

Turbulent Flame interaction with (i) droplets and (ii) inert walls

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Motivation and Objectives

Combustion of multiscale phenomenon:

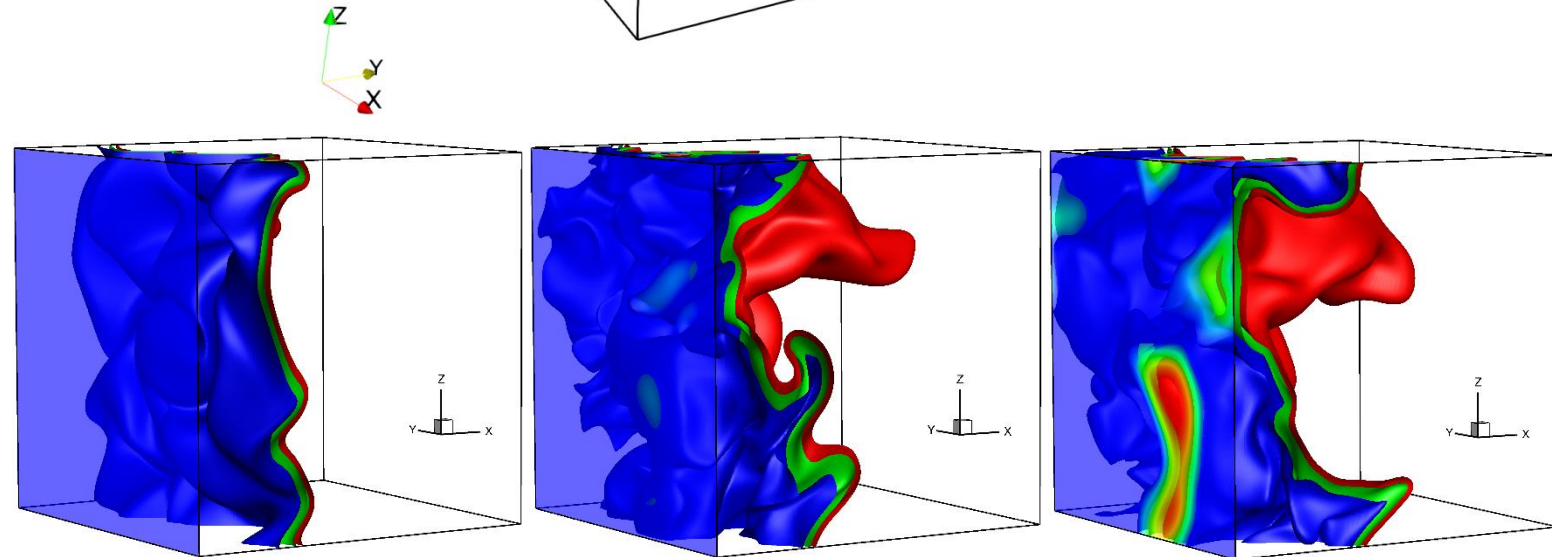
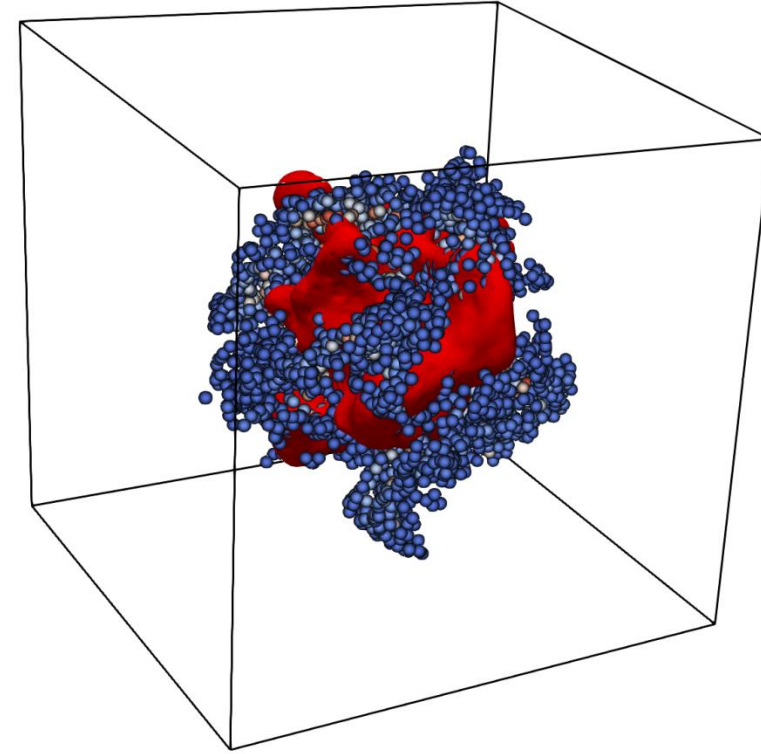
- Internal Combustion (IC) engines
- Gas turbines
- Industrial furnaces

