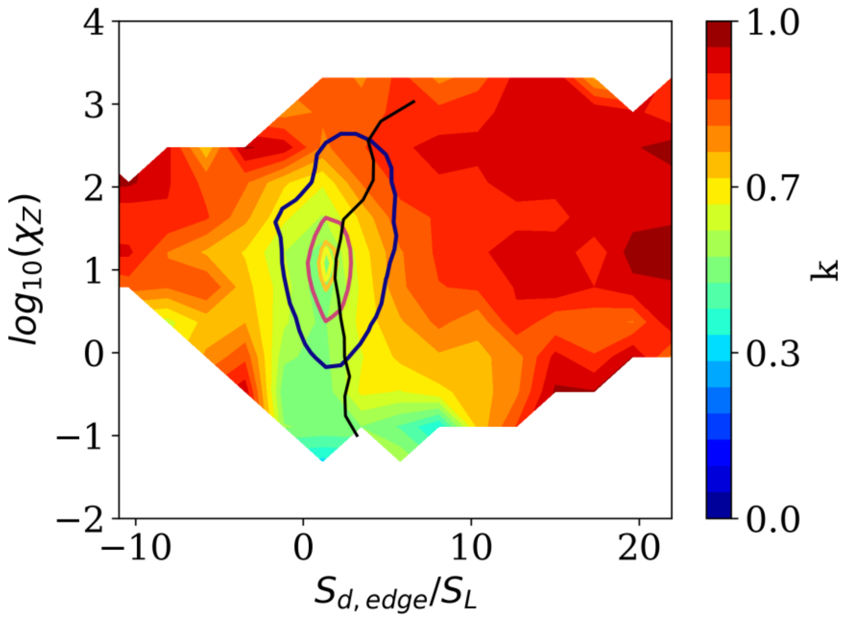
$$S_{d,edge} = \frac{S_d - kS_Z}{\sqrt{1-k^2}}$$

where k is the inner product of normal vectors of progress variable and mixture fraction isosurfaces

Jet-A



C1



- Mean alignment of Z_{stoich} and C_{edge} isosurfaces (k) conditional on scalar dissipation rate and $\boldsymbol{S_{d,edge}}$

Premixed mode dominates total HRR

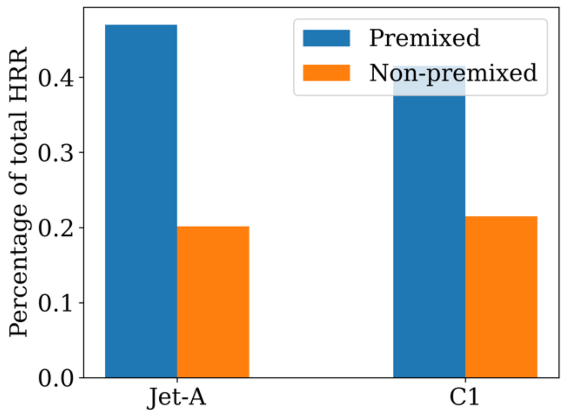
Premixed flames have a higher contribution to the total Heat Release Rate

Normalized flame index (NFI):

