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Impact of thermodiffusive effects in lean turbulent hydrogen flames

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Context
Challenges related to hydrogen for turbulent combustion modeling

- Compared to conventional hydrocarbons
  - Effective Lewis << 1 on the lean side
- Response of **flame structure** to **stretch**
- **Cellular** flame instability

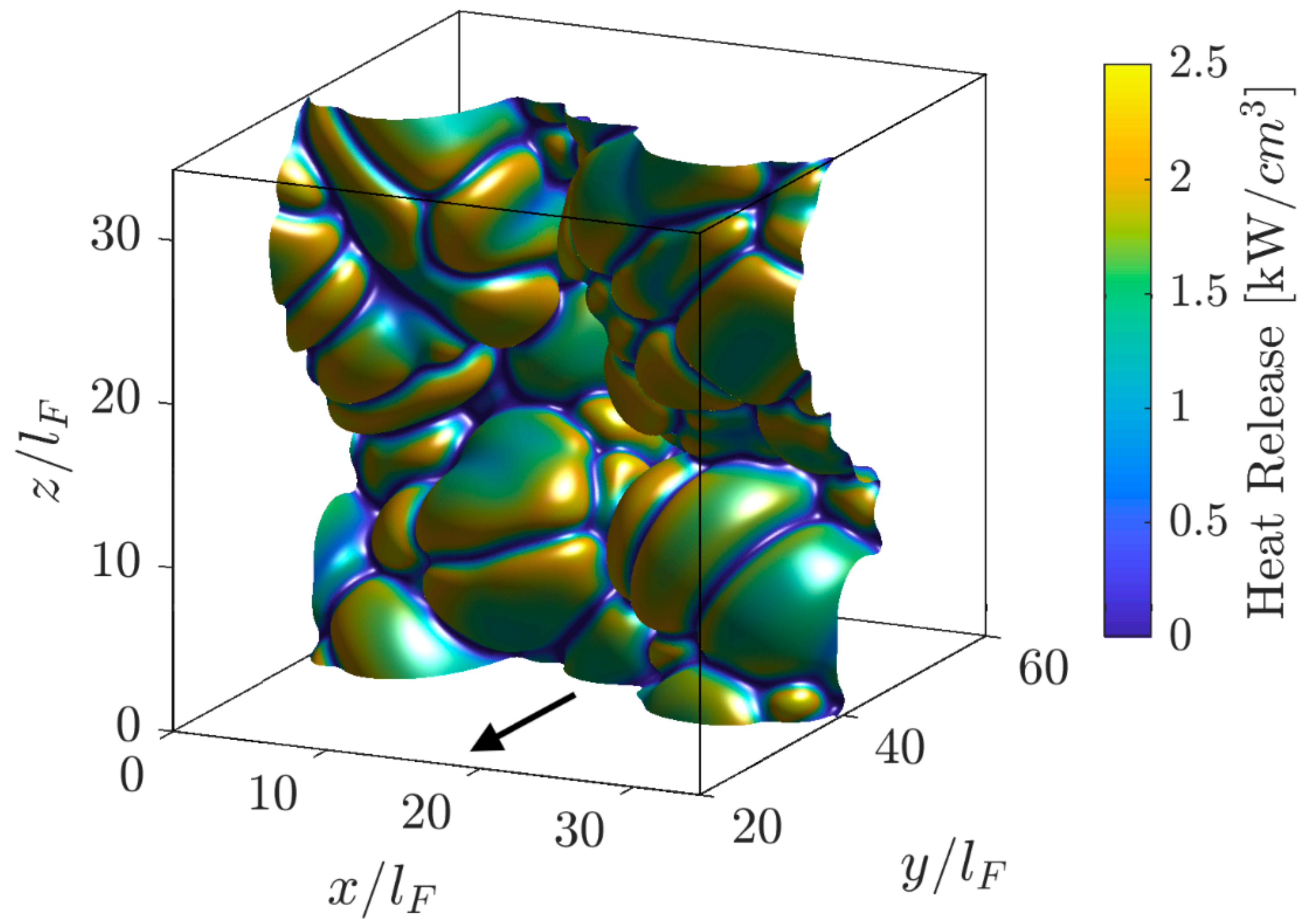


Figure 3: Snapshot of the flame surface area of the *LamUnstable* case colored by the heat release. The flame surface area is defined by an iso-surface of progress variable at C_{H_2} = 0.8. The initially flat flame is propagating towards an inlet and the flame propagation indicated by arrow.

Berger et al. C&F 2022

- Interplay between **turbulence** and **cellular instability?**
- Implications for turbulent combustion model?

Context

Combustion models for Large Eddy Simulation

- Many ways to tackle this problem
  - (Presumed) PDF models
  - Flame surface density
  - Linear Eddy models
  - **Artifically thickened flame model 'TFLES'**

Modification of the governing equations

$$\frac{\partial}{\partial x_i}(\rho u_i Y_k) = \frac{\partial}{\partial x_i}\left(\rho F D \frac{\partial Y_k}{\partial x_i}\right) + \frac{\dot{\omega}_k}{F}$$

$$\dot{\omega} \rightarrow \frac{\dot{\omega}}{F} \qquad D \rightarrow FD$$

From flamelet equations (or dimensional analysis)

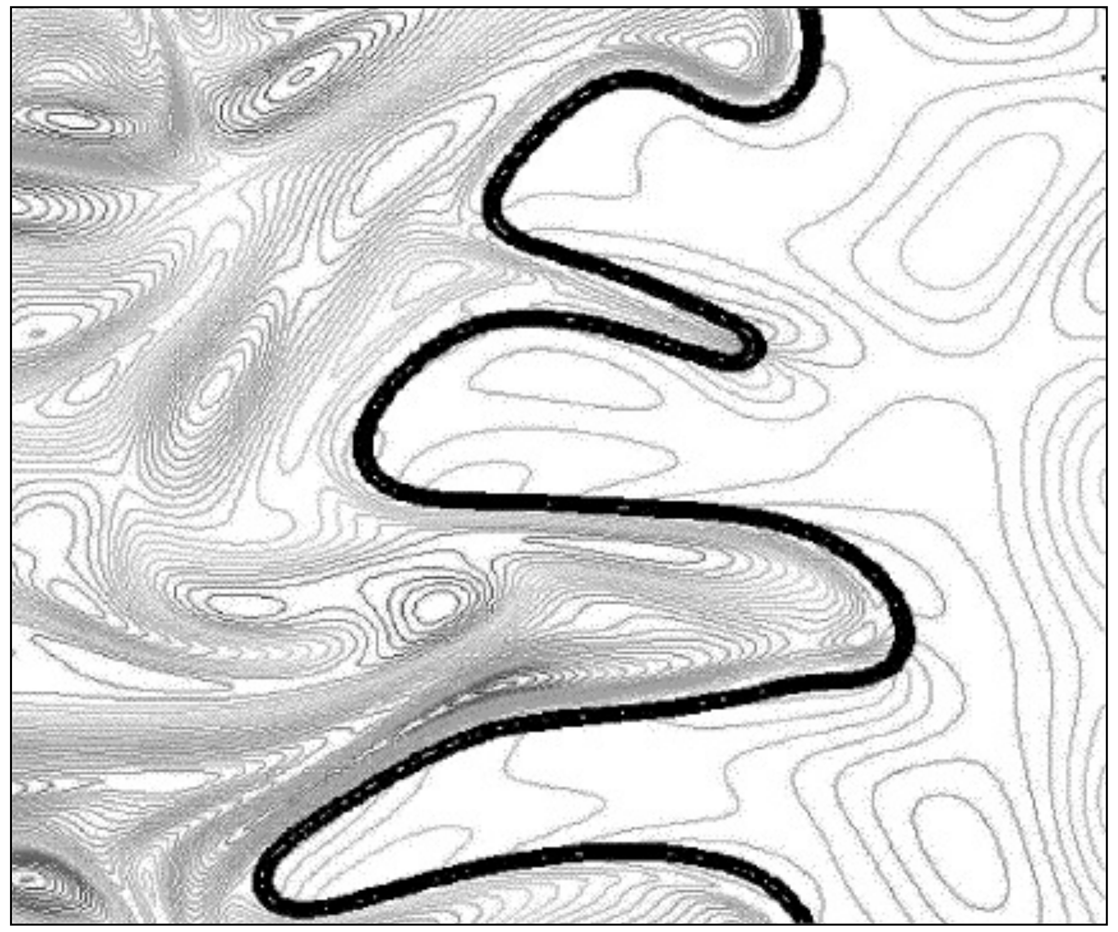
$$S_L \propto \sqrt{\dot{\omega}/F \times FD} \rightarrow S_L$$

$$\delta_l \propto \sqrt{\frac{FD}{\dot{\omega}/F}} \rightarrow F\delta_l$$

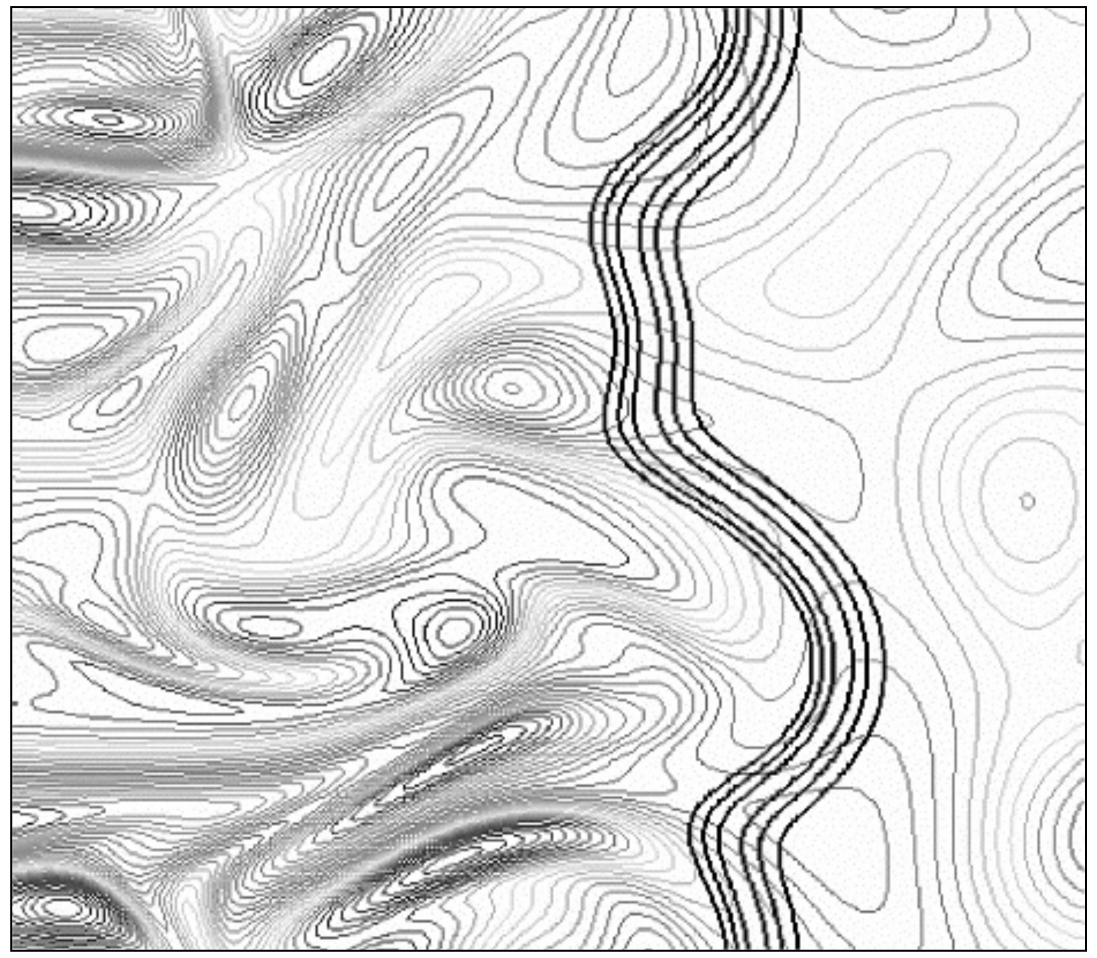
- Laminar flame speed is unchanged !
- The flame is F time thicker

Artificial flame thickening: what do we lose?