Combustion of droplet-laden mixtures:

- Flame structure and wrinkling
- Evolution of flame surface area
- Evolution of burned gas volume

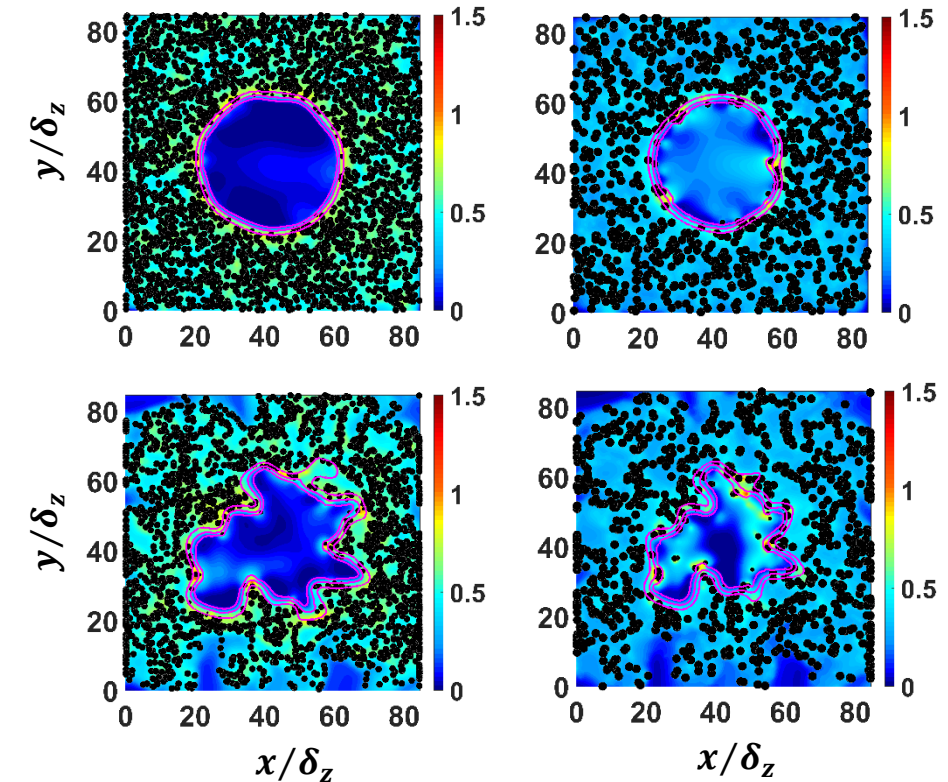
Flame-Wall interaction (FWI):

- FWI in fully developed boundary layer.
- Influence of wall boundary condition on the flame evolution.
- Comparison of flame surface evolution with statistically planar turbulent flames.



Direct Numerical Simulation

- Liquid phase-Lagrangian Approach is used for droplets following the approach proposed by Reveillon & Vervisch.
- Gaseous phase- Eulerian Approach is used to solve for gas phase combustion.
- Code: 3D,compressible DNS code, SENGAs
 - 10th order central difference scheme
 - Time advancement: Explicit low-storage 3rd order Runge-Kutta scheme.
- A single-step chemical mechanism is used.