$$NFI = \frac{\nabla Y_F \nabla Y_{O2}}{|\nabla Y_F \nabla Y_{O2}|}$$

$NFI \approx 1$: premixed
$NFI \approx -1$: non-premixed

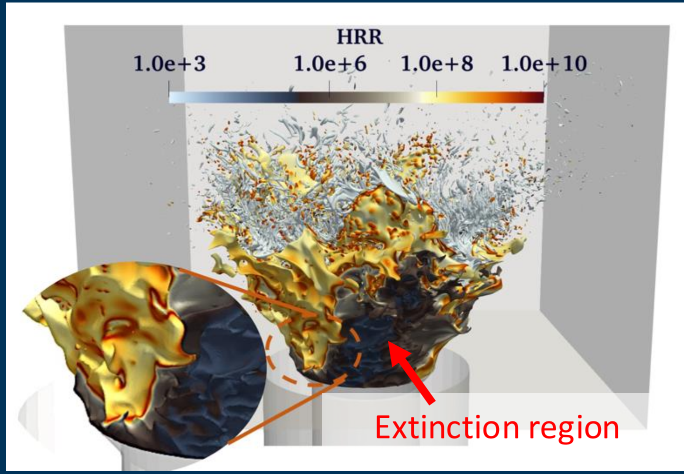
Y_F = C2H4



Contribution of combustion mode to total heat release rate

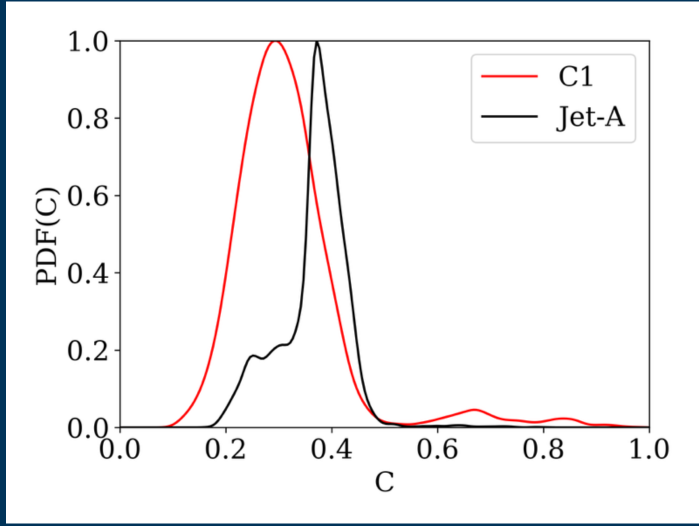
- Premixed flames have a larger contribution to HRR
- Models should correctly predict multi-mode combustion

Analysis of the premixed flame: propagation into partially reacted mixture



Stoichiometric mixture fraction iso-surface colored by heat release rate

- Three-dimensional edge flame propagation along the stoichiometric mixture fraction
- Edge flames propagate to re-ignite extinction regions
- Propagation into a partially-reacted mixture: C > 0; ~1000K
- Deflagration or ignition front?



Probability Density Function for the progress variable (C) in the extinction region

Soriano B. S., Owen L. , Esclapez L. and Chen J. AIAA 2024-1999. *AIAA SCITECH 2024 Forum.*

Deflagration fronts reignite mixture

Contribution of propagation mode to the total heat release rate (HRR)

Damköhler number (Da) can be used to quantify deflagration/ignition fronts:

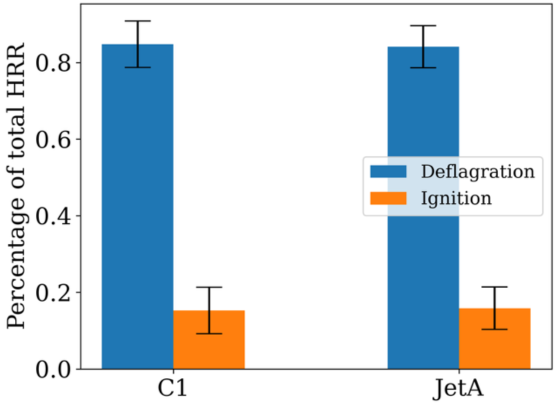
$$Da = \frac{\dot{\omega}_k}{|-\nabla(\rho Y_k V_k)|} \qquad Y_c \equiv Y_{CO_2} + Y_{CO}$$

(progress variable)

Deflagration fronts have a diffusion/reaction balance: typically around 3[1]

Findings:

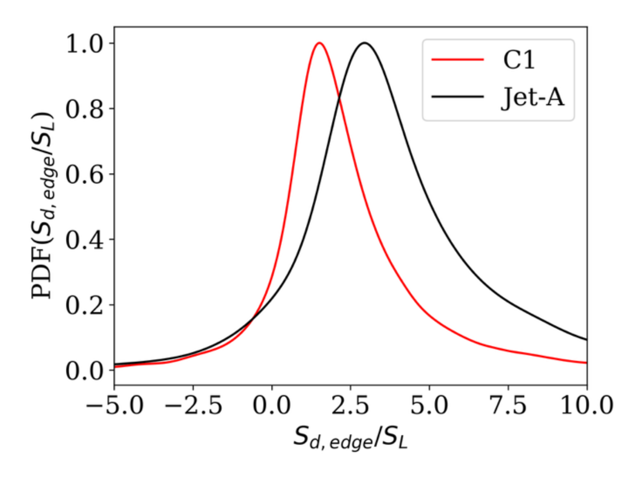
- Deflagration and ignition fronts coexist
- Deflagration is assisted by ignition
- Contribution of ignition/deflagration to total HRR is similar between Jet-A and C1



Contribution of propagation mode to total heat release rate

[1]C.S. Yoo et al. PROCI 34 (2013) 2985–2993

Lean blow-off correlation with flame displacement speed



Probability density function of $S_{d,edge}/S_L$ for Jet-A and C1

Cetane number correlation with lean blow-off may be related to enhanced edge flame propagation speed for more reactive fuels

- Jet-A has a higher probability of larger $S_{d,edge}/S_L$ consistent with a lower sensitivity to lean blow-off