DNS of flame turbulence interaction



*LES of the same case with **F=2***



- Loss of flame wrinkling !
- Introducing a so-called correction: **the efficiency function 'E'**

$$\frac{\partial}{\partial x_i}(\rho u_i Y_k) = \frac{\partial}{\partial x_i}\left(\rho E F D \frac{\partial Y_k}{\partial x_i}\right) + E\frac{\dot{\omega}_k}{F}$$

F : controls the flame front resolution on the grid

E : compensates the unresolved flame wrinkling

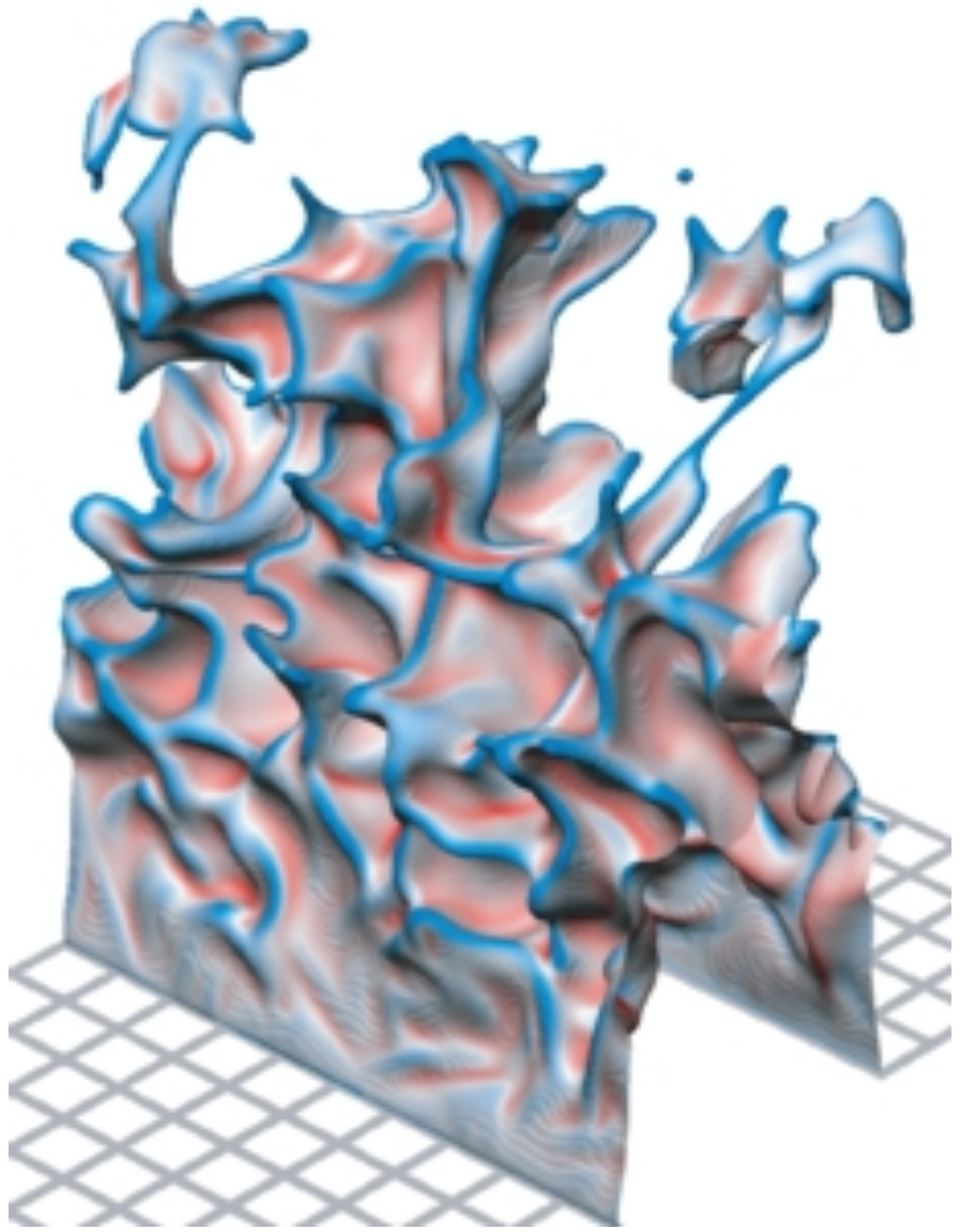
$$S_l \propto \sqrt{\dot{\omega} D} \rightarrow \sqrt{E\dot{\omega}/F \times EFD} = E\sqrt{\dot{\omega}D}$$

$$\delta_l^T \propto \sqrt{D/\dot{\omega}} \rightarrow \sqrt{\frac{EFD}{E\dot{\omega}/F}} = F\sqrt{D/\dot{\omega}}$$

Role of stretch in the geometrical approach

Main impact of turbulence =

Increase of the flame surface



Turbulent flame brush

Damköhler hypothesis

$$\boxed{S_T} = \boxed{A_T/A_0} \times \boxed{S_L^0}$$

Turbulent flame speed

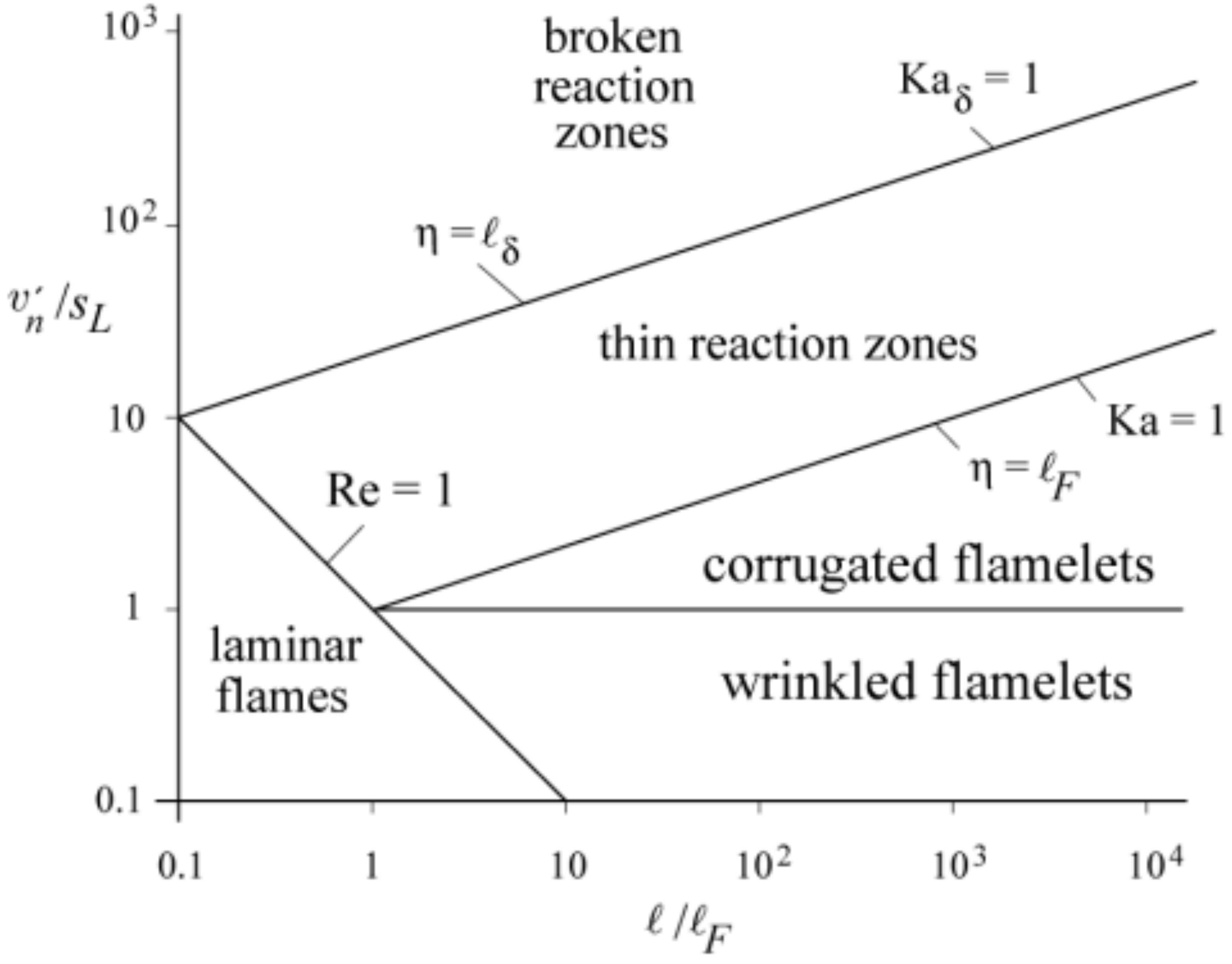
Surface enhancement

Laminar flame speed

Validity of the geometrical approach

- Flamelet hypothesis
  - Assuming Karlovitz number Ka is moderate
    - $Ka = \tau_{flamme}/\tau_{turb} \simeq \delta_L^2/\eta^2 \simeq u_\eta^2/S_L^2$
  - The flame structure remains locally a laminar structure (but which one?)

Borghi diagram



Peters, 1999

Derivation of the efficiency function

- In the TFLES context

$$E = S^{\Delta}_{F=1}/S^{\Delta}_{F>1}$$

$\Delta =$ LES filter scale

How is it estimated ?

- Algebraic models: $E = f(u'/S_L, L_T/\delta_l)$
- Transport equation
- Dynamic (scale similarity) models

Context

The fractal concept

- Algebraic model based on fractal concept (Charlette et al. C&F 2002)

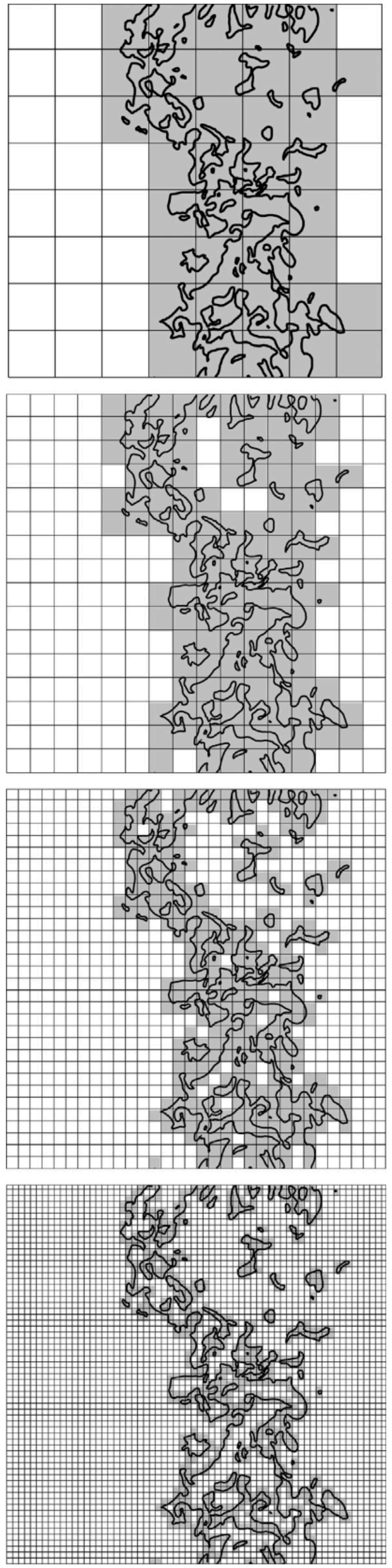
$$E = (1 + \Delta/\eta_i)^{\beta}$$

β = power-law exponent = D-2 (fractal dimension)

η_i = cutoff limit of the fractal range

Different asymptotic regimes

- $\eta > L_G, \delta_L$
- $L_G > \delta_l > \eta$ = Damkohler limit
- $\delta_l > L_G, \eta$ = bending effect



Chatakonda et al., C&F, 2013

Derivation of the efficiency function

- Balance equation for the sub grid-flame surface (Colin et al. 2000)

$$\frac{\partial \bar{\Sigma}}{\partial t} + \nabla \cdot [\langle \mathbf{u} \rangle_s \bar{\Sigma}] + \nabla \cdot [\langle w\mathbf{n} \rangle_s \bar{\Sigma}] = \langle \nabla \cdot \mathbf{u} - \mathbf{nn} : \nabla \mathbf{u} \rangle_s \bar{\Sigma} + \langle w \nabla \cdot \mathbf{n} \rangle_s \bar{\Sigma},$$

Strain — Curvature

= Total stretch

= Flame surface creation/destruction

→ Equilibrium hypothesis

$$\langle \nabla \cdot \mathbf{u} - \mathbf{nn} : \nabla \mathbf{u} \rangle_s \bar{\Sigma} = -\langle w \nabla \cdot \mathbf{n} \rangle_s \bar{\Sigma}.$$

$$\approx s_l^0 |\langle \nabla \cdot \mathbf{n} \rangle_s|$$

$$1/\eta_i = |<\nabla \cdot \mathbf{n}>_s| = \frac{1}{S_L^0}\frac{u'_\Delta}{\Delta}\Gamma$$

$$\frac{1}{S_L^0}\frac{u'_\Delta}{\Delta}\Gamma\left(\frac{\Delta}{\delta_l}, \frac{u'_\Delta}{S_L} Re_\Delta\right)$$

= net straining effect

What about hydrogen? ‘Thermodiffusive effects’