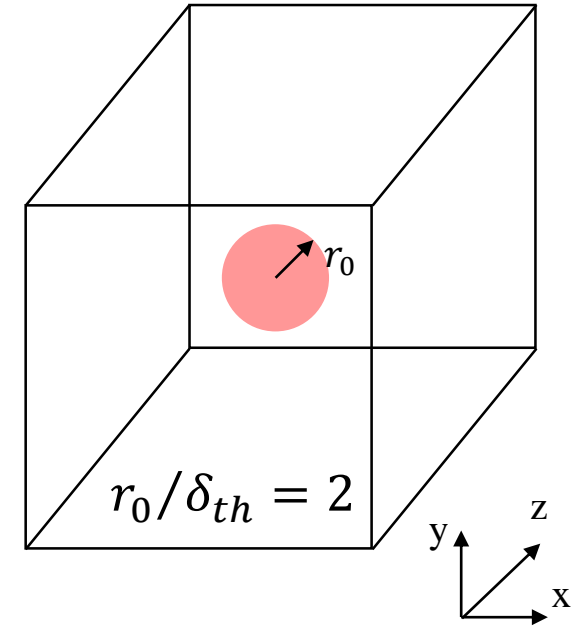


¹Reveillon, J., Vervisch, L.: Spray vaporization in non-premixed turbulent combustion modelling: a single droplet model. Combust. Flame 121, 75–90 (2000).

²Jenkins, K.W., Cant, R.S., Direct numerical simulation of turbulent flame kernels, 2nd AFOSR Conf. DNS and LES (1999).

Simulation set-up for spray flames

- 3D flame kernel simulations with droplet laden mixtures have been performed.
- Domain: $(84.49\delta_z)^3$ (where $\delta_z = \alpha_{T0}/S_{b(\phi_g=1)}$ is the Zel'dovich flame thickness)
- Grid number: $(512)^3$
- Initial turbulent field: Incompressible, homogeneous, isotropic (decaying turbulence).
- Reacting flow field initialisation: 1D steady state spray flame solutions (from COSILAB) specified in the radial direction.



Reaction progress variable:

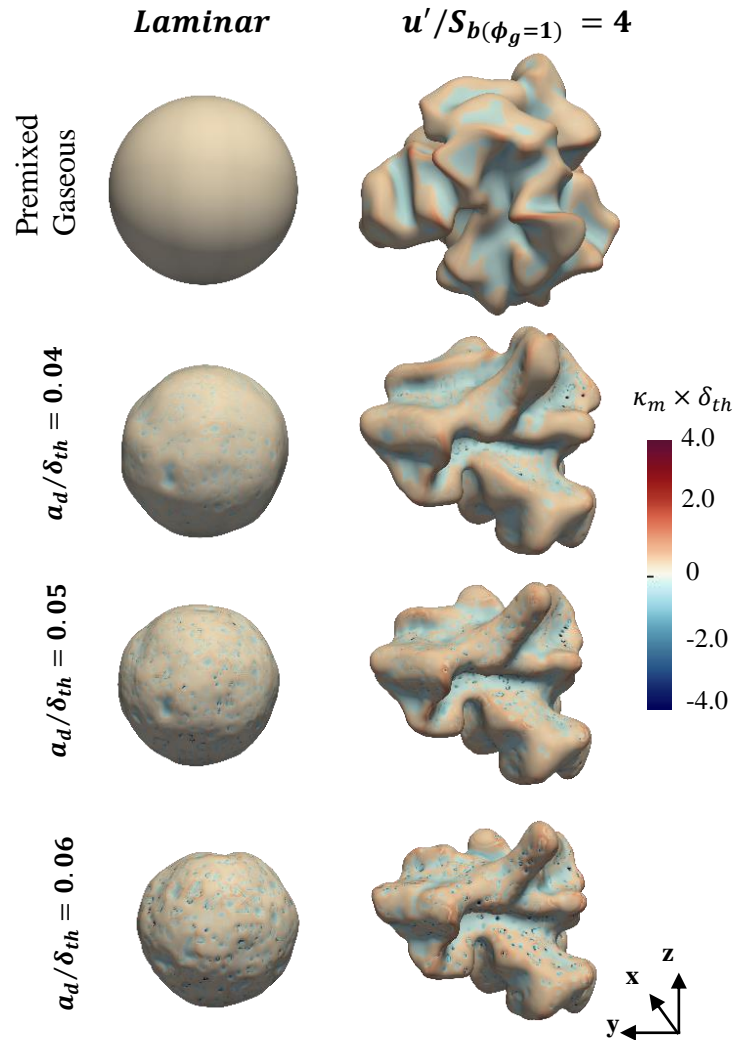
$$c = \frac{(1 - \xi)Y_{O\infty} - Y_O}{(1 - \xi)Y_{O\infty} - \max(0, [\xi_{st} - \xi]/\xi_{st})Y_{O\infty}}$$

Mixture fraction:

