Lewis number and pressure effects on weakly turbulent premixed Bunsen flames – Direct Numerical Simulation studies

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Outline

- Motivation
- Challenges
- Mathematical background
- Overview of work conducted
- DNS of lab scale Bunsen burner
- Results

Motivation

1

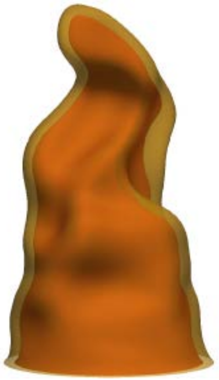
increasing P

P

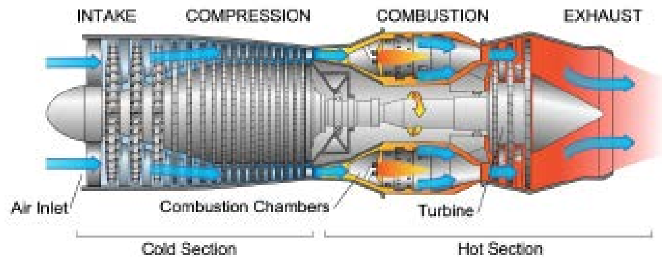
1

decreasing Le

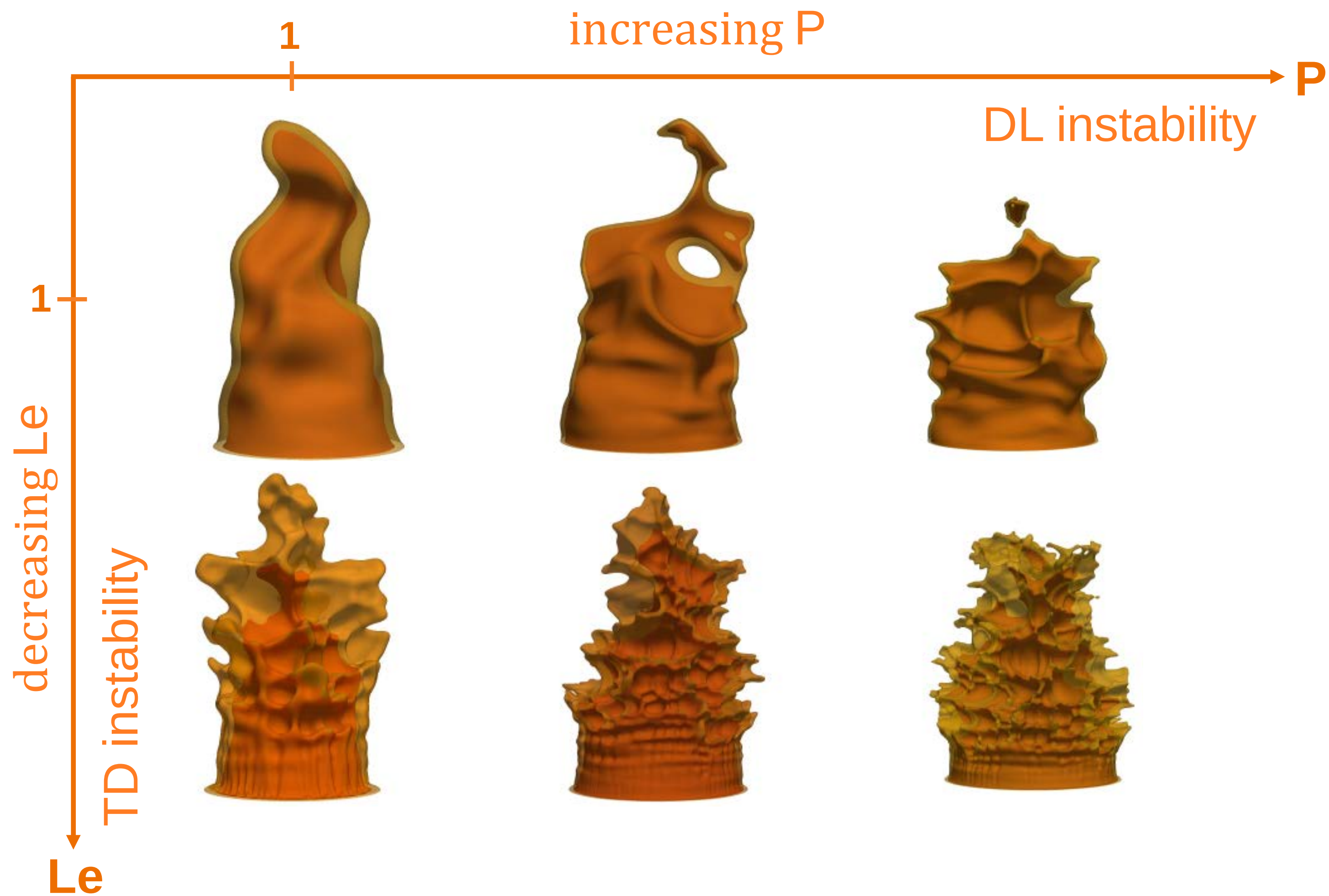
Le



largest knowledge



H_2


1
increasing P
P
DL instability
1
decreasing Le
TD instability
Le

Challenges

- Resolution requirements increase with increasing pressure:
  - For hydrocarbon-air flames: $S_L \sim p^{-0.5}, \nu \sim p^{-1}$
  - Fixed burner geometry; if $l, u'/S_L = const \Rightarrow Re_t \sim p^{0.5}$
  - Furthermore, $\delta_L = D/S_L^0 \sim p^{-0.5}$
  - Fixed geometric dimensions → realistic scale separation
  - $p = 1\text{bar} \rightarrow 20\text{bar}$ computational extra cost: $(20^{0,5})^4 = 400$

- Evaluation of turbulent flame speed requires long integration times

$$S_T = \frac{1}{\rho_u A_L} \int_V \dot{\omega}_c \, dV$$

- Modelling requires parametric studies: $P, Le, \frac{u'}{S_L}, \frac{l}{\delta_{th}}$, ...
- DNS of lab scale burner

In this work we use (mostly) simple chemistry (SC) DNS because

- it would be nearly impossible to use detailed chemistry transport for this large parametric study including elevated pressures
- it would have a tremendous carbon footprint (ten thousands kg CO_2)
- results from detailed chemistry can be ambiguous due to different choices of reaction progress variable
- analysis does neither involve emissions nor ignition
- flame propagation and turbulence chemistry interaction can be captured with SC
- there is no correct model for chemistry and transport but different levels of approximation

Mathematical Background

- 3D compressible DNS code with
- Single step irreversible Arrhenius type chemistry
- 10^{th} order special discretization dropping to one sided 2^{nd} order
- Third order low-storage Runge-Kutta scheme
- Very efficient variant of digital filter based synthetic inflow
- Hyperbolic-tangent like mean velocity profile
- Partially non-reflecting outflow everywhere else (NSCBC)
- Viscosity & Arrhenius parameters such that: $S_L \sim p^{-0.5}, \nu_u \sim p^{-1}$