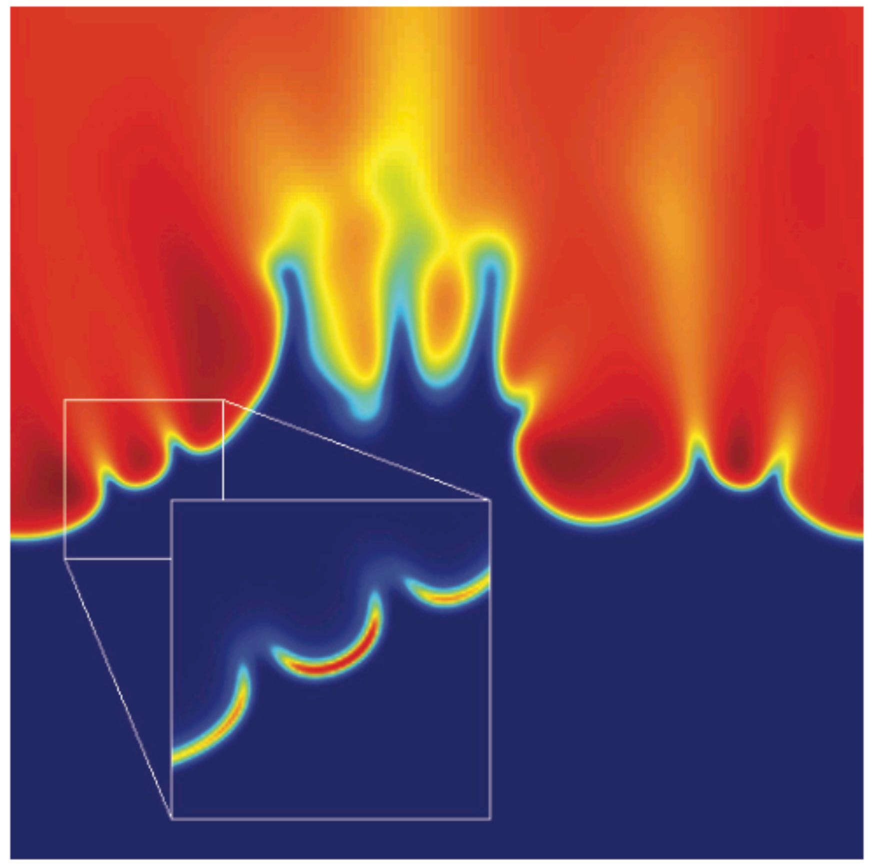
- **Damköhler hypothesis must be modified**

$$S_T = A_T/A_0 \times S_L^0 \times I$$

S_T	A_T/A_0	S_L^0	$\times I$
Turbulent flame speed	Surface enhancement	Laminar flame speed	‘Stretch factor’ = global effect of local flame speed enhancement

- Arising questions
  - Does the flamelet hypothesis remains valid (strained or unstrained?)
  - What is the interplay between turbulent and cellular instability:
    - Surface wrinkling: low Lewis number/TD unstable flame = more wrinkling?
    - Increased reactivity: I0 resulting from cellular instability and/or turbulent stretching
    - Competition, interaction?

Wrinkling and burning rate of a lean TD unstable hydrogen flame



Aspden et al. 2011

Lean hydrogen

Brief literature review

Aspden et al. JFM, 2011:
Lean ($\phi < 0.4$) flames with
$\mathrm{Ka} = 10 - 1500$

- At high Karlovitz number, transition to distributed combustion regime with no extinction
- Strong local enhancement of burning speed

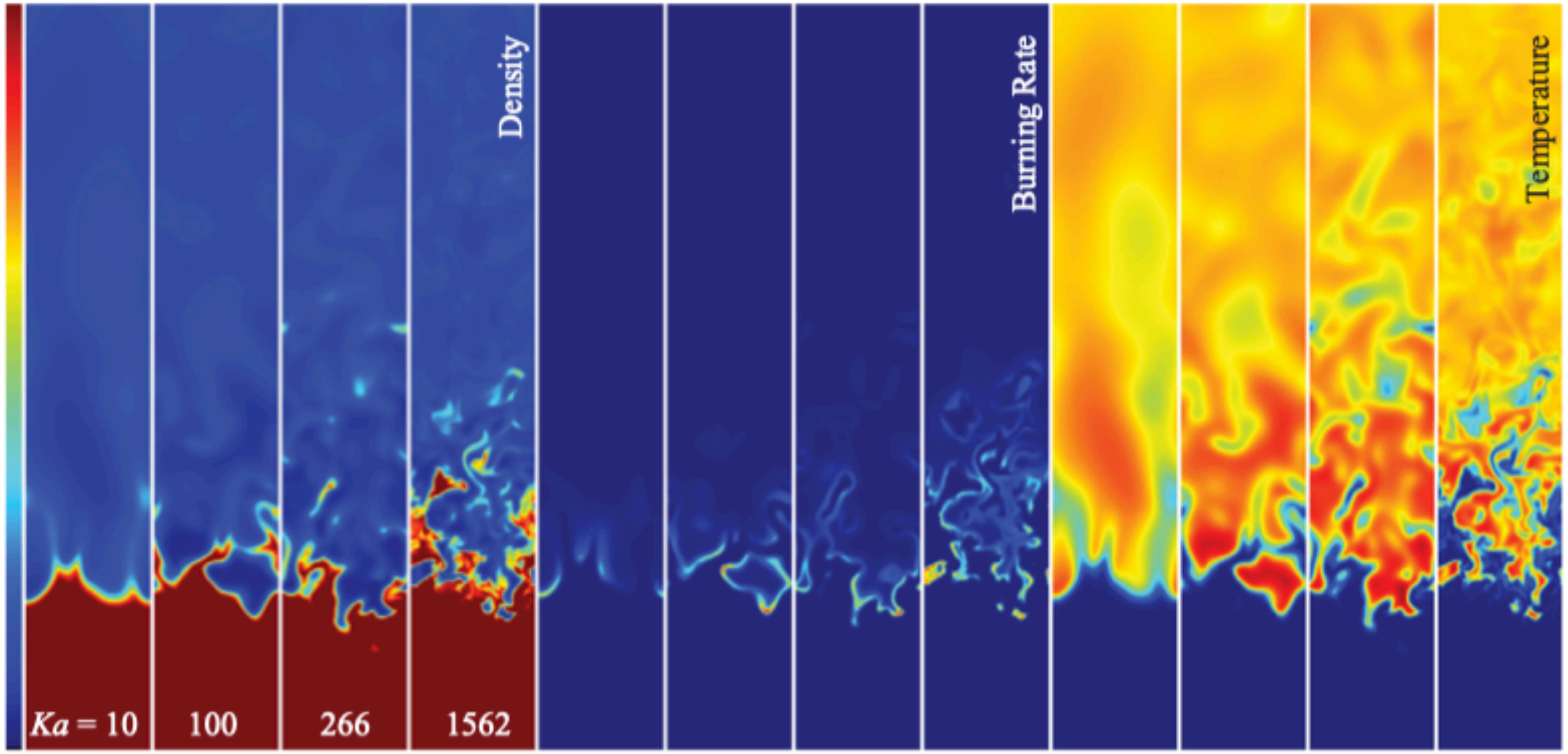


FIGURE 5. Two-dimensional vertical slices through three-dimensional simulations showing density, burning rate and temperature at $\varphi = 0.31$, respectively. The density range is [0.2,1.02] $\mathrm{kg\,m^{-3}}$ in each case. The burning rate is shown between zero and 15, 25, 35 and 45 $\mathrm{kg\,m^{-3}\,s^{-1}}$, respectively. The temperature range is [298,1600] K in each case.

Lean hydrogen
Brief literature review

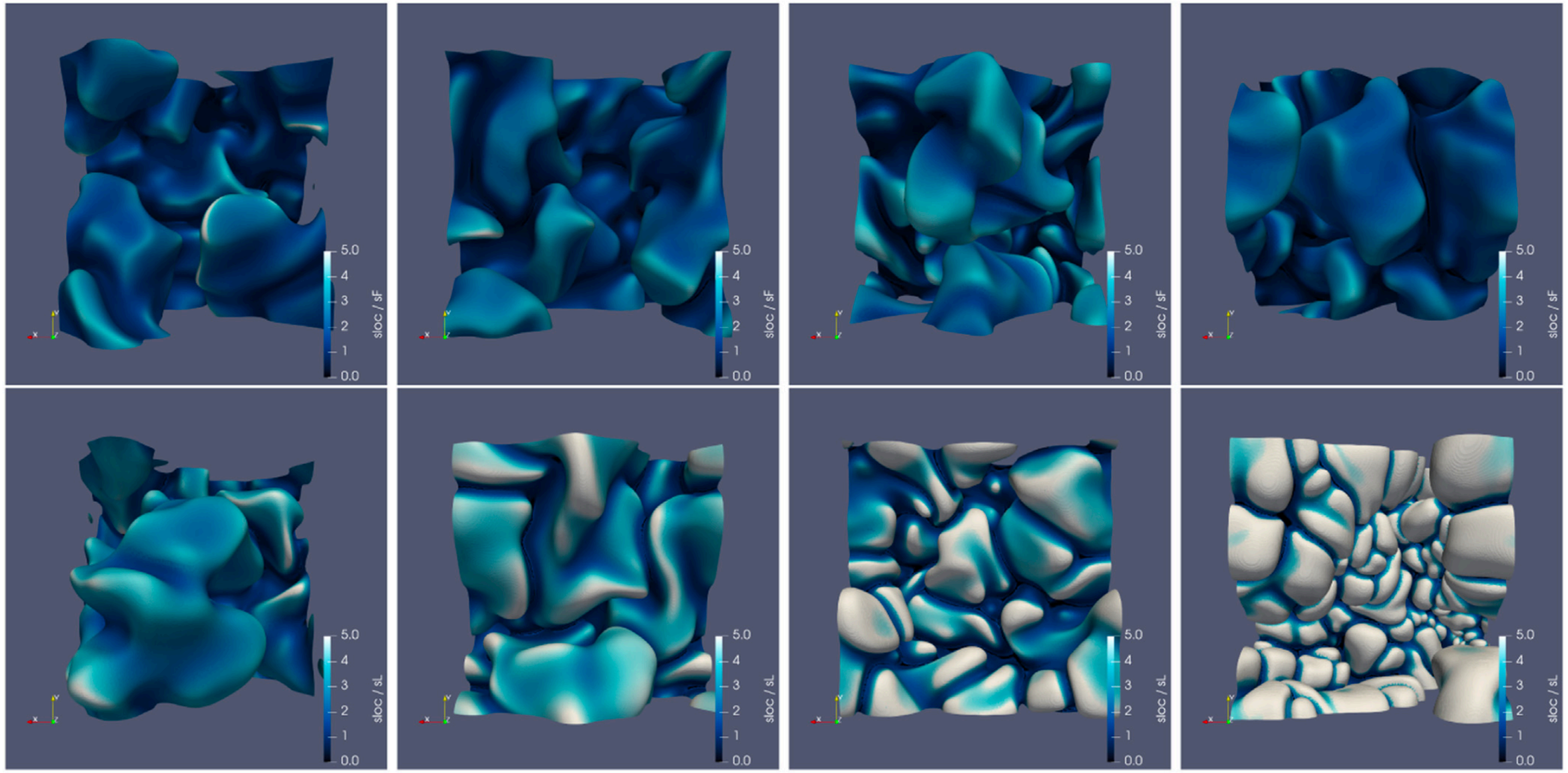
- Howarth et al. C&F 2023
- Dataset with large range of operating points (turbulent intensity, pressure, temperature)
- Flame scales based on Aspden et al. PCI 2011: S_L **and** δ_L **taken from 1D TD-unstable freely propagating flame**

F-Normalization

(TD unstable flame)

Unstretch flame parameters

Normalization



Lean hydrogen

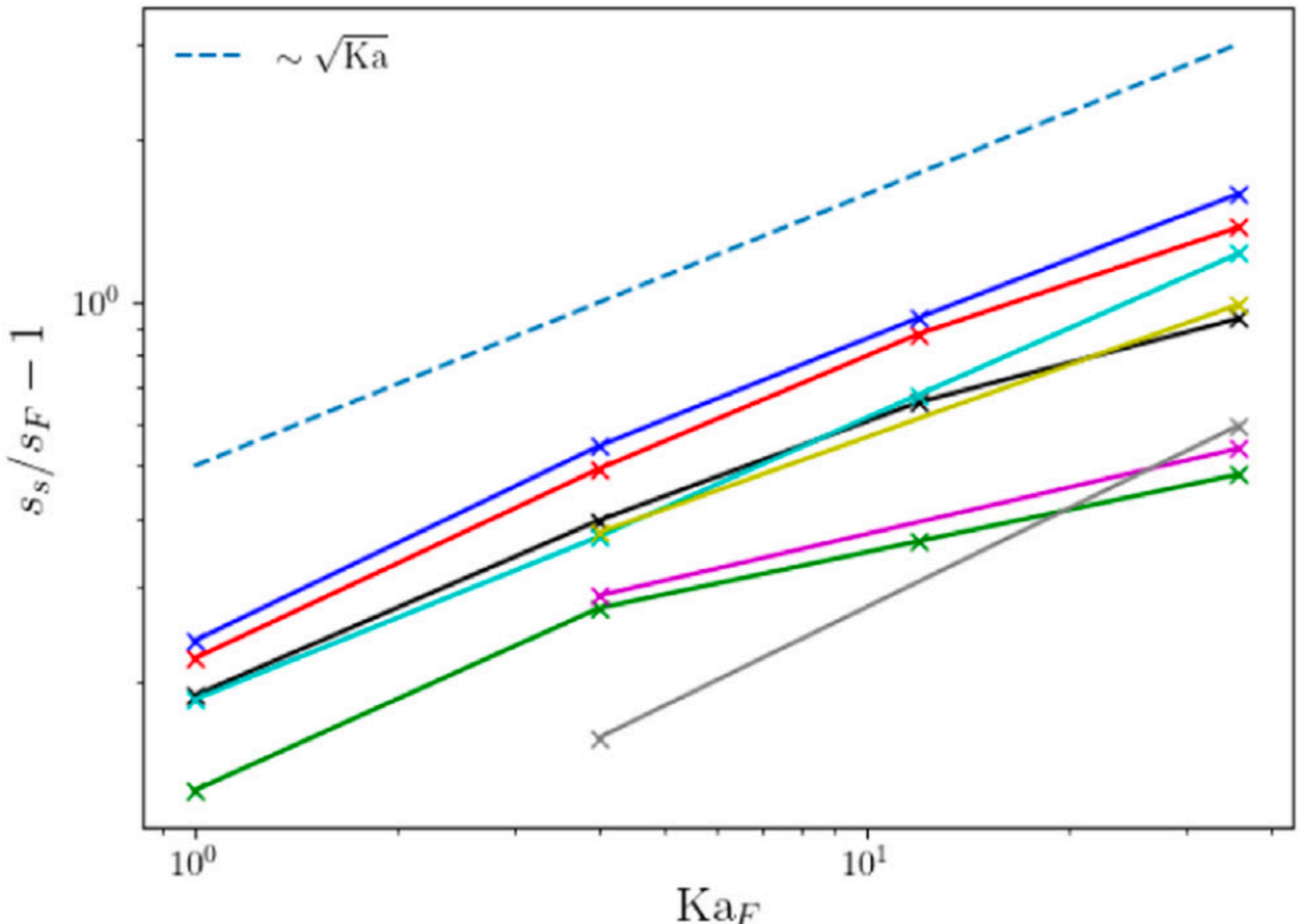
Brief literature review

- Howarth et al. C&F 2023, Aspden et al. PCI 2011
  - Proposed correlation for stretch factor