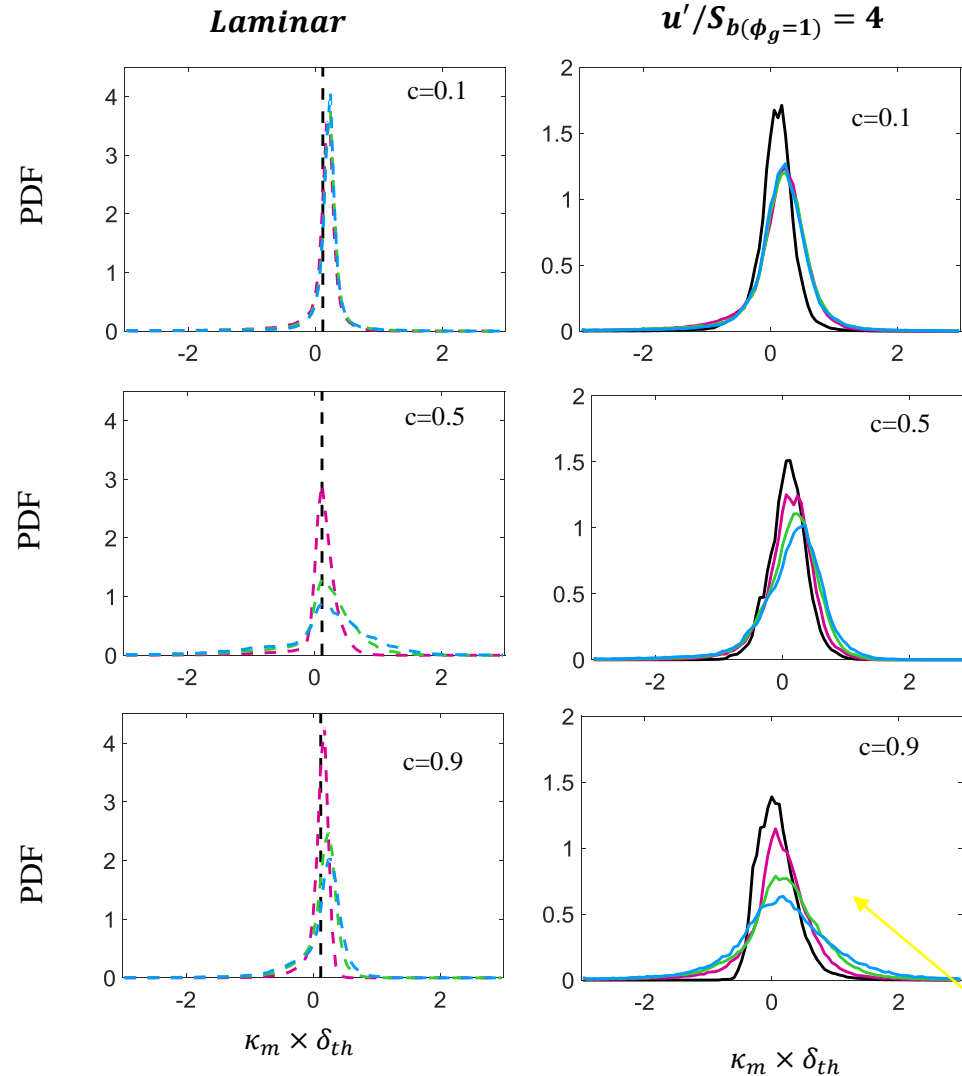
$$\xi = \frac{(Y_F - Y_O/s + Y_{O\infty}/s)}{(Y_{F\infty} - Y_{O\infty}/s)}$$

$u'/S_{b(\phi_g=1)}$	L_{11}/δ_{th}	a_d/δ_{th}	ϕ_{ov}	$\tau = \frac{T_{ad(\phi_g=1)} - T_0}{T_0}$
0, 4.0	2.5	0.04, 0.05, 0.06	1.0	6.54

Droplet Induced Wrinkling



Instantaneous view of $c = 0.5$ isosurface coloured with local values of $\kappa_m \times \delta_{th}$ at $t = 2.1t_{chem}$.