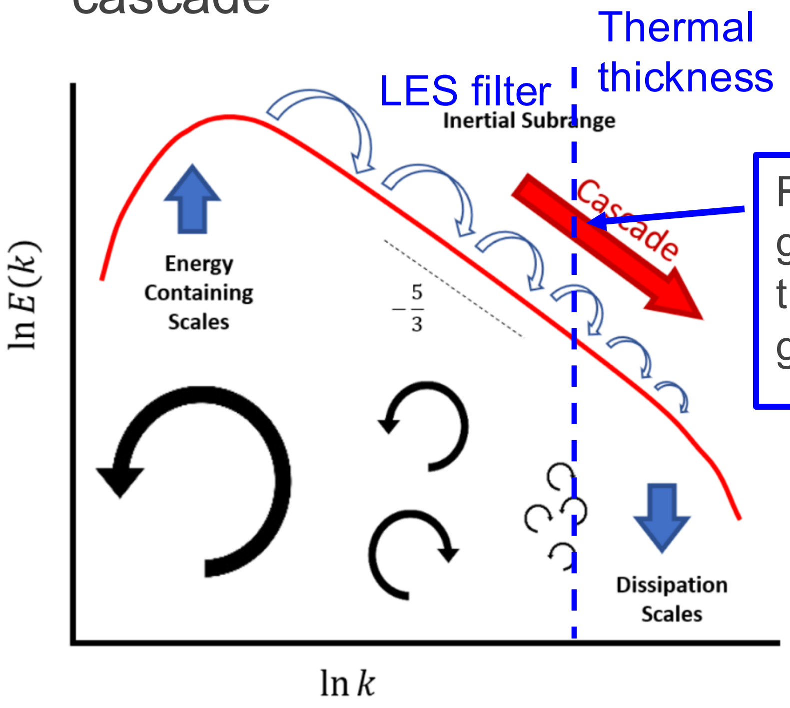
B. S. Soriano, L. D. Owen, J. H. Chen, Fuel (2024) in preparation

Outline of Part 3: SAF Combustion

- Flame Stabilization
- **Backscatter**

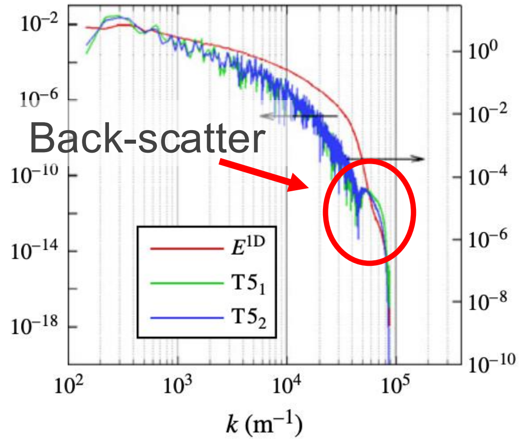
Turbulence back-scatter

LES turbulence models use the classical Richardson-Kolmogorov phenomenological model for constant density flows: forward energy cascade



Reacting flows can generate turbulence at sub-grid scale

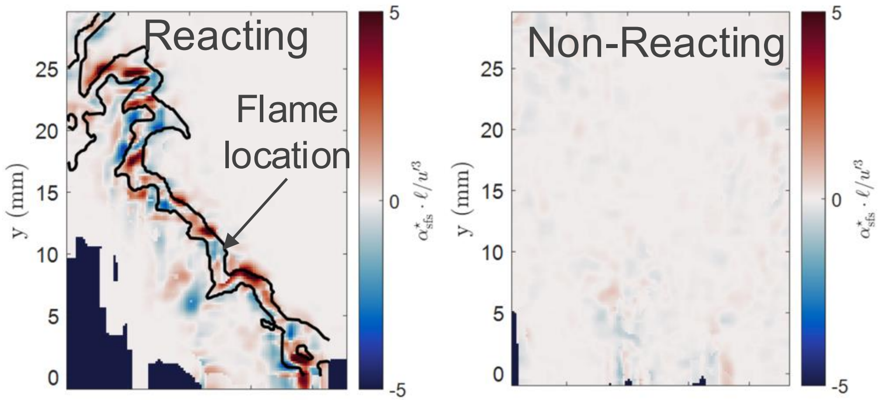
Fundamental question: Do edge flames observed in the Cambridge burner DNS induce back-scatter?



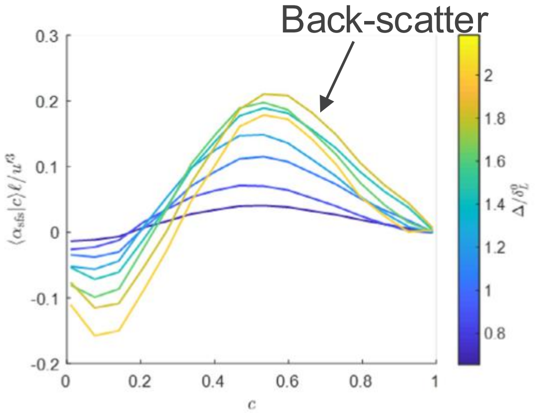
DNS results for the energy spectra in a temporal H_2 premixed flame [2]