$$I_0 \propto I_0^{TD,lam}(1 + \alpha\sqrt{Ka_F})$$

Ka_F = Ka number based on laminar unstable flame

Local flame speed enhancement ('I_0') vs Ka_F

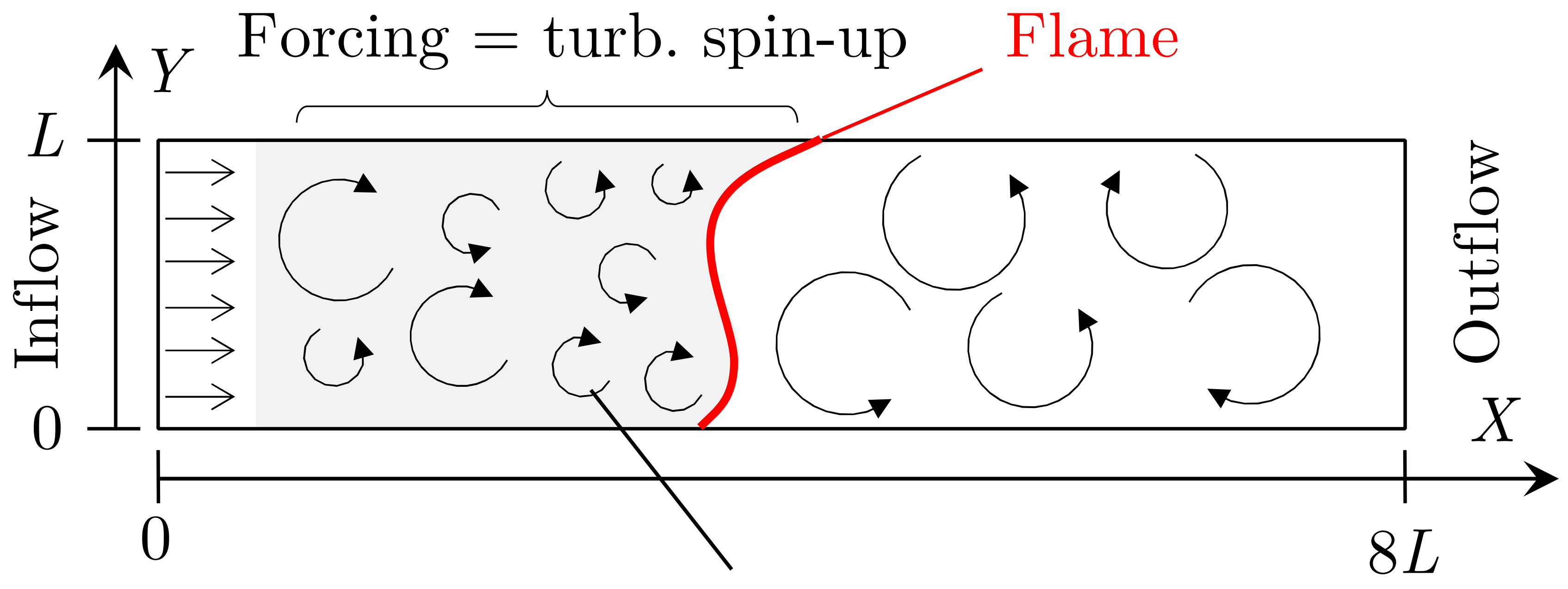


DNS of lean hydrogen flames

Numerical setup

- Classical setup for turbulent flame in forced HIT to (Savard C&F 2015, Aspden 2011 JFM, etc.)

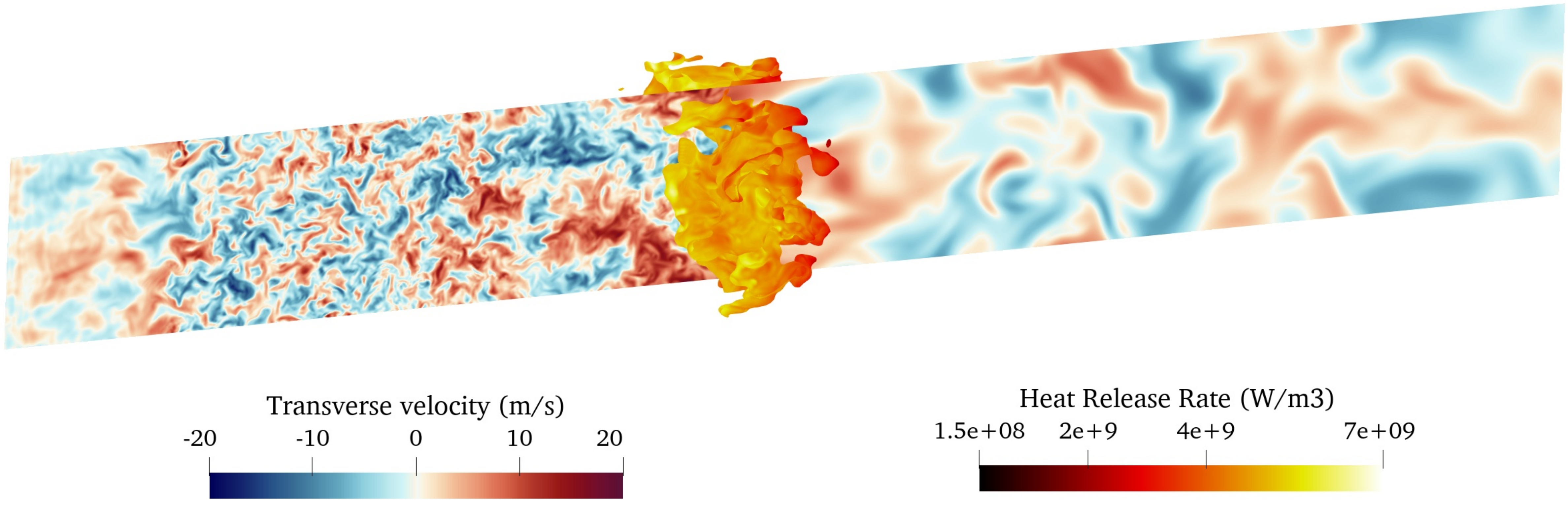
Low intensity turbulence injected to kickstart fluctuations
u’ = 10% U_{bulk}



Through a linear momentum source term

$L = 25\ \delta_l^0$

$\delta_l^0 = 7\ \Delta_x$



DNS of lean hydrogen flames

Operating points

Characteristics for the two equivalence ratio considered

Equivalence ratio ϕ	0.36	0.52
Laminar flame speed s_l^0 (m/s)	0.134	0.609
Laminar flame thickness δ_l^0 (μm)	879	364
Adiabatic flame temperature T_{ad} (K)	1318	1675
Characteristic flame time τ_f (ms)	6.6	0.59
Flame Reynolds number $Re_f = s_l^0 \delta_l^0 / \nu_u$	6	11
Effective Lewis number Le_{eff}	0.37	0.43

Two chemistries:

- San Diego, with real Lewis numbers (LeRe)
  ➜ thermodiffusive effects and instabilities
- Fitted 1-step, unitary Lewis numbers (Le1)
  ➜ no thermodiffusive effects

Operating points

Flame time

$$Ka^0 = \frac{\tau_f}{\tau_k} = \frac{\delta_l^0}{s_l^0} \cdot \frac{u'^{3/2}}{L_t^{1/2}\nu^{1/2}}$$

Time of the smaller turbulent scales (Kolmogorov)

Increasing turbulent intensity

Case	u'/s_l^0	Ka^0	ϕ	Re_t
A36	0.38	0.25	0.36	13
B36	0.76	0.70	0.36	25
C36	3.0	5.5	0.36	99
D36	6.0	16	0.36	198
E36	11	40	0.36	372
F36	15	62	0.36	496
A52	0.47	0.5	0.52	25
B52	0.75	1	0.52	40
C52	2.2	5	0.52	116
D52	3.5	10	0.52	184
E52	5.6	20	0.52	292
F52	8.8	40	0.52	464