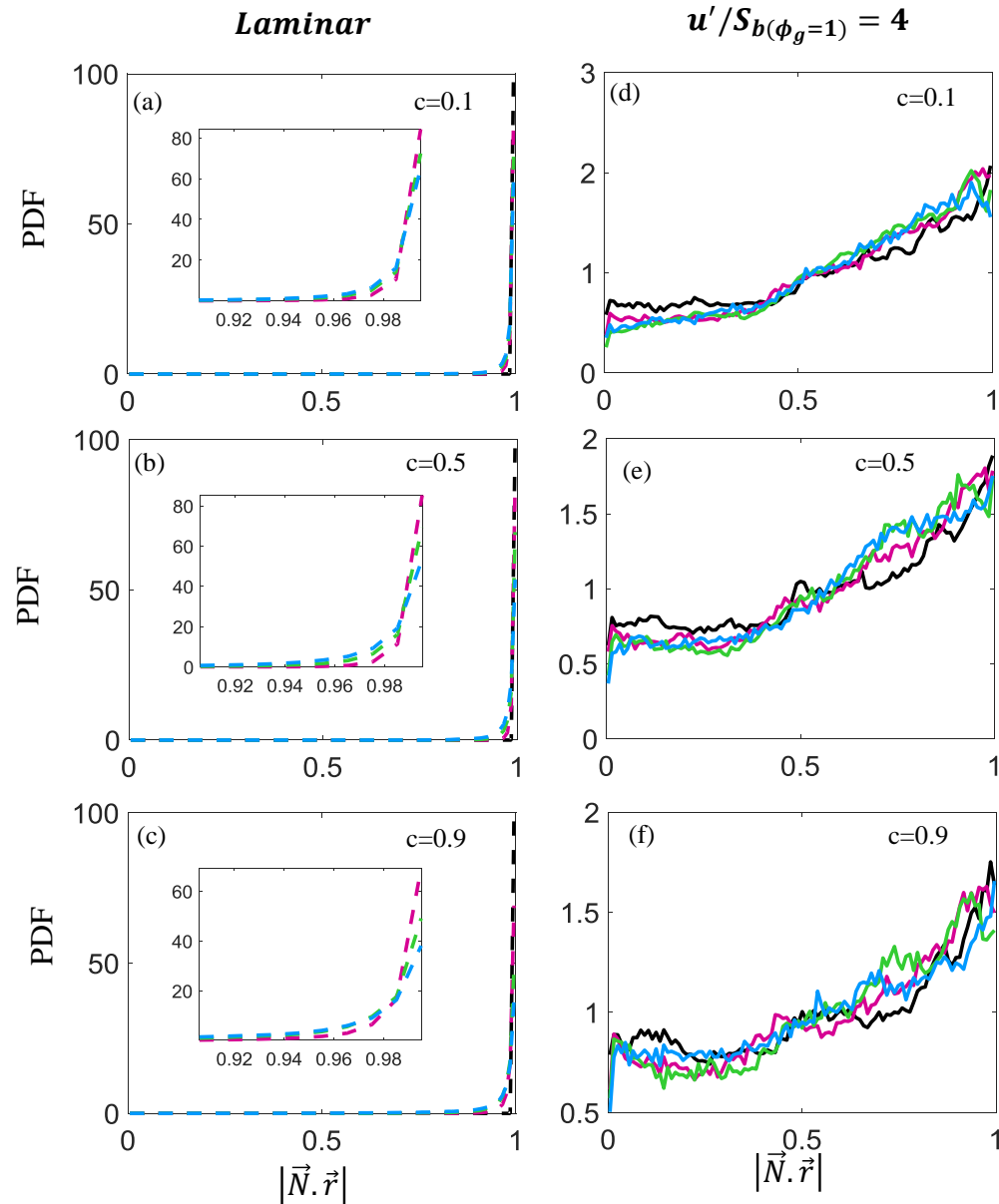
- Premixed Gas.
- $a_d/\delta_{th}=0.04$
- $a_d/\delta_{th}=0.05$
- $a_d/\delta_{th}=0.06$

