Length Scale Effects in Thermodiffusively-Unstable Turbulent Lean Premixed Hydrogen Flames

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Recap of Andy's 12:35 Talk

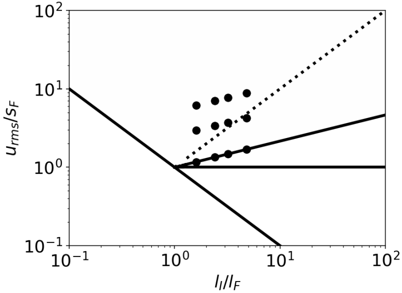
Thermal Leading Points in Thermodiffusively-Unstable Lean Premixed Hydrogen Flames:

- Evaluated the local flame response for varying pressure, temperature and equivalence ratio for thermodiffusively unstable H_2 flames
- Studied the local flame statistics:
  - Freely propagating mean local flame speed thickness (s_F, l_F)
  - Turbulent mean local flame speed and thickness (s_s, l_s)
- Developed a model for predicting local flame quantities s_F, s_s, l_F, l_s based of P, T, ϕ from 1D (Cantera) simulations
- Carried out at fixed integral length scale and domain size $(\Omega_F = \frac{L_x}{l_F} = 16, \Lambda = \frac{l_I}{l_F} = 1.6)$
- Did not look at global flame surface area and turbulent flame speed

Simulation Conditions

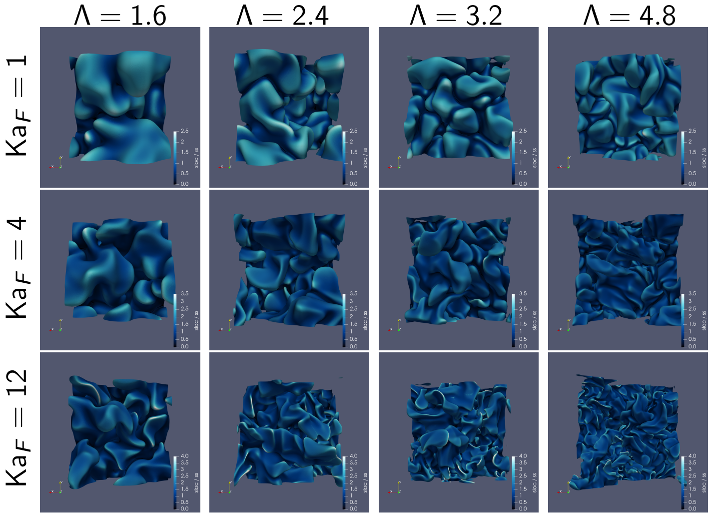
- 3D DNS of turbulent lean hydrogen combustion using PeleLM [1]
- Complex chemistry with Burke et al. H_2 mechanism [2]
- Maintained homogeneous isotropic turbulence
- $P = 40\,\text{atm},\ T = 700\,\text{K},\ \phi = 0.4$ and $L_x/l_I = 10$

$\Omega_F = \frac{L_x}{l_F}$	$\Lambda = \frac{l_I}{l_F}$	Ka_F	Da_F	$\frac{u}{s_F}$
16	1.6	1	1.37	1.17
		4	0.54	2.95
		12	0.26	6.13
24	2.4	1	1.79	1.33
		4	0.71	3.37
		12	0.34	7.02
32	3.2	1	2.17	1.47
		4	0.86	3.71
		12	0.41	7.72
48	4.8	1	2.85	1.69
		4	1.13	4.25
		12	0.54	8.84

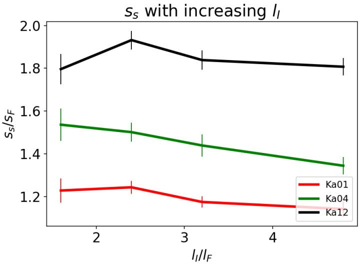


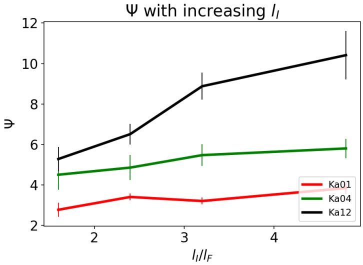
[1] M. S. Day and J. B. Bell. Numerical simulation of laminar reacting flows with complex chemistry.Combustion Theory and Modelling, 4(4):535–556, 2000.
[2] Michael P. Burke, Marcos Chaos, Yiguang Ju, Frederick L. Dryer, and Stephen J. Klippenstein. Comprehensive H2/O2 kinetic model for high-pressure combustion. International Journal of Chemical Kinetics, 44(7):444–474, 2012.