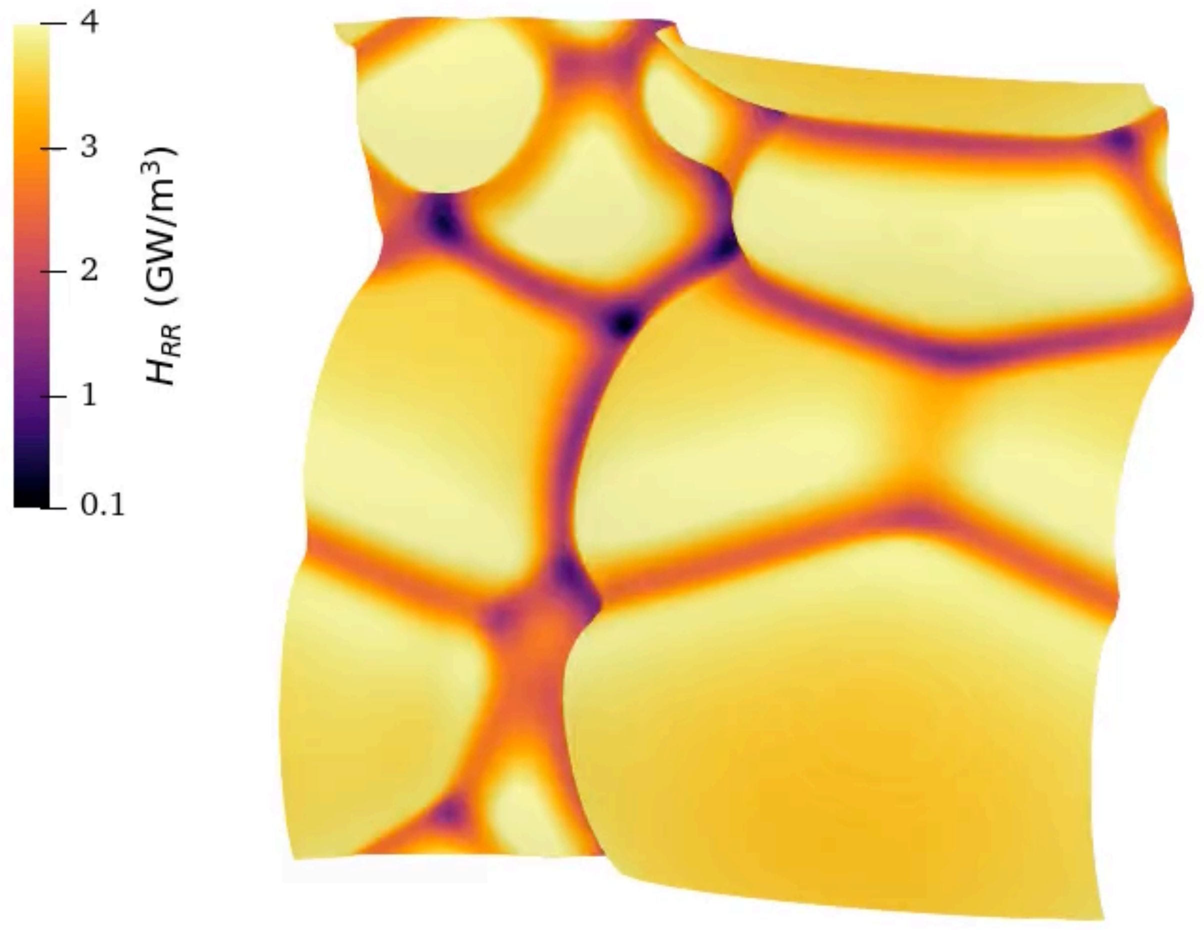
List of cases of study

Outer to inner scale ratio L_t/δ_l^0 fixed for a given domain size

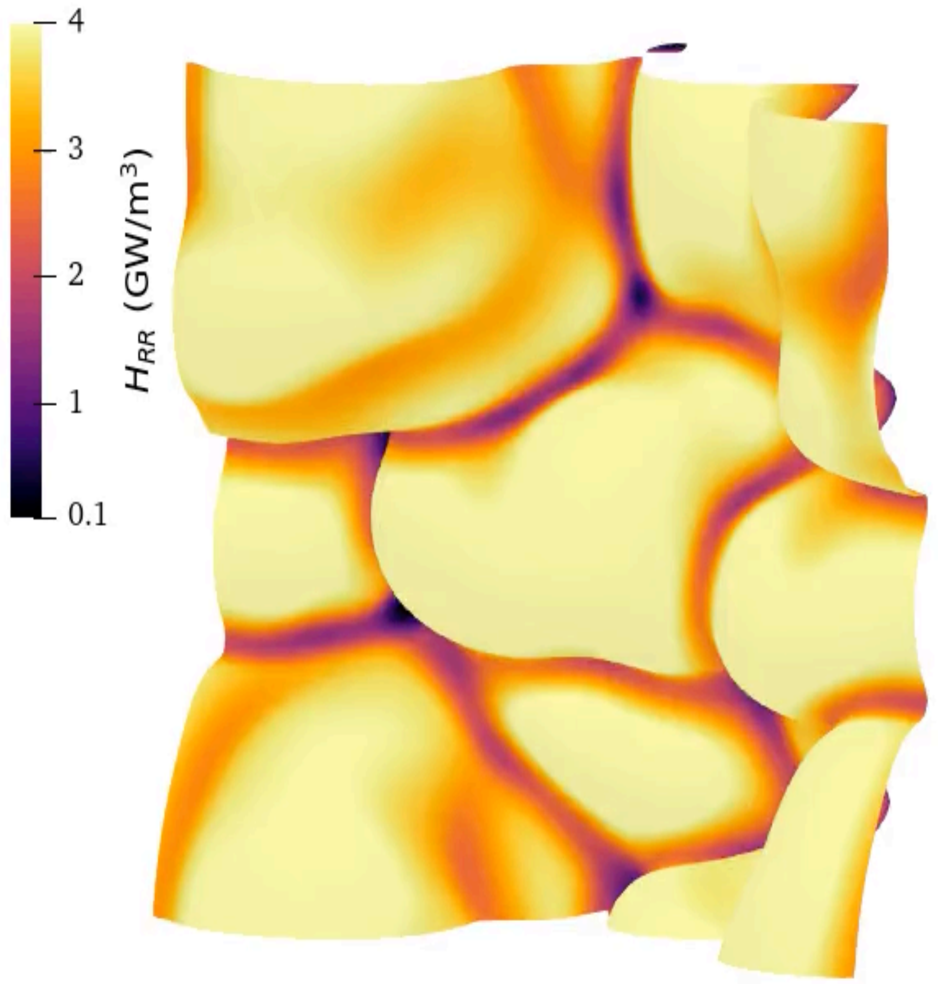
DNS of lean hydrogen flames

Effect of Karlovitz number

Laminar unstable flame



Turbulent unstable flame Ka^0=0.5



Turbulent unstable flame Ka^0=40

ϕ = 0.52 San Diego chemistry

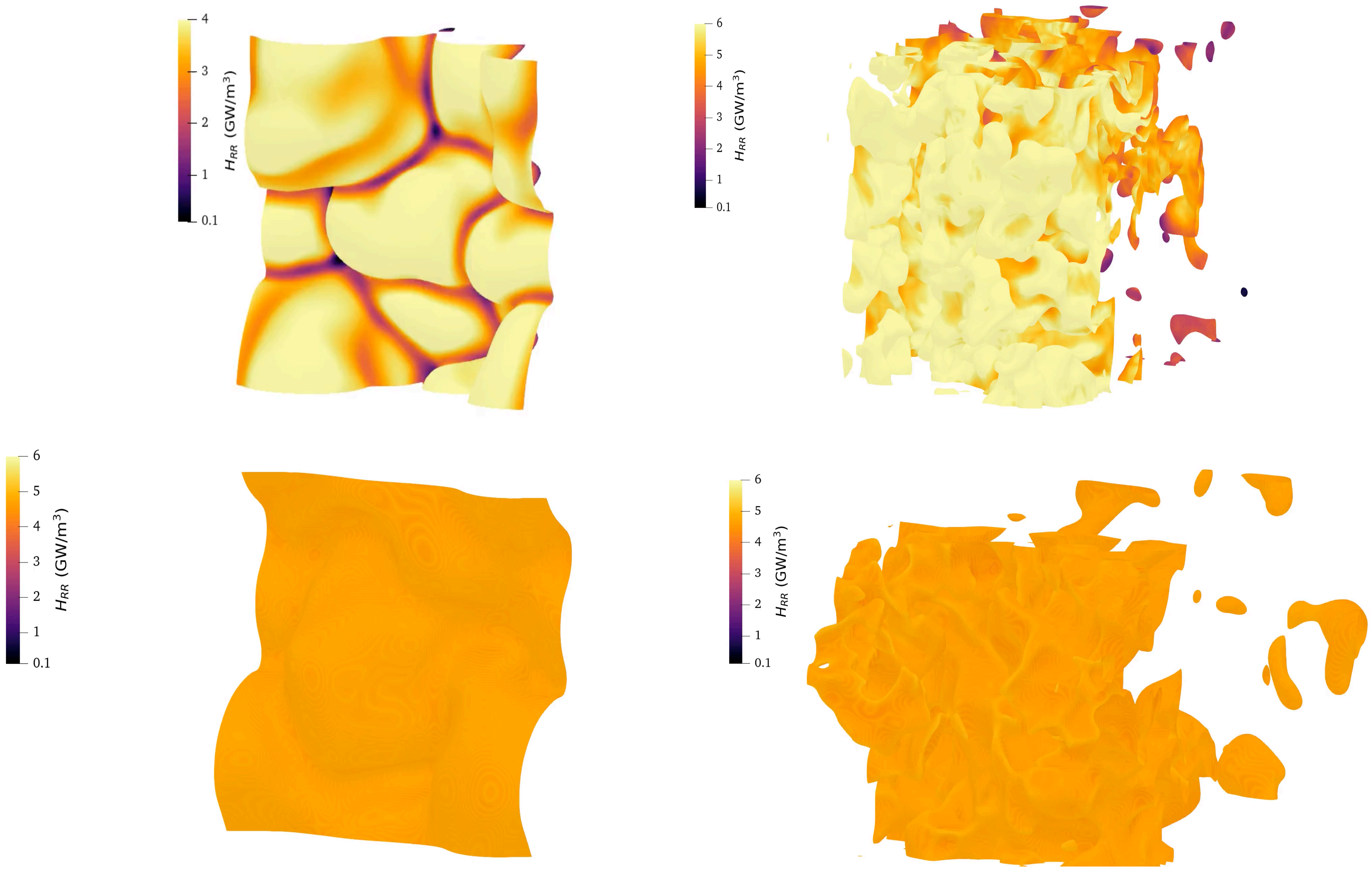
DNS of lean hydrogen flames

Effect of Lewis number

$Ka^0 = 0.5$ | **$Ka^0 = 40$**

SanDiego (LeRe) chemistry

Le1 chemistry



DNS of lean hydrogen flames

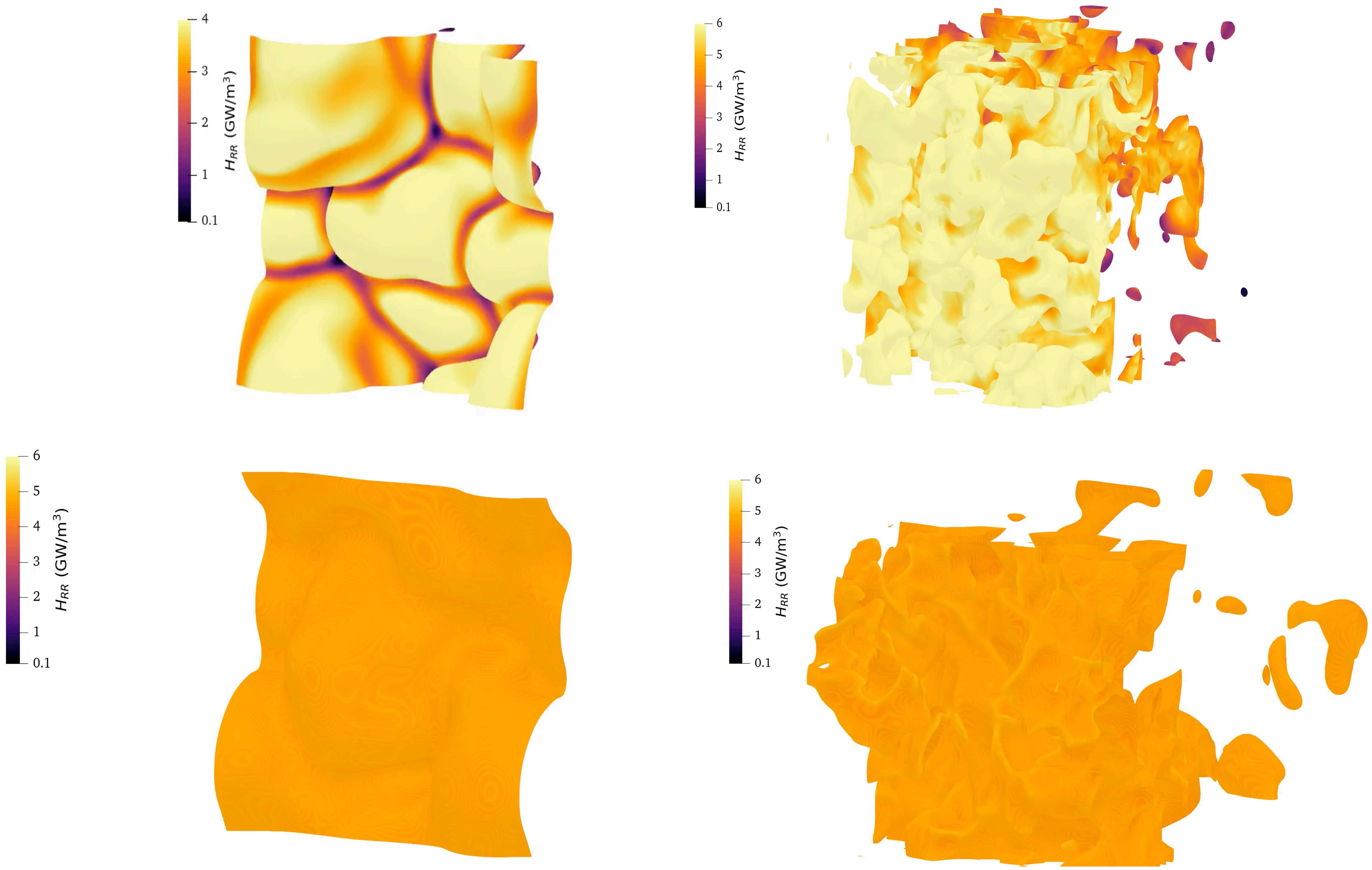
Effect of Lewis number

Ka⁰ = 0.5

Ka⁰ = 40

SanDiego (LeRe) chemistry

Le1 chemistry



DNS of lean hydrogen flames
Flame structure

Thermodiffusive effects:

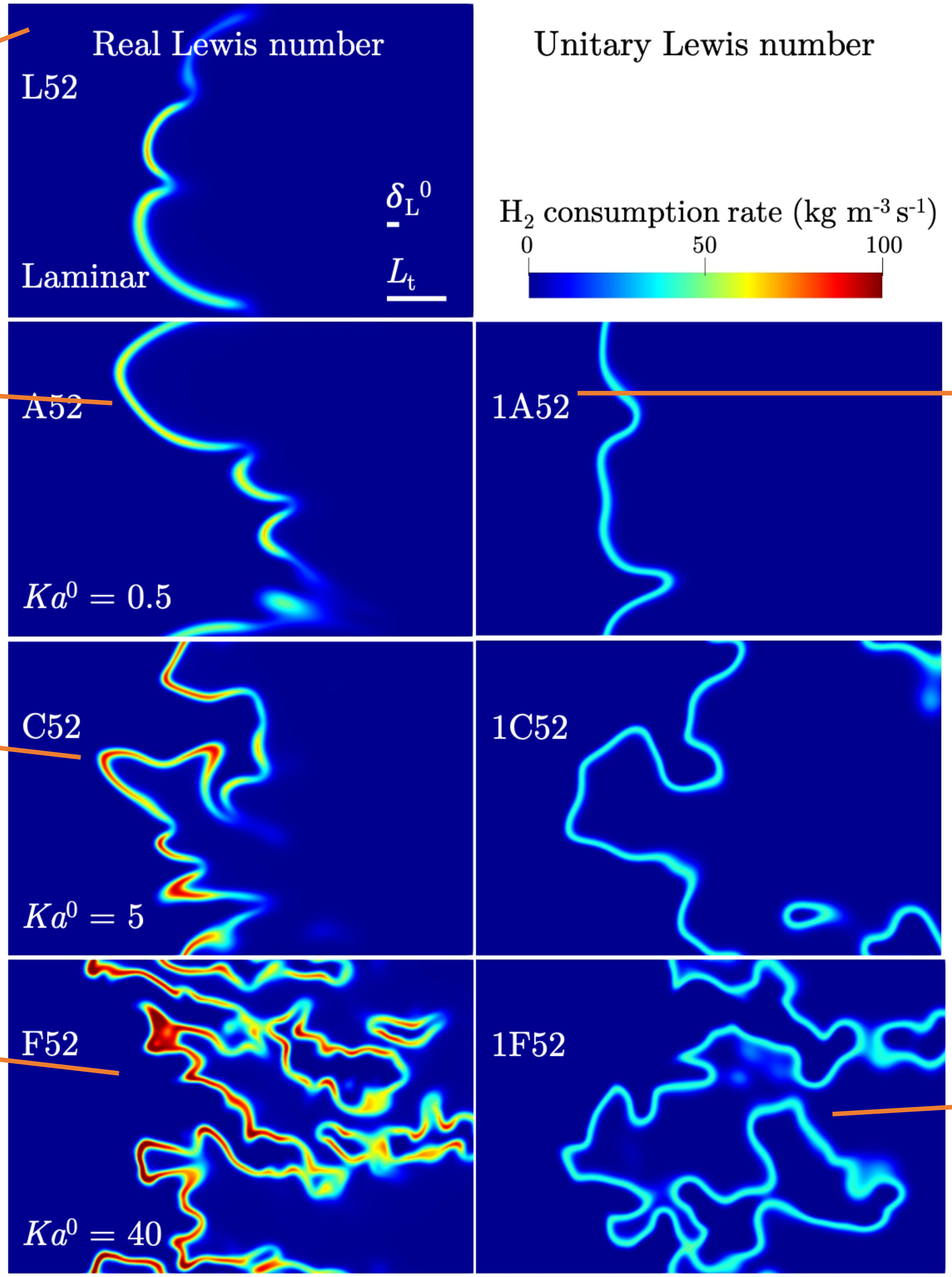
- Cellular wrinkling

- Increased consumption in regions of positive curvature

Increased consumption though higher curvature at higher Ka

Effective widening of the region with fuel consumption with Ka

San Diego ***Unity Lewis Number***



No cellular structure ≠ LeRe

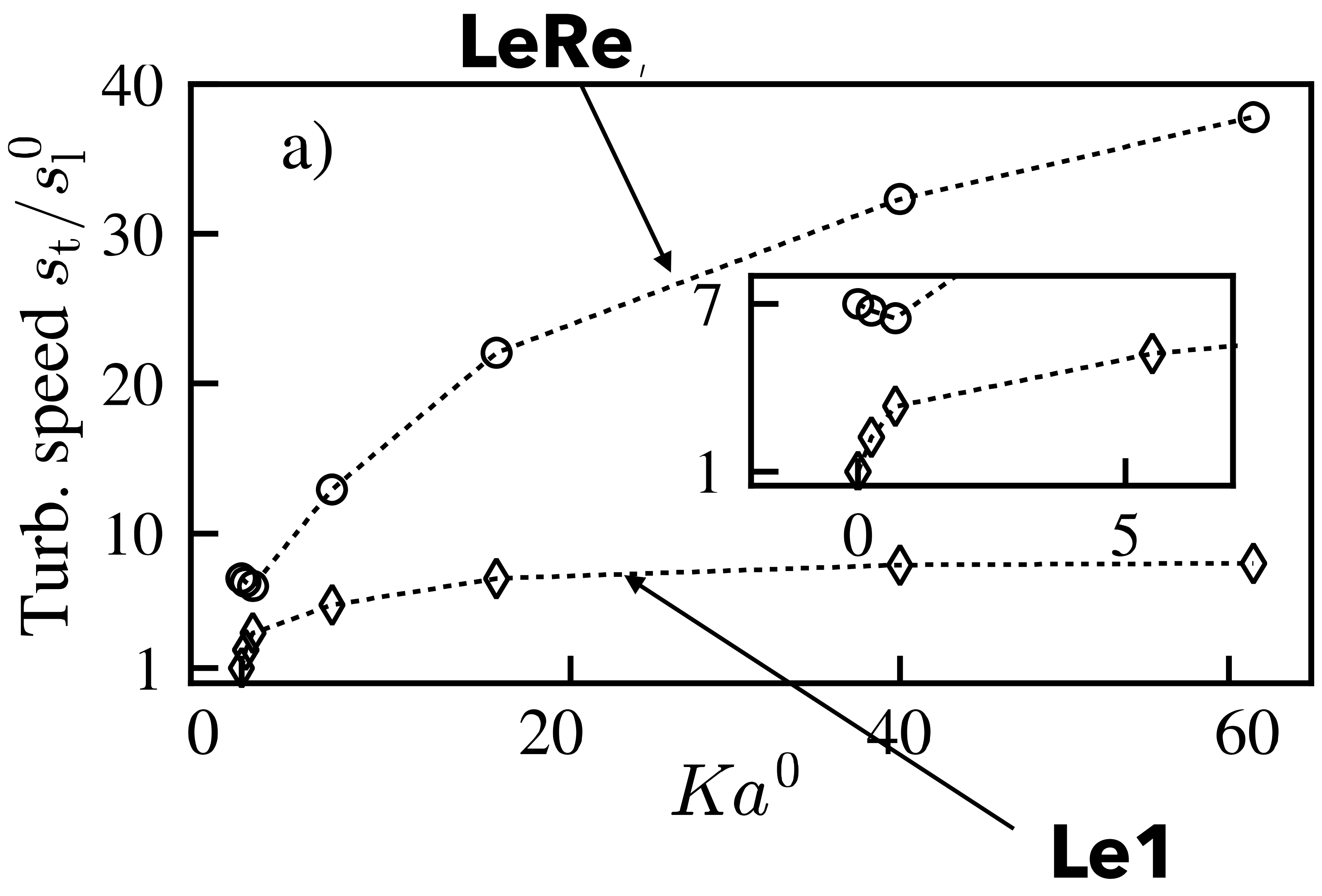
Constant consumption – Flame unaffected by stretch