$$\kappa_m = \nabla \cdot \vec{N}/2$$

$$\vec{N} = -\nabla c/|\nabla c|$$

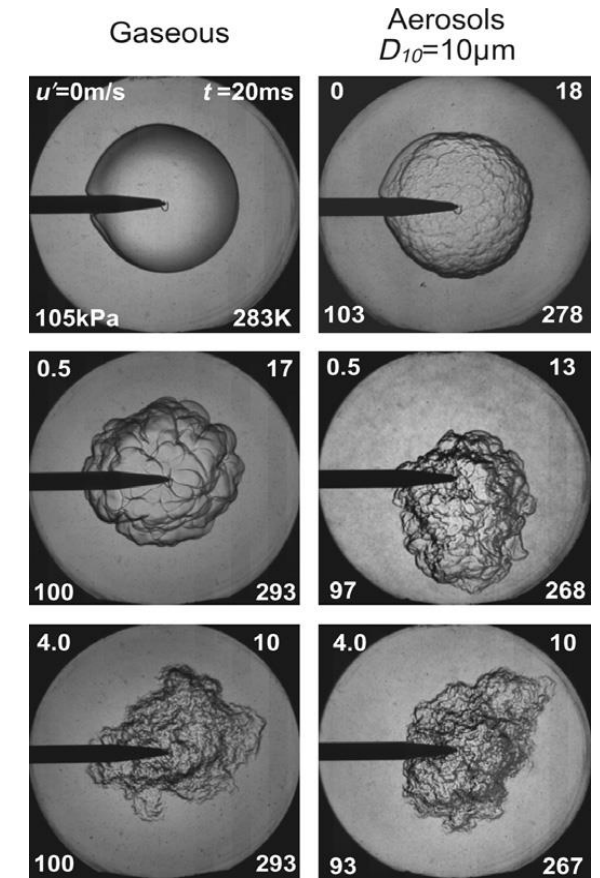
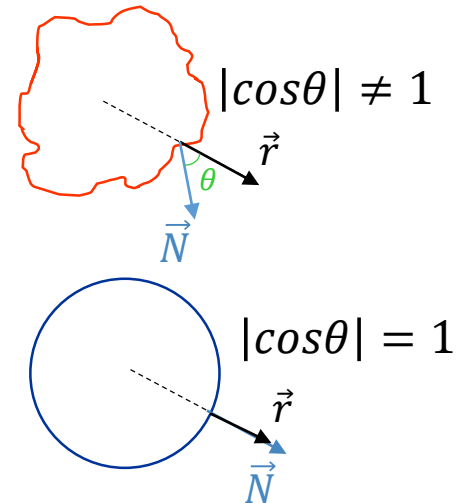
Prominent effect of large droplets

Flame Wrinkling



— Premixed Gas.
 — $a_d/\delta_{th}=0.04$
 — $a_d/\delta_{th}=0.05$
 — $a_d/\delta_{th}=0.06$

\vec{N} : local flame normal
 \vec{r} : unity radial vector from the center of mass of the flame kernel



Flame images from gaseous and aerosol flames at $\phi_{av}=1.2$ and different values of u' ¹

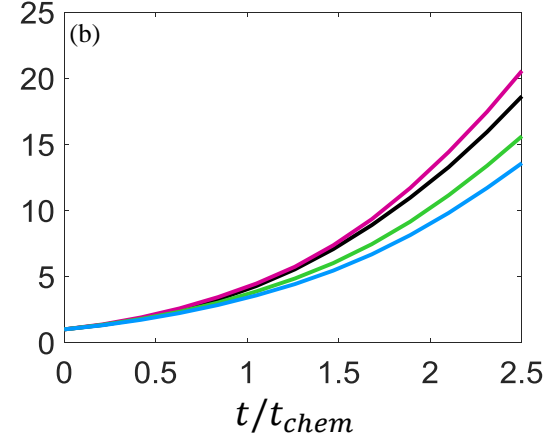
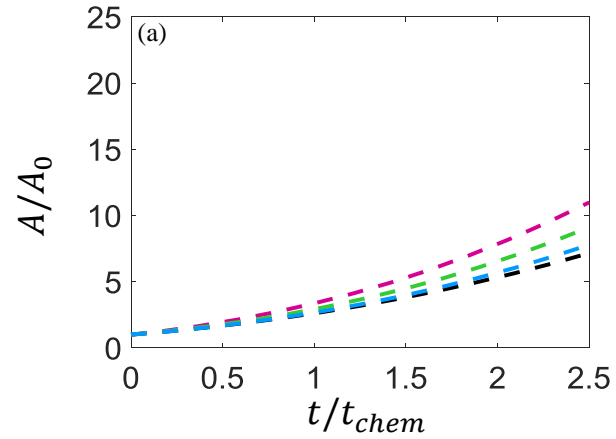
¹Lawes, M., Saat, A.: Burning rates of turbulent iso-octane aerosol mixtures in spherical flame explosions. Proc. Combust. Inst. 33, 2047–2054 (2011).