Overview of work conducted

Physics

Modelling

Damköhler's 1st and 2nd hypothesis

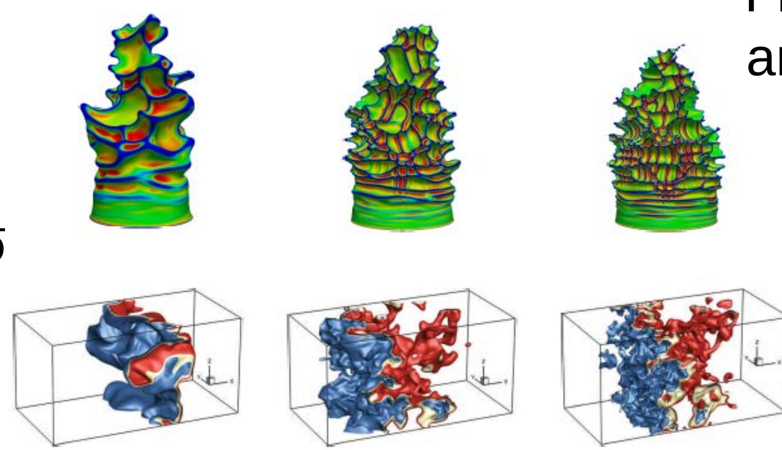
Bending of S_t

Statistics of $|\nabla c|$ and a_T

TD and DL instabilities

Flame curvature and its transport

Machine learning based closure of $\overline{\omega}$



turbulent flux $\bar{\rho}(\widetilde{u_i c} - \tilde{u}_i \tilde{c})$

Modelling of S_t

scalar variance $\widetilde{c^2} - \tilde{c}^2$

SGS scalar dissipation $\overline{\rho D \nabla c \cdot \nabla c}/\bar{\rho} - \tilde{D} \nabla \tilde{c} \cdot \nabla \tilde{c}$

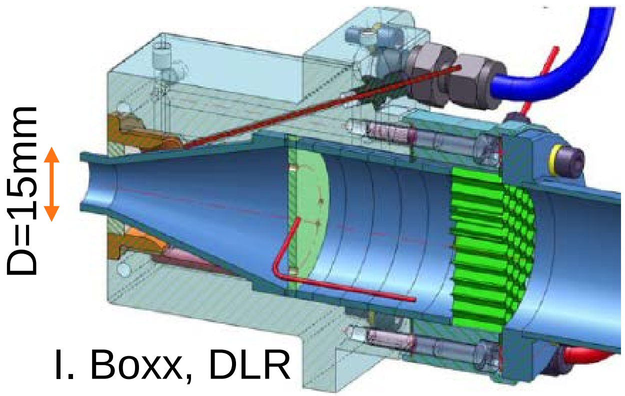
Fractal analysis and modelling

Transport of Σ_{gen}

Algebraic models of FSD, Σ_{gen}

DNS of lab scale Bunsen burner

- Database consists of three atmospheric Bunsen flames
- Varying H_2 content in CH_4 (by volume)
- Low turbulence intensity to focus on flame instabilities



I. Boxx, DLR

Case A (0%)

Case B (40%)

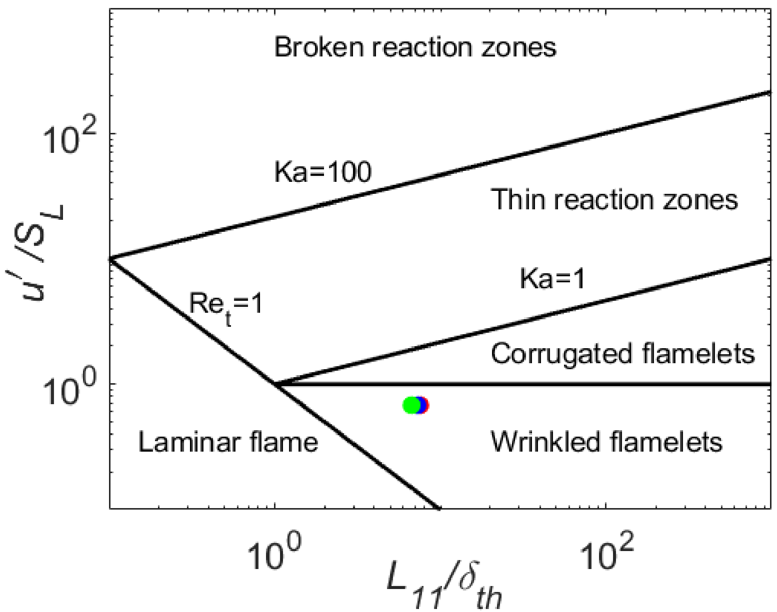
Case C (70%)