Turbulence-wrinkled structure increasingly similar to LeRe

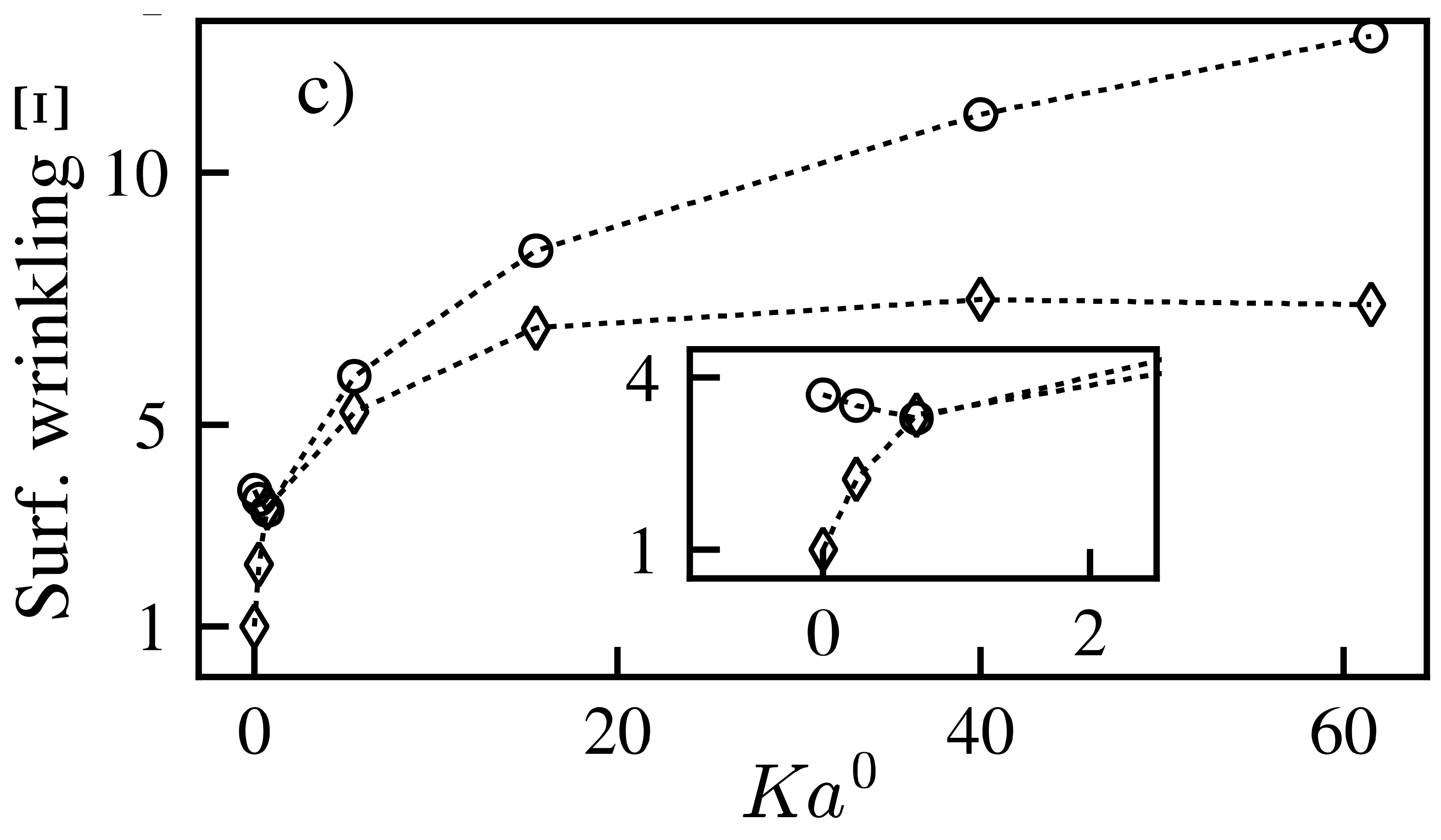
DNS of lean hydrogen flames

Damköhler decomposition

$$S_T/S_L^0 \quad = \quad \Xi \quad \times \quad I_0$$



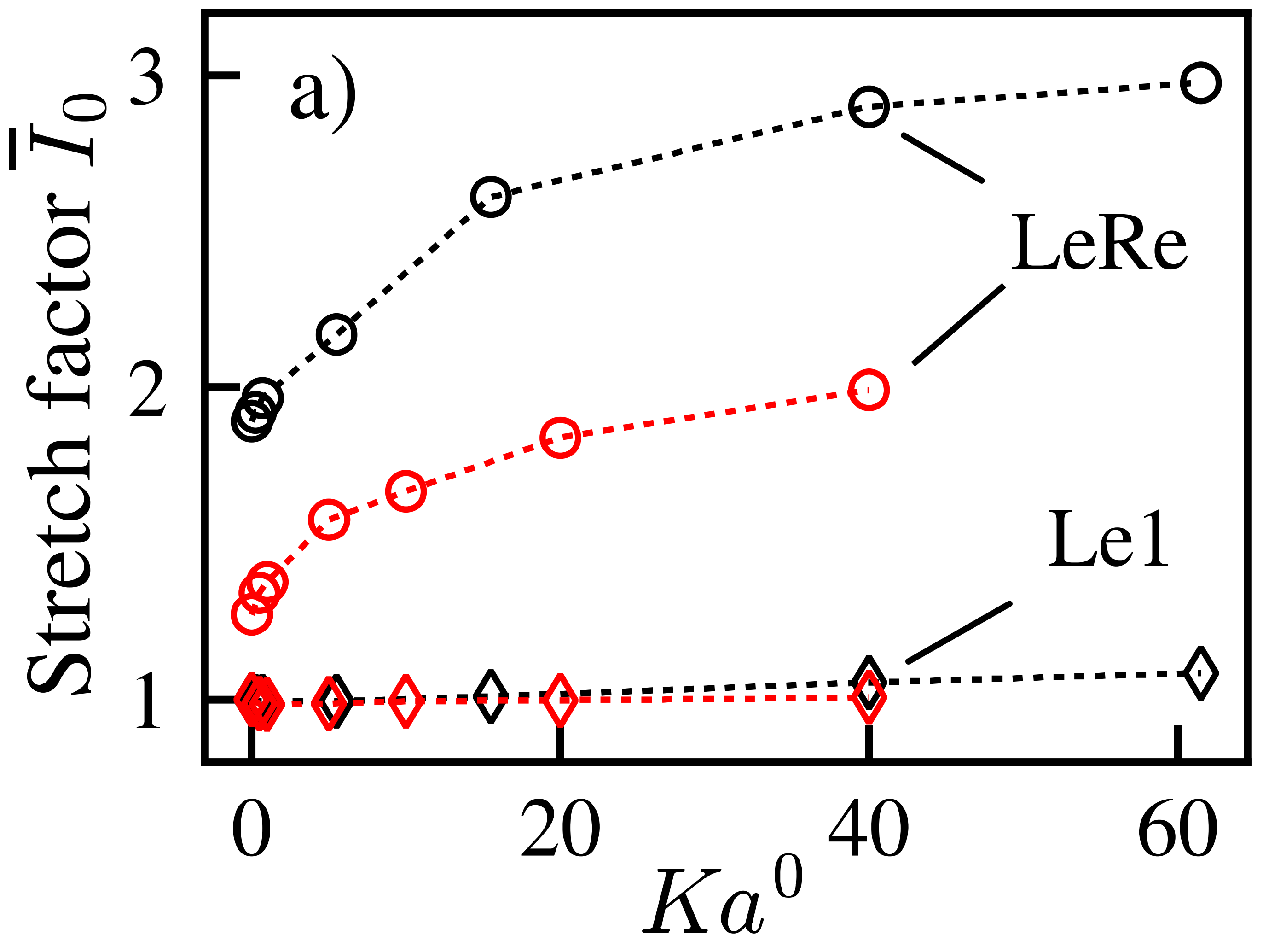
Plateau at high Ka^0 only for Le1



Higher winkling for LeRe flame due to **cellular structure at Low Ka**

For $Ka^0 < 1$: $\Xi_{LeRe} >> \Xi_{Le1}$

For $Ka^0 > 1$: $\Xi_{LeRe} >= \Xi_{Le1}$



Global stretch factor **increases with Ka^0** due to the turbulent stretching

Stronger general response for the leaner mixture

Key takeaways for modeling

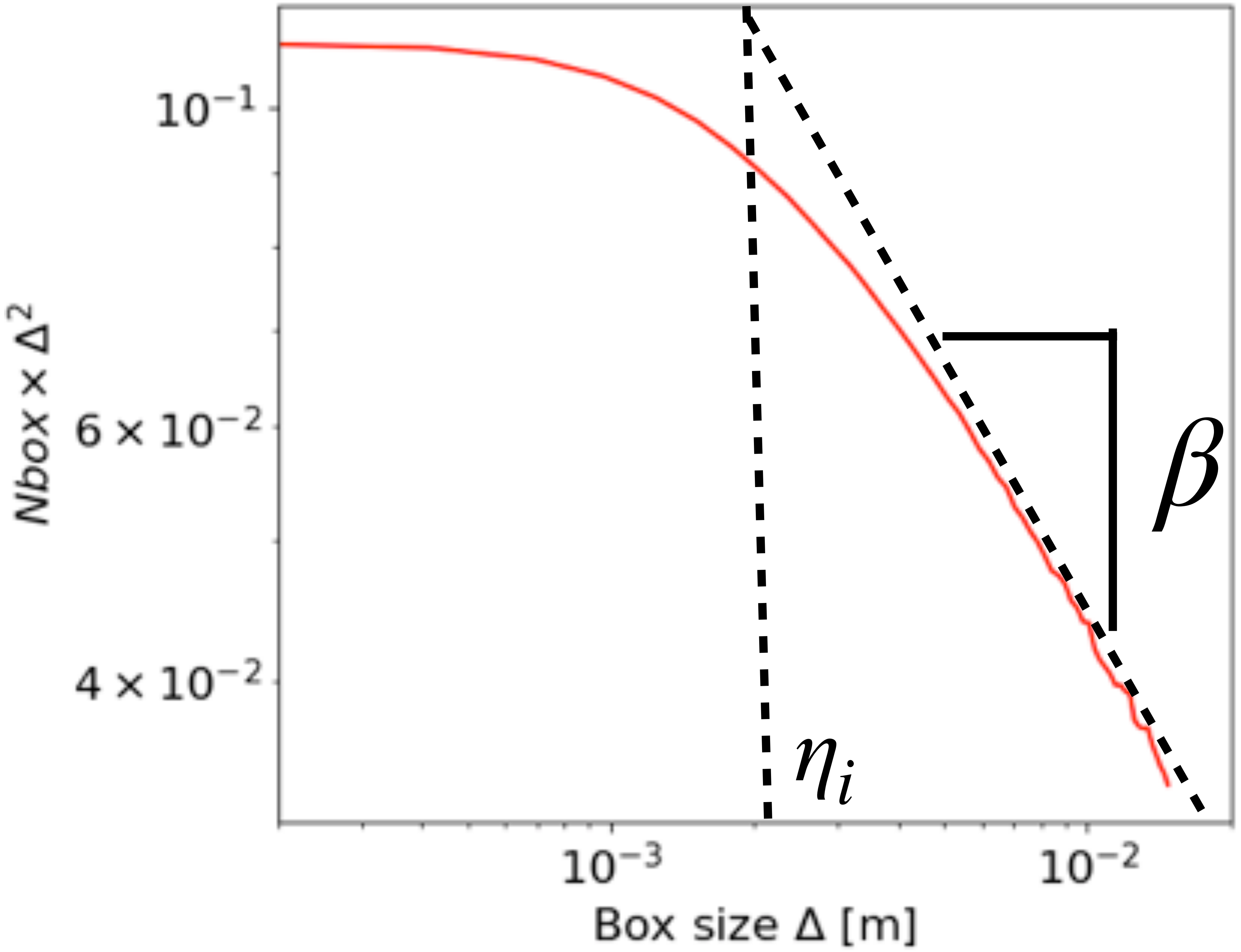
- Thermodiffusive effects are very significant in lean hydrogen flames
  - **Low Ka**: Cellular instability mechanism → Local flame speed enhancement ('I0' factor); → Increased flame surface area
  - **High Ka:** turbulent stretching → Local flame speed enhancement $I_0/I_0^{lam} - 1 \approx \sqrt{Ka}$ → Modified flame scales (S_L, δ_L) = Modified wrinkling