Flame Surfaces (local flame speed)



Mean local flame speed and flame surface wrinkling with varying integral length scale and Ka





Mean local flame speed (s_s):

- Strongly dependent on Ka
- Largely independent from integral length scale l_I
- Perhaps slight decrease with l_I (possibly constrained)

Wrinkling factor (Ψ):

- Increases with length scale
- More so with increasing Ka

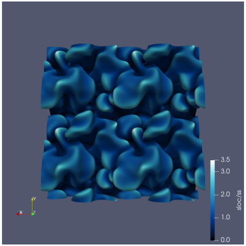
Effect of domain size

- Separate out the differences between integral length scale and domain size effects
- New condition highlighted in blue (below)
- The domain size was doubled from $16l_F$ to $32l_F$
- The integral length scale was fixed at $1.6l_F$

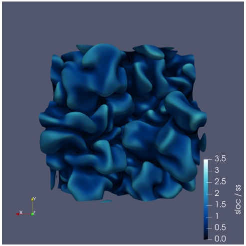
$\Omega_I = \frac{L_x}{l_I}$	$\Lambda = \frac{l_I}{l_F}$	$\Omega_F = Lx/l_F$	p (atm)	T (K)	ϕ	ω_2	s_F (m/s)	l_F (μm)
10	1.6	16						
20	1.6	32	40	700	0.4	5.58	0.56	0.0187
10	3.2	32						

Flame Surface Images (local flame speed)

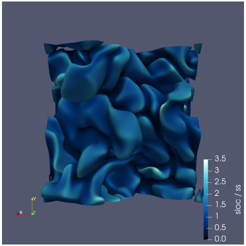
(a) $\Lambda = 1.6, \Omega_l = 10$



(b) $\Lambda = 3.2, \Omega_l = 20$

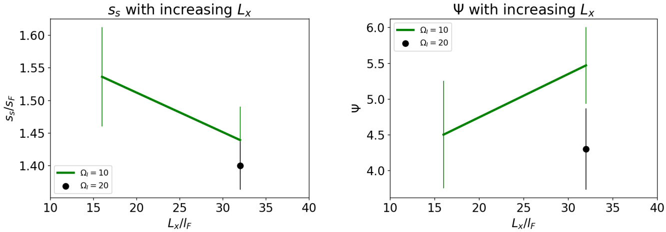


(c) $\Lambda = 3.2, \Omega_l = 10$



- Local flame speed looks mostly the same in all cases
- Slightly stronger leading points in (a)
- Small difference in flame structure with large integral length scale (c)
- Surface (b) flame structure looks to be an intermediate between (a) and (c)

Mean local flame speed and flame surface wrinkling with varying integral length scale and domain size



Mean local flame speed (s_s):

- Largely independent of integral length scale
- Elevated value at small L_x suggests constrained by domain size
- Thermodiffusive effect (not expected for $\mathrm{Le} = 1$)

Wrinkling factor (Ψ):

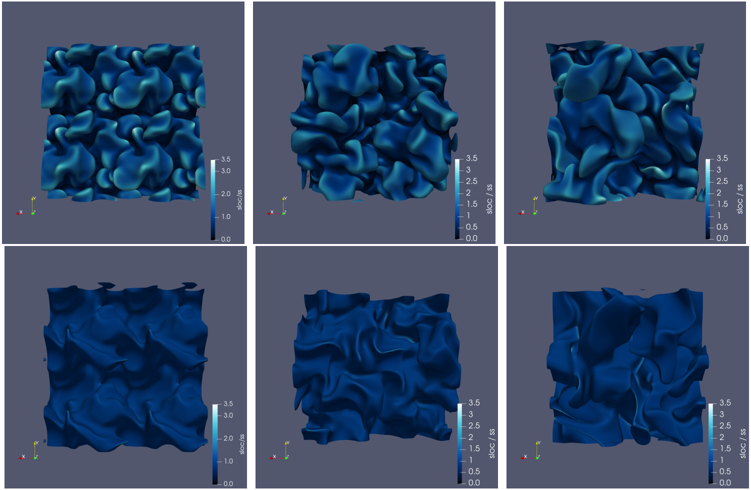
- Increased with integral length scale but not domain size

Comparison with Unity Lewis Number

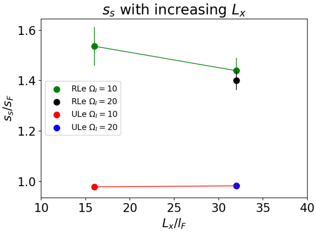
$\Lambda = 1.6, \Omega_l = 10$ | $\Lambda = 3.2, \Omega_l = 20$ | $\Lambda = 3.2, \Omega_l = 10$

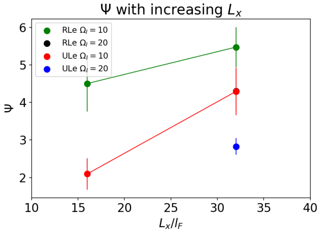
Real Le

Unity Le



Mean local flame speed and flame surface wrinkling with varying domain and integral length





Mean local flame speed (s_s):

- Near zero local flame speed variation at unity Lewis number

Wrinkling factor (Ψ):