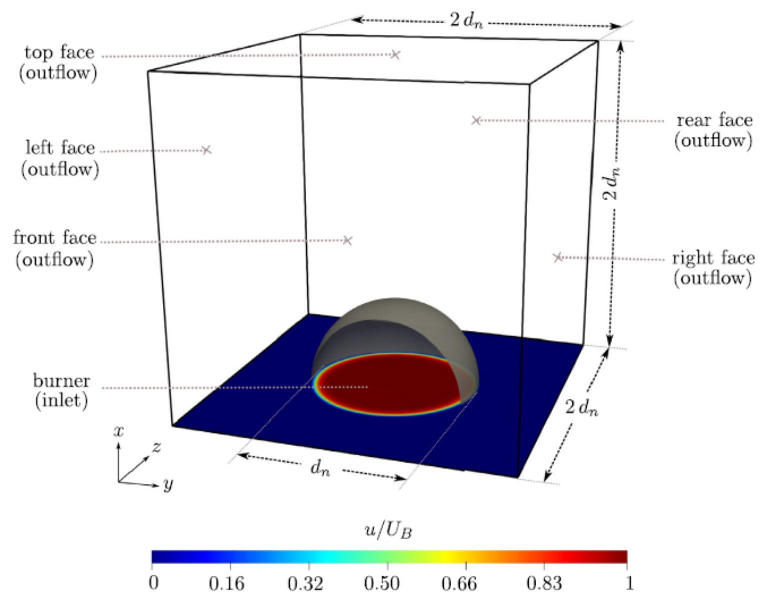
Case	ϕ	$H_2[\%]$	$U_0\ [m/s]$	$S_L[m/s]$	$T_{ad}\ [K]$	$\delta_{th}[mm]$
A	1.0	0	2.13	0.3654	2229	0.4063
B	0.8	40	2.18	0.3665	2026	0.4112
C	0.65	70	2.12	0.3456	1818	0.4474

U_b	u'	l_0	D	u'/S_L	l_0/D
$2.12\ m/s$	$0.25\ m/s$	$3mm$	$15mm$	0.68	$1/5$

Re	Re_t	Da	Ka
$1838-1987$	$40.89-46.57$	$9.83-10.82$	$0.21-0.22$

Grid: $750 \times 750 \times 750$, $\delta_{th}/\Delta x > 9$, $\Delta x/\eta > 0.4$





There are different ways to determine an effective Lewis number

Following Bechthold & Matalon (for lean mixtures):

$$Le_{eff} = 1 + \frac{(Le_F - 1) + (Le_O - 1)A}{1 + A} \qquad A = 1 + \beta\left(\frac{1}{\phi} - 1\right)$$