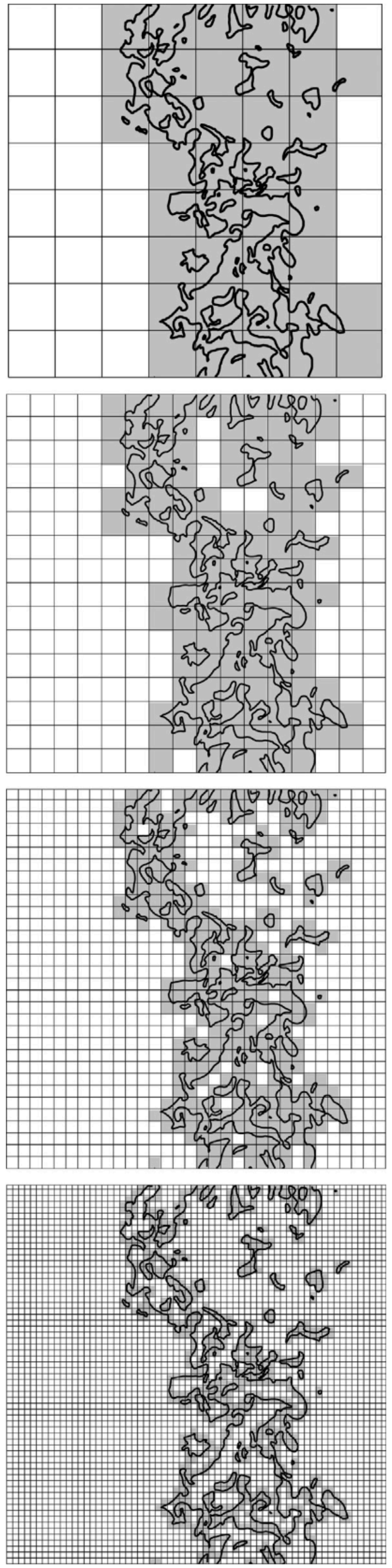
Wrinkling of turbulent H2 flames

Fractal analysis

- Fractal parameters extracted with a box counting method

$$E = (1 + \Delta/\eta_i)^\beta$$





Chatakonda et al., C&F, 2013

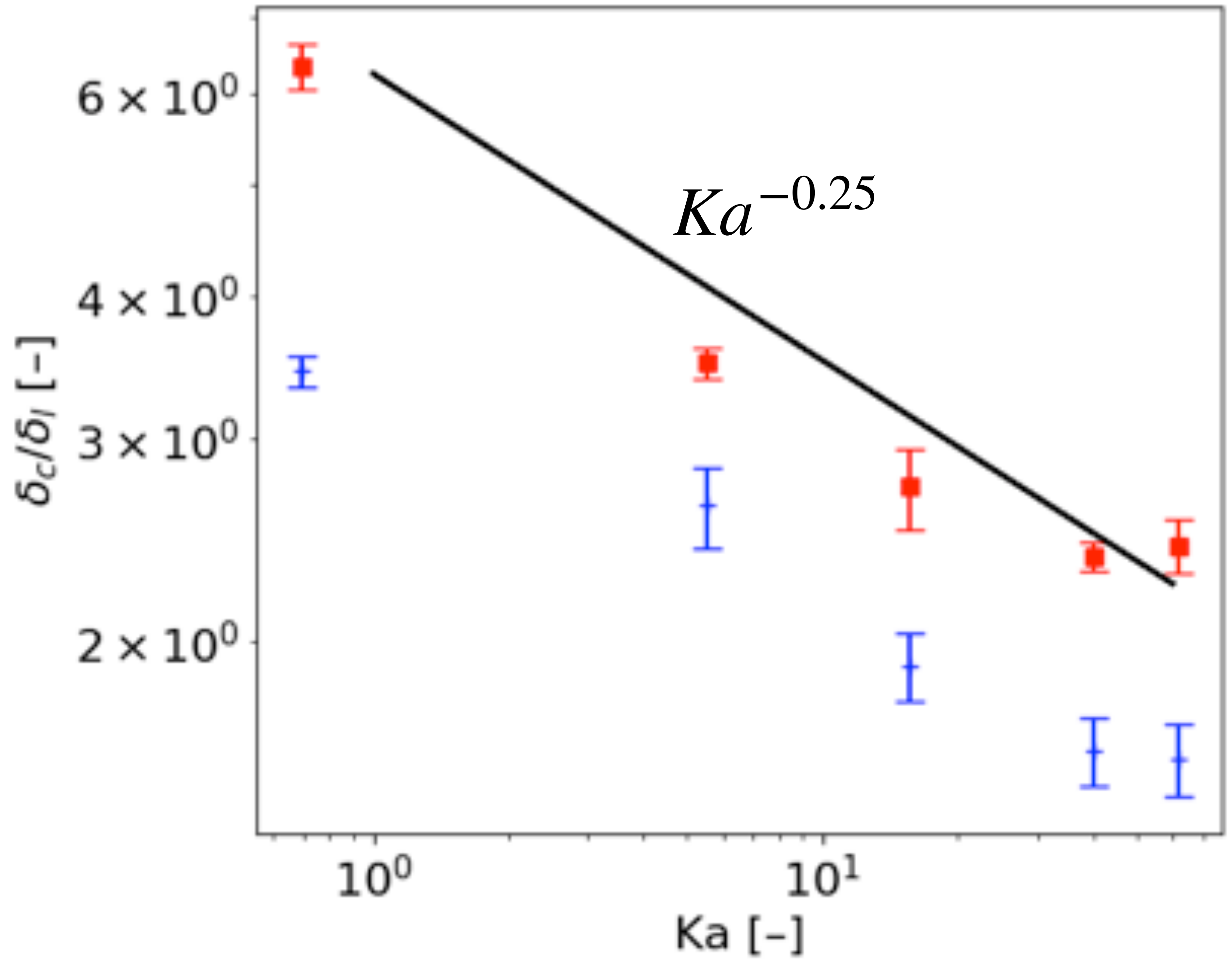
Fractal analysis
Inner-cut off scale

O Le1 chemistry

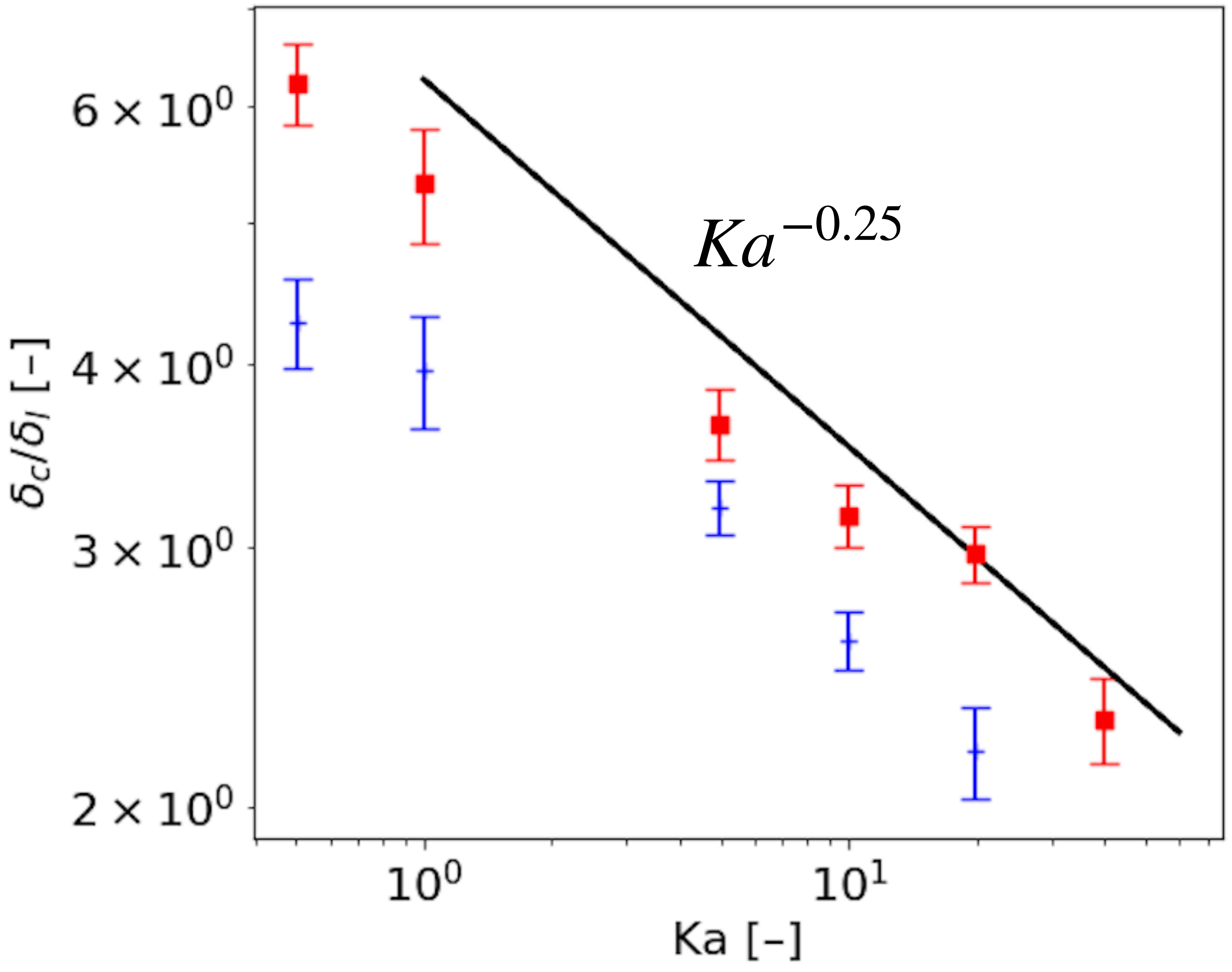
O LeRe chemistry

Cut-off scale vs Karlovitz number

$\phi = 0.36$



$\phi = 0.52$

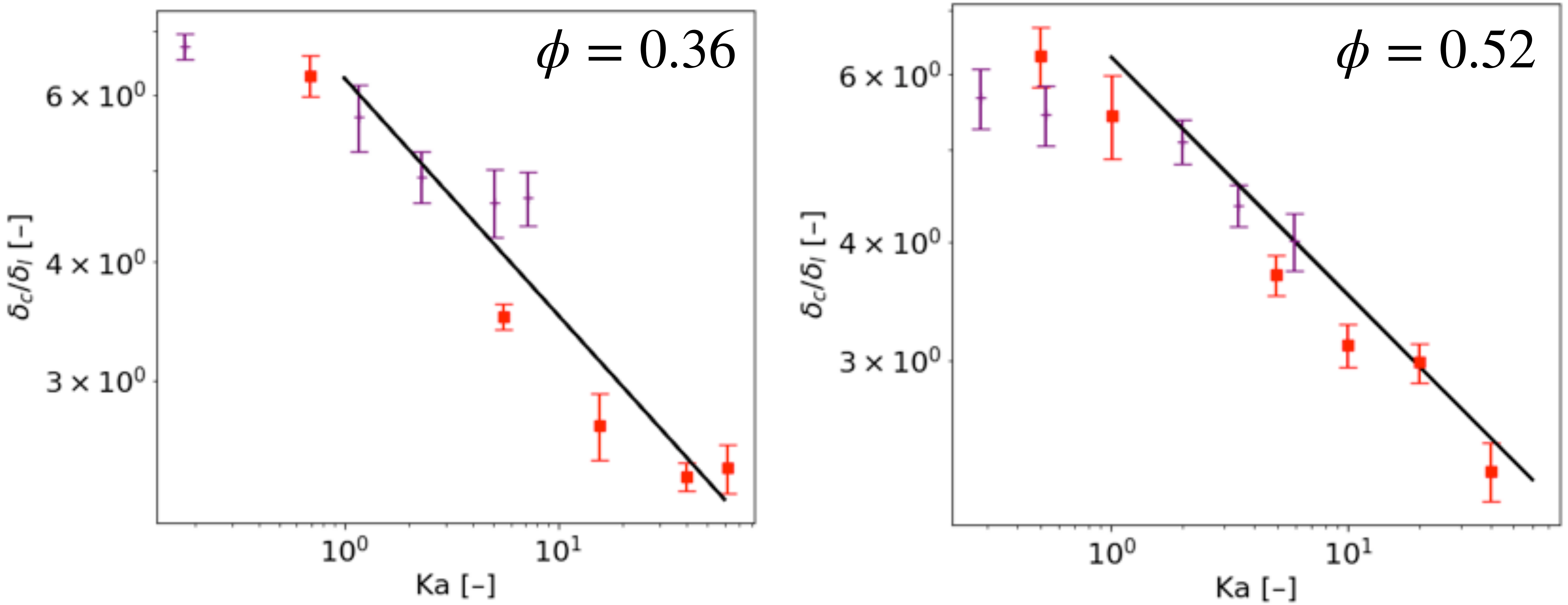


- The slope is consistent with findings from Hawkes et al., C&F, 2012: $\eta_i/\delta_l^0 \propto Ka^a$ a=0.22-0.265

Fractal analysis

Inner cut-off scale

- δ_l and Ka based on laminar un stretched quantities
    - Aspden et al. 2011, 2023 suggest to use laminar unstable quantities
- Following a similar idea: δ_l **and** Ka **based on effective stretched quantities** (measured by I_0)



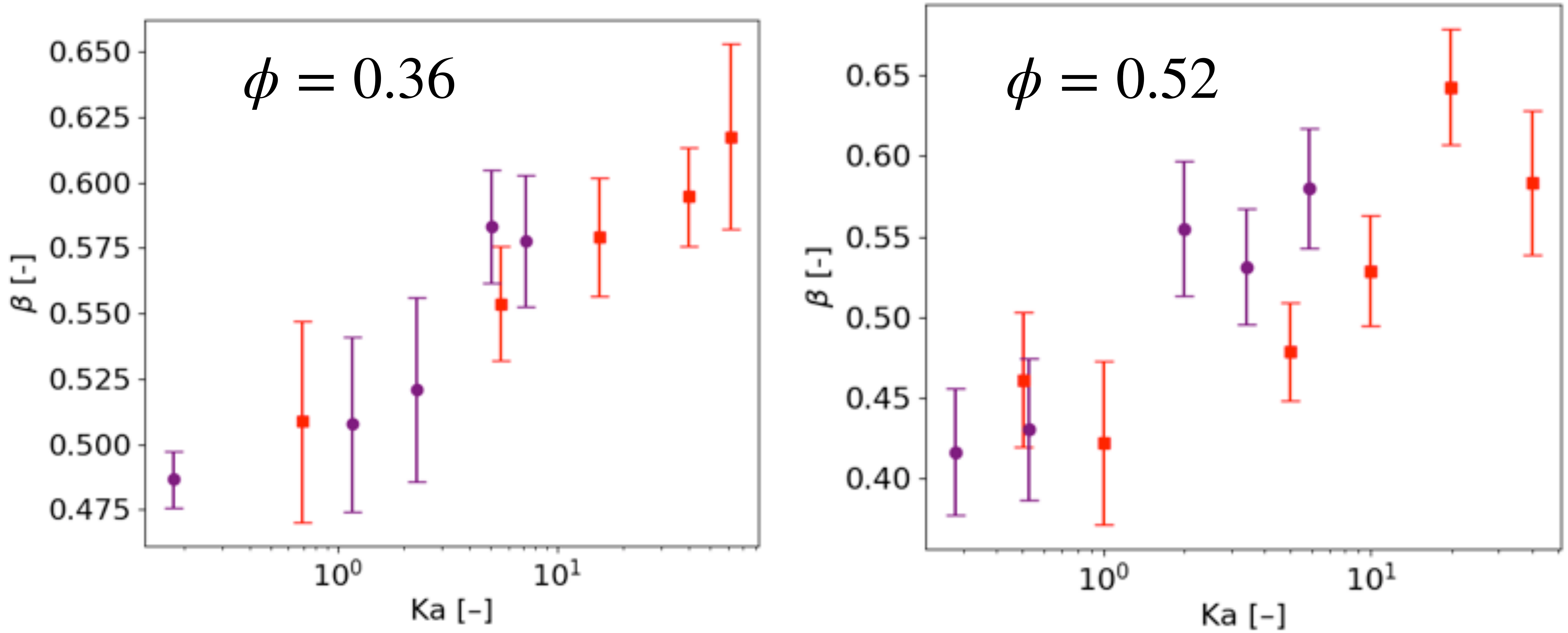
O Le1 chemistry

O LeRe chemistry

'stretched' scaling

Fractal dimension

Fractal dimension vs Karlovitz number



O Le1 chemistry

O LeRe chemistry

'stretched' scaling

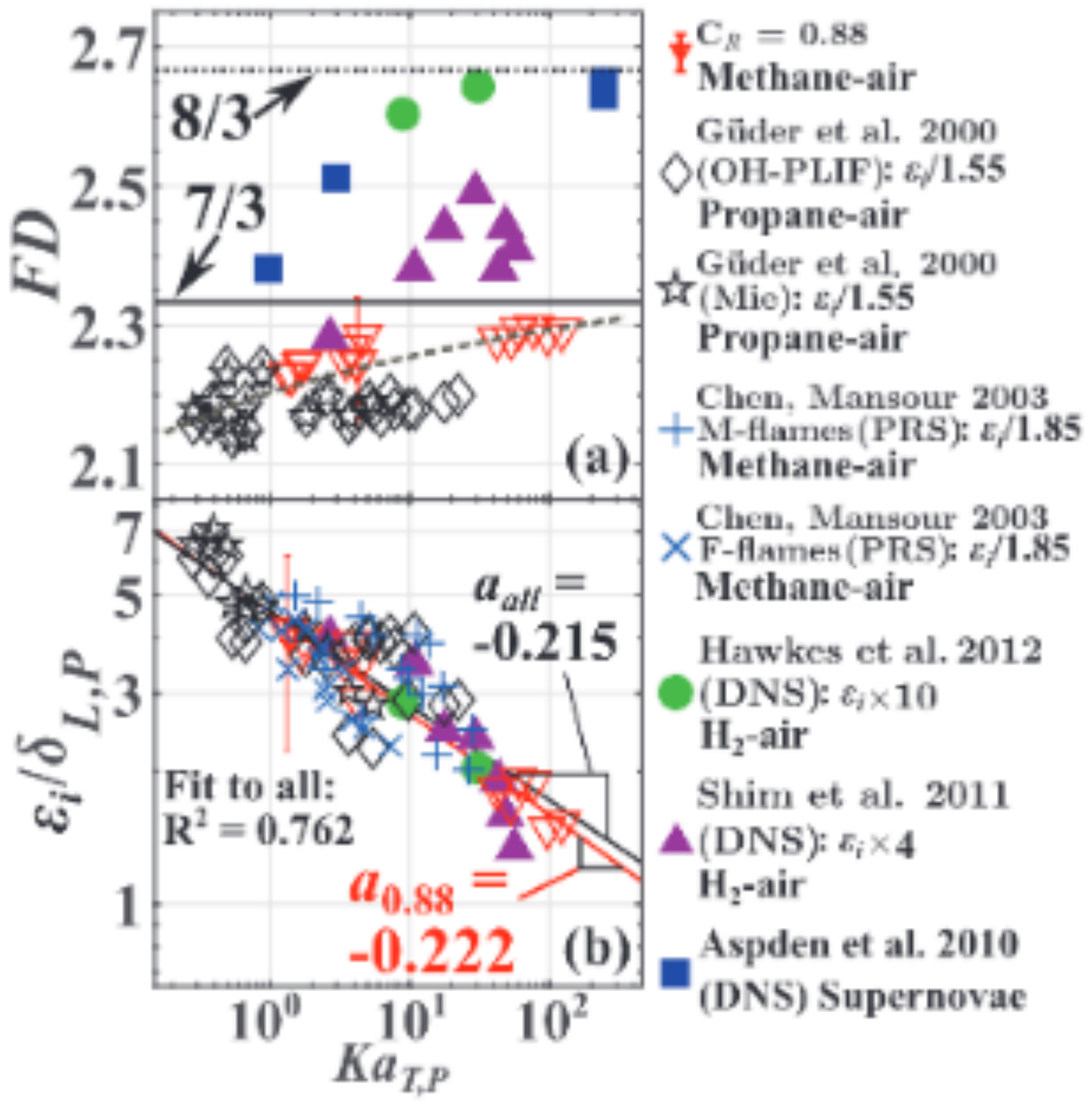
- Positive trend for fractal dimension vs. Karlovitz number
- Consistent with theoretical bounds: passive flame front limit $\beta = 0.67$

Fractal analysis

Summary

- Trends for Le1 cases largely consistent with the literature in terms of wrinkling
- Le<1 cases can be collapsed to Le1 with proper scaling by stretched laminar quantities implying
  - **Thinner cut-off scale**
  - Lower effective Karlovitz number (divided by ≈ 10 in our case, up to ≈ 20 in DNS of Aspden group) → **Lower fractal dimension**

Fractal dimension and inner-cutoff scale from various exp. and num. datasets (Skiba et al. PCI, 2020)



Key takeaways for modeling

- **Cellular instability:** significant in the low Ka limit (cellular wrinkling + stretch factor effect) where it is the main contributor to small-scale wrinkling
  - **MOD5 approach** ($S_T = \Xi_{turb} \times \Xi_{TD} \times I_0$) **may be valid for** $L_G >> \delta_l$ (hard to verify in DNS)
  - Buiding criterion for the significance of TD instability in turbulent flows? (Chomiak et al., Physical Review E, 2023)

- **Local reactivity enhancement** ('I_0'): synergistic effect between turbulence/TD effects
  - $I_0 \propto I_0^{TD,lam}(1 + \alpha\sqrt{Ka})$

- **Flame surface wrinkling:** High Karlovitz number = high turbulent stretching

  → thinner flame brush = lower inner cut-off

  → lower effective Karlovitz number = lower fractal dimension

  - Overall trend = more wrinkling