- Strongly increases with integral length (and domain size)
- Also increases with domain size at fixed integral length
- Need to consider domain size, which is usually ignored

Turbulent Flame Speed With Peters' Model

Peters' turbulent flame model (Turbulent Combustion, 2000):

- One of the recommended turbulent flame models in Ricardo's Vectis
- Included terms for integral length scale
- $s_T = s_X \left(1 - \mathcal{A}_1 \frac{l_I}{l_Z} + \left[(\mathcal{A}_1 \frac{l_I}{l_Z})^2 + \mathcal{A}_2 \frac{u_{\mathrm{rms}} l_I}{s_Y l_Z}\right]^{\frac{1}{2}}\right) = s_X \Psi_{Y,Z}$
- $\mathcal{A}_1$ & $\mathcal{A}_2$ unmodified model constants

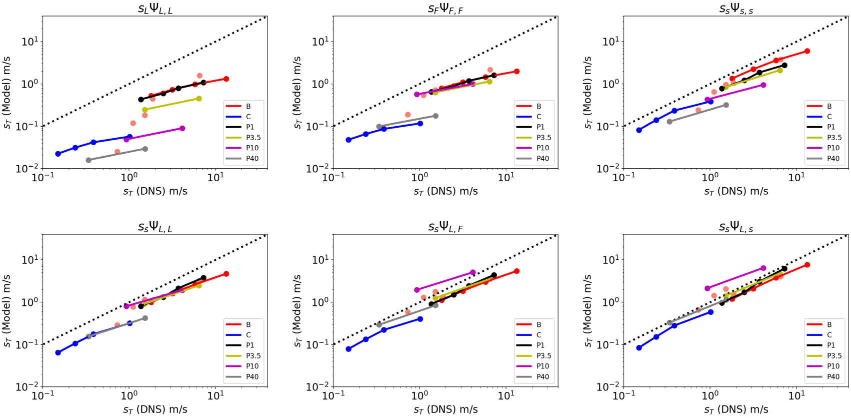
Modelling parameters:

- Prefactor flame speed s_X
- Wrinkling factor flame speed s_Y
- Wrinkling factor thermal thickness l_Z

Each parameter can take one of three values: (obtainable from Cantera)

- 1D laminar value (s_L, l_L)
- Modelled freely-propagating values (s_F, l_F)
- Modelled mean local values form (s_s, l_s)

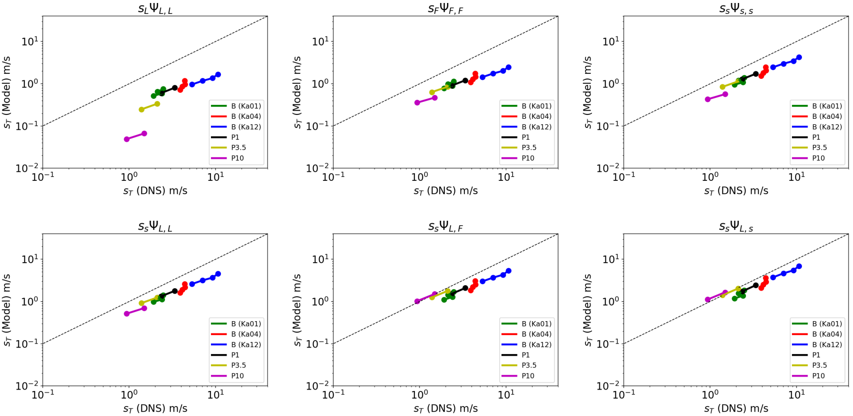
Fixed $l_I / l_F = 1.6$ Cases from Andy's Talk



- Free-prop prefactor captures bulk of thermodiffusive underprediction
- Accounting for $\sqrt{\mathrm{Ka}_F}$ dependence fixes gradient
- Modifying Ψ to account for thickness (not speed) produces best agreement

Turbulent Flame Speed Model - With Varying l_l/l_F

- Cases presented earlier are denoted as set "B" ($\mathrm{Ka}_F = 1-12$)
- Additional Ka_F cases at 300K, $\phi = 0.4$ at pressures 1, 3.5 and 10 atm



- Similar trends observed here over range of length scales
- Good agreement over broad range of conditions ($\omega_2 \approx 5-27$)

Conclusion

- Mean local flame speed:
  - Strongly dependent on Ka_F
  - Largely independent from integral length scale
  - Small domain sizes can constrain the flame (slightly higher s_s)
  - Particular feature of thermodiffusively unstable flames
- Flame surface wrinkling:
  - Increases with integral length scale, more so with Ka_F
  - There is a domain-dependence that is usually ignored
- Implications for turbulent flame modelling:
  - Crucial to account for thermodiffusive local flame acceleration
  - Wrinkling appears to depend on flame thickness (rather than speed)
  - Predictive model can by formulated based on Cantera (no DNS)
  - Good agreement over a large range of P, T, ϕ