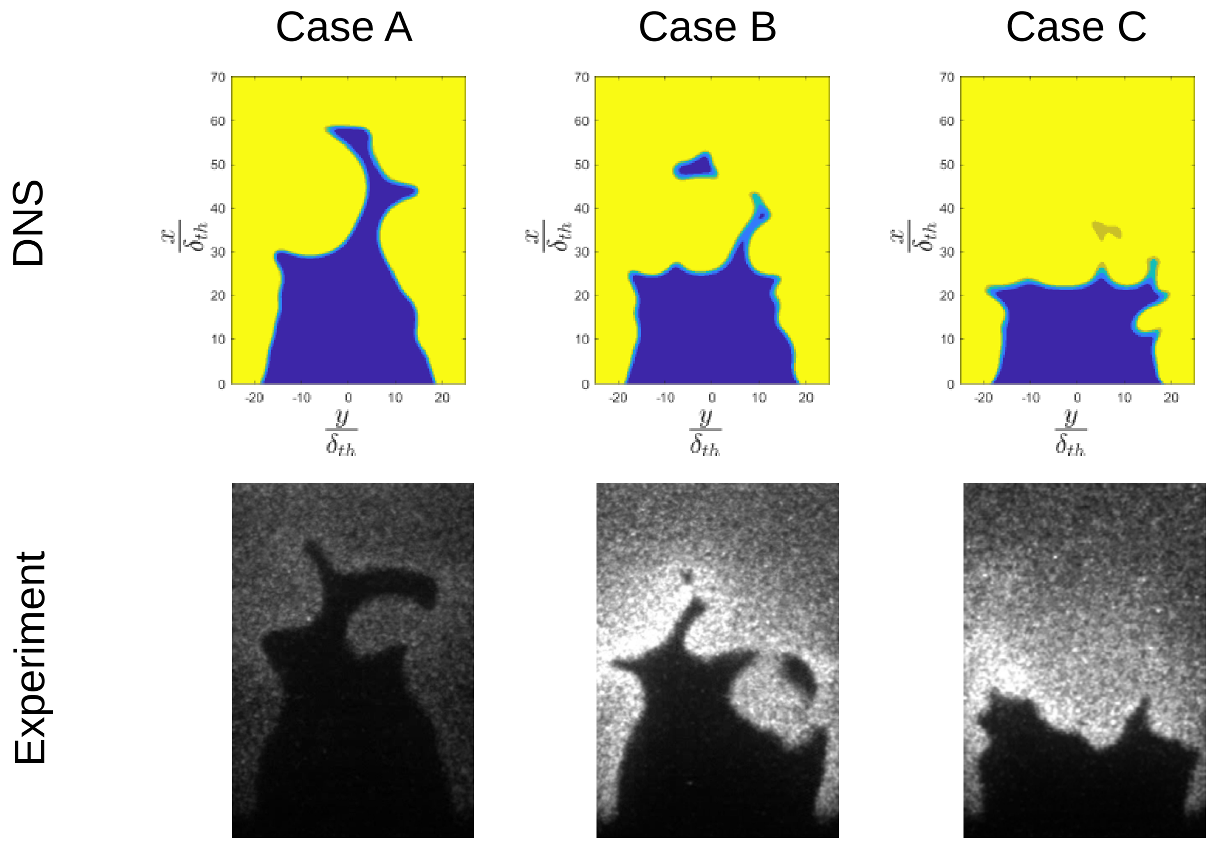
Weak sensitivity to Zel'dovich number β. Here $\beta = 6$ from experiment.

For the fuel Lewis number among different options we use the formula by Dinkelacker et al.

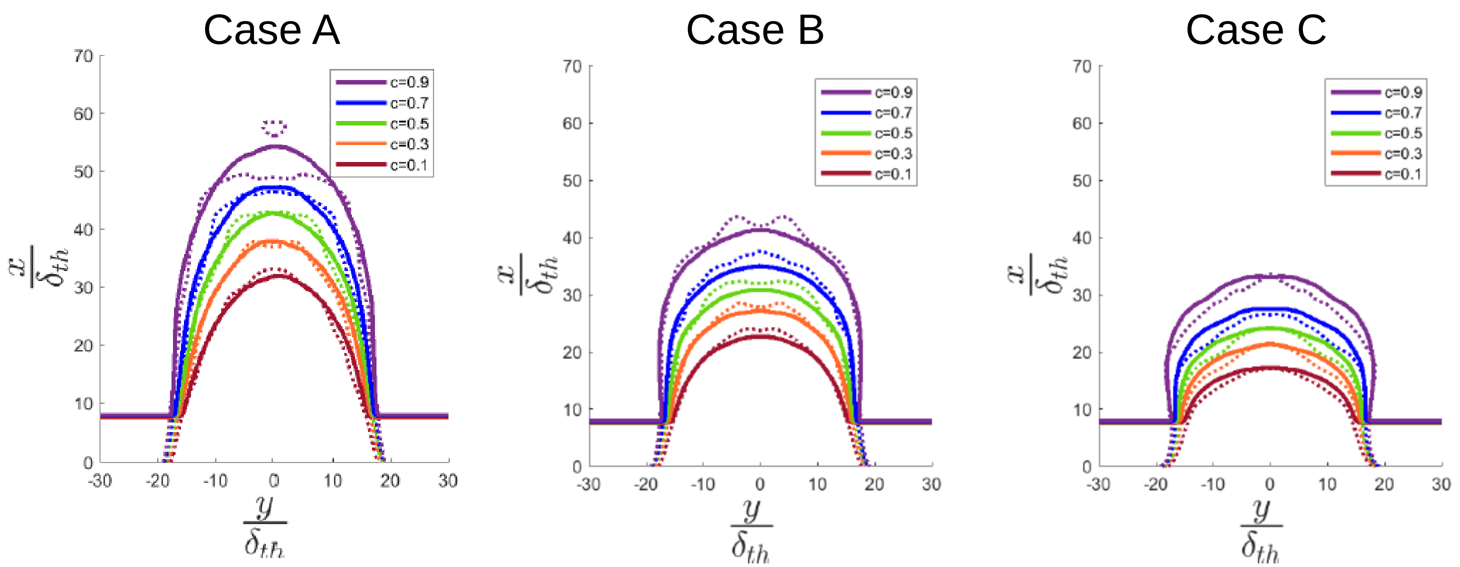
$$\frac{1}{Le_F} = \frac{x_{CH_4}}{Le_{CH_4}} + \frac{x_{H_2}}{Le_{H_2}}$$