Energy spectra for isotropic turbulence.
Adapted from [1]

GA Tech swirl stabilized premixed burner



Instantaneous measurement of Forward/reverse energy transfer. Back-scatter is denoted in red [1]



Forward/reverse energy transfer parameter conditioned on progress variable [3]

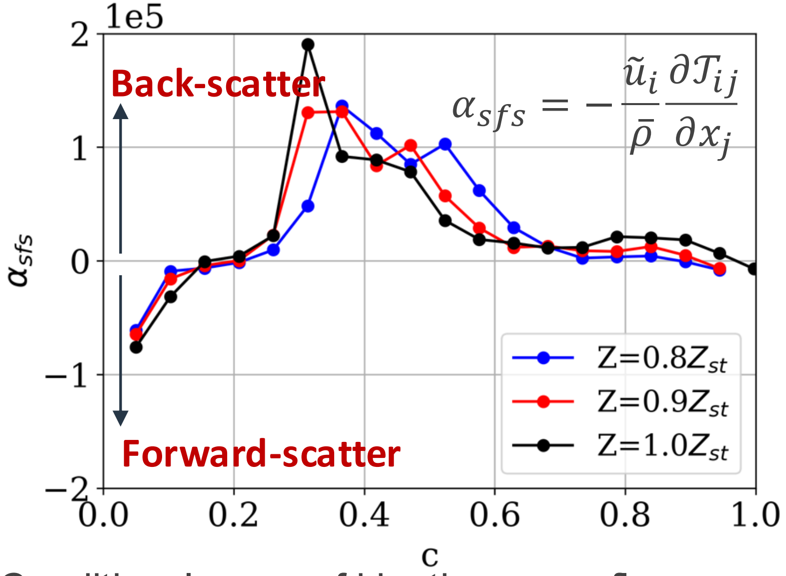
[1] A. Kazbekov, *Inter-scale energy transfer in turbulent premixed combustion.* PhD Thesis (2022)
[2] Kolla et al, *On the velocity and reactive scalar spectra in turbulent premixed flames*. JFM (2014)
[3] A. Kazbekov and A.M. Steinberg. *Physical space analysis of cross-scale turbulent kinetic energy transfer in premixed swirl flames.* CNF (2021)

Back-scatter from partially-premixed combustion

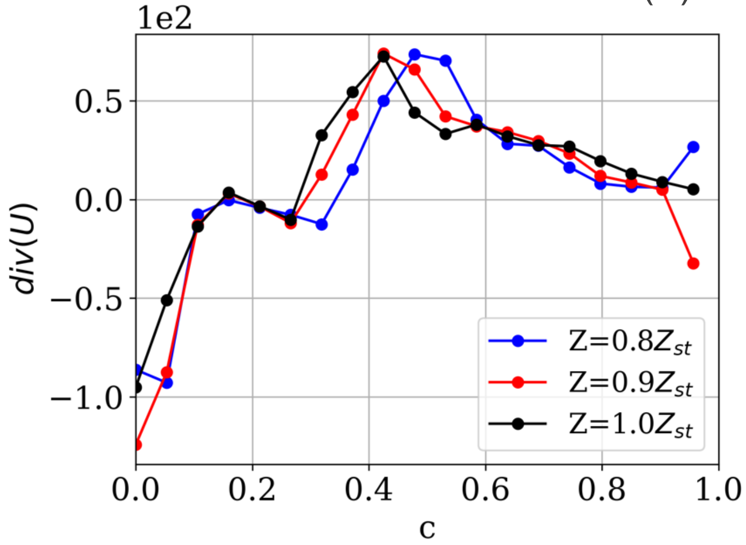
- DNS solution is spatially filtered:
  - Favre filtering operation on 3D field for multiple snapshots
  - Top hat filter kernel
  - Filter size: $\Delta = 2.2\delta_{th}$
- Analysis performed for Jet-A simulation
- Data presented in terms of conditional means as a function of progress variable for three equivalence ratio iso-surfaces

Findings:

- Edge flames lead to an inversion of the turbulent kinetic energy cascade
- Backscatter is more likely to occur near lean blow-off conditions
- The injection of energy at resolved scales: for 0.3 < c < 0.6
- Correlation between kinetic energy flux across the filter scale α_{sfs} and dilatation due to strong gas expansion caused by the flame
- Closure for LES turbulence models do not capture back-scatter present in extinction/reignition events



Conditional mean of kinetic energy flux across the filter scale as a function of progress variable (c) for different mixture fraction (Z)



Conditional mean of dilatation as a function of progress variable (c) for different mixture fraction (Z)

B. S. Soriano, J. H. Chen, Combustion and Flame (2025) in preparation