Evolution of flame surface area

— Premixed Gas. — $a_d/\delta_{th}=0.04$ — $a_d/\delta_{th}=0.05$ — $a_d/\delta_{th}=0.06$

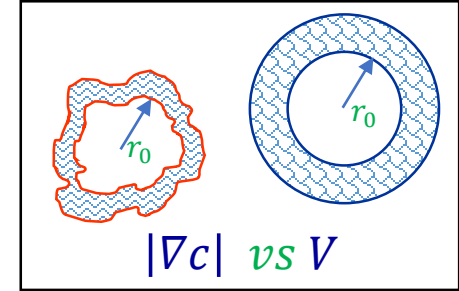
Laminar

$u'/S_{b(\phi_g=1)} = 4$

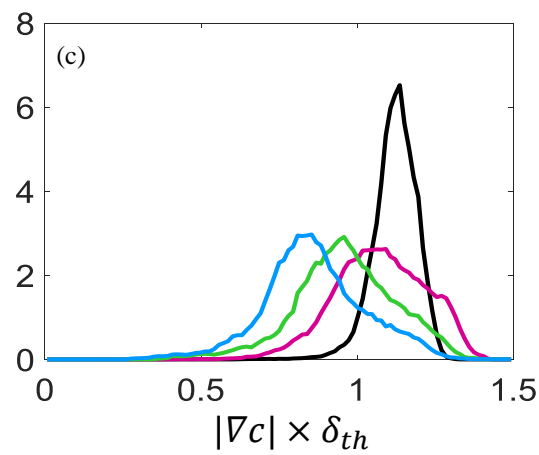
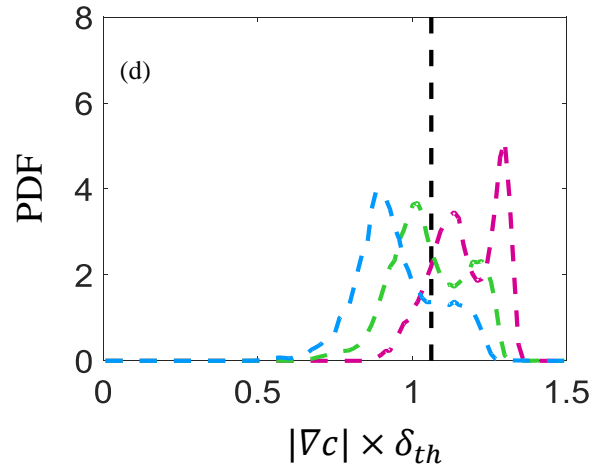