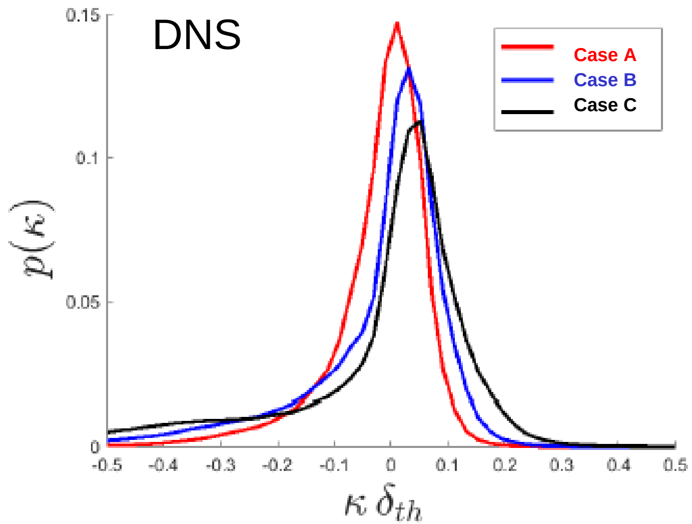
Case	ϕ	Le_{CH_4}	Le_{H_2}	Le_{O_2}	Le_F	Le_{eff}	DNS
A	1.0	0.96	0.29	1.11	0.96	1.04	1.0
B	0.8	1.08	0.32	1.24	0.55	0.75	0.8
C	0.65	1.21	0.34	1.36	0.44	0.61	0.6

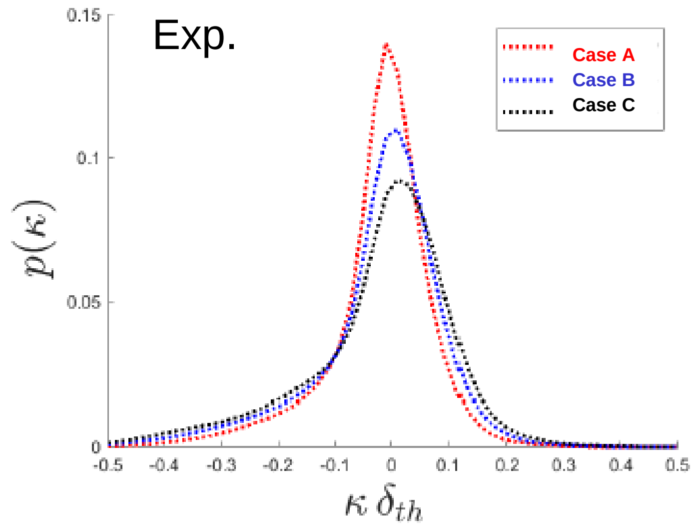
Instantaneous snapshots of flame contours



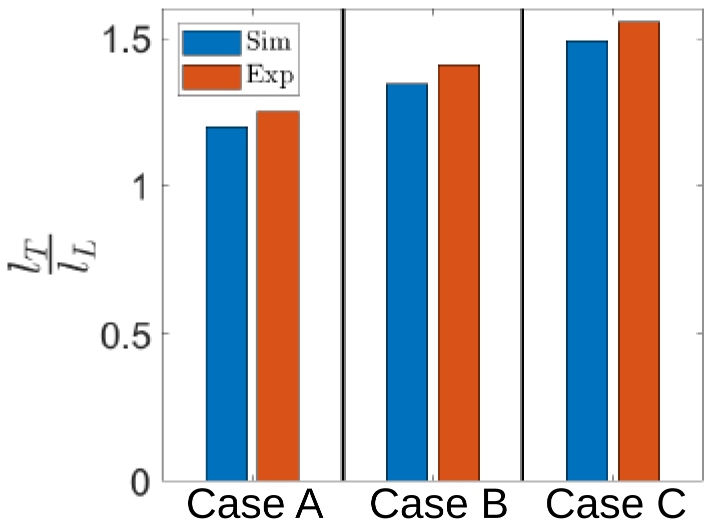
Mean flame contours

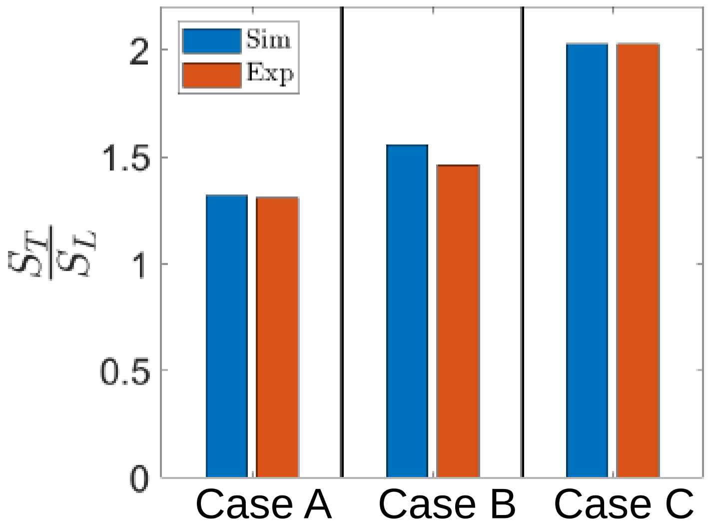






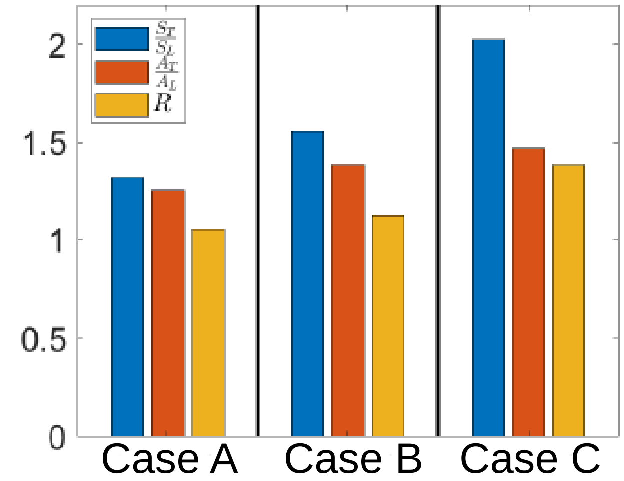
Turbulent flame wrinkling, flame speed, Damköhler‘s hypothesis





$R = (S_T S_L)/(A_T/A_L)$

Damköhler’s hypothesis: $R = 1$



Conclusions & Outlook

- A large DNS database has been generated including variations
  - of $u'/S_L\ , l/\delta_{th}\ , P, Le$
  - flame geometry
  - description of chemistry and transport (DC vs. SC)
- The data has been used by many researchers for understanding the physics and modelling the physics in the context of LES and RANS
- Simple chemistry with suitable Arrhenius parameters captures the flame propagation very well in comparison to experiment
- Quantitative comparison btw. experiment and simulation remains challenging because of different resolution and nature of data

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- More than 15 journal contributions, several conference papers
- 6 student theses
- Workshop on high pressure turbulent combustion (HPTC)
- Special issue in Combustion Science and Technology on HPTC

Thanks to LRZ !