Flame surface area
normalised with its initial
value A/A_0

$$A = \int |\nabla c| dV$$



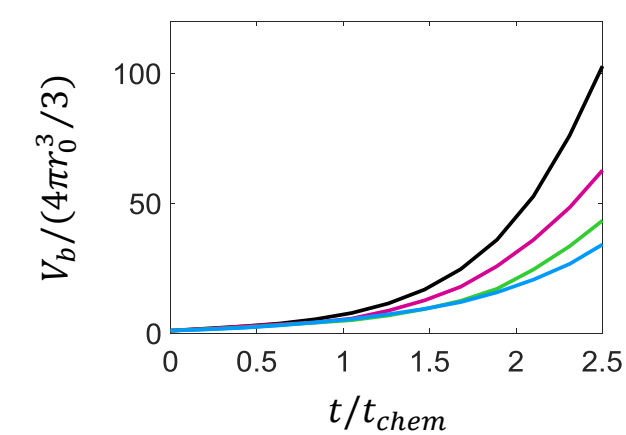
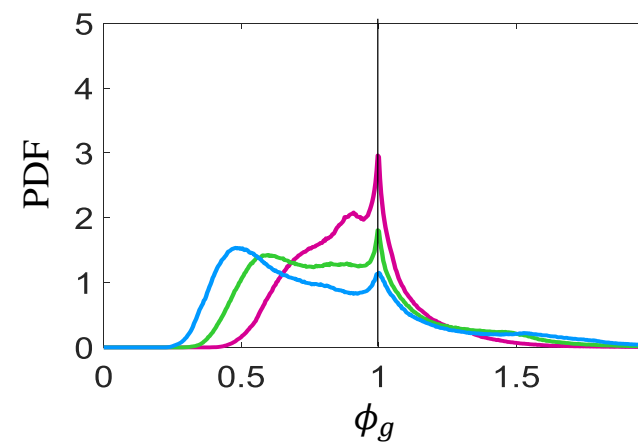
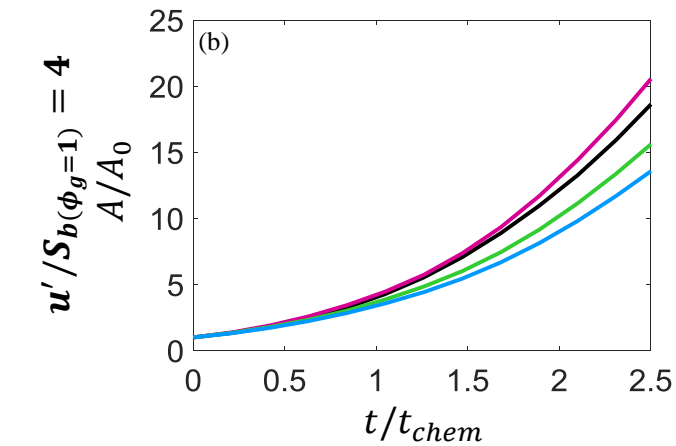
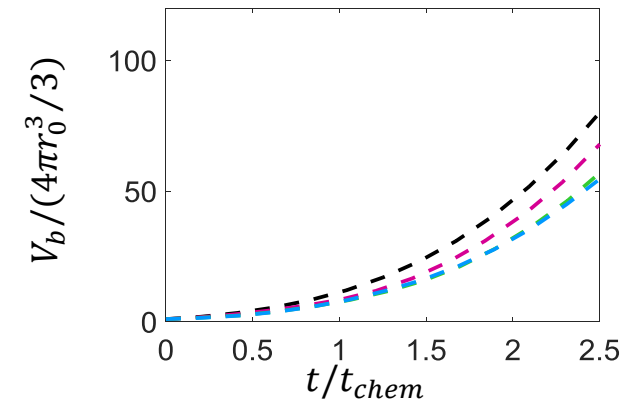
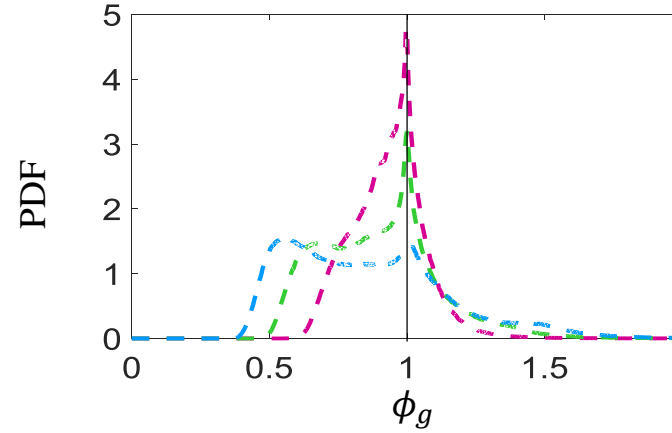
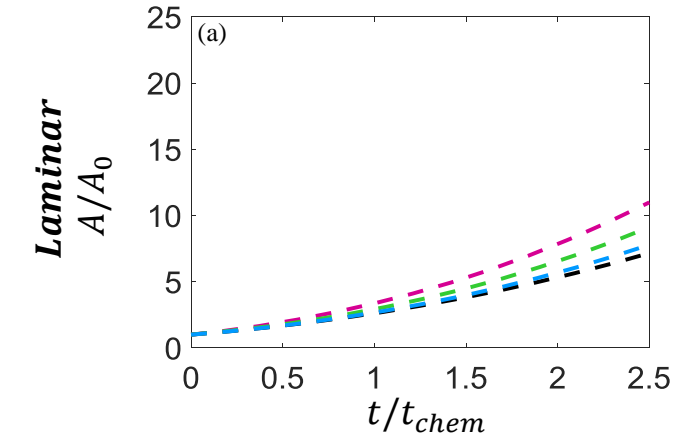
$A_0 \longrightarrow$ flame surface area A of a spherical laminar
flame of initial radius $r_0 = 2\delta_{th}$.



PDF of $|\nabla c| \times \delta_{th}$
on $c = 0.5$

Gaseous equivalence ratio and burned gas volume

— Premixed Gas. — $a_d/\delta_{th}=0.04$ — $a_d/\delta_{th}=0.05$ — $a_d/\delta_{th}=0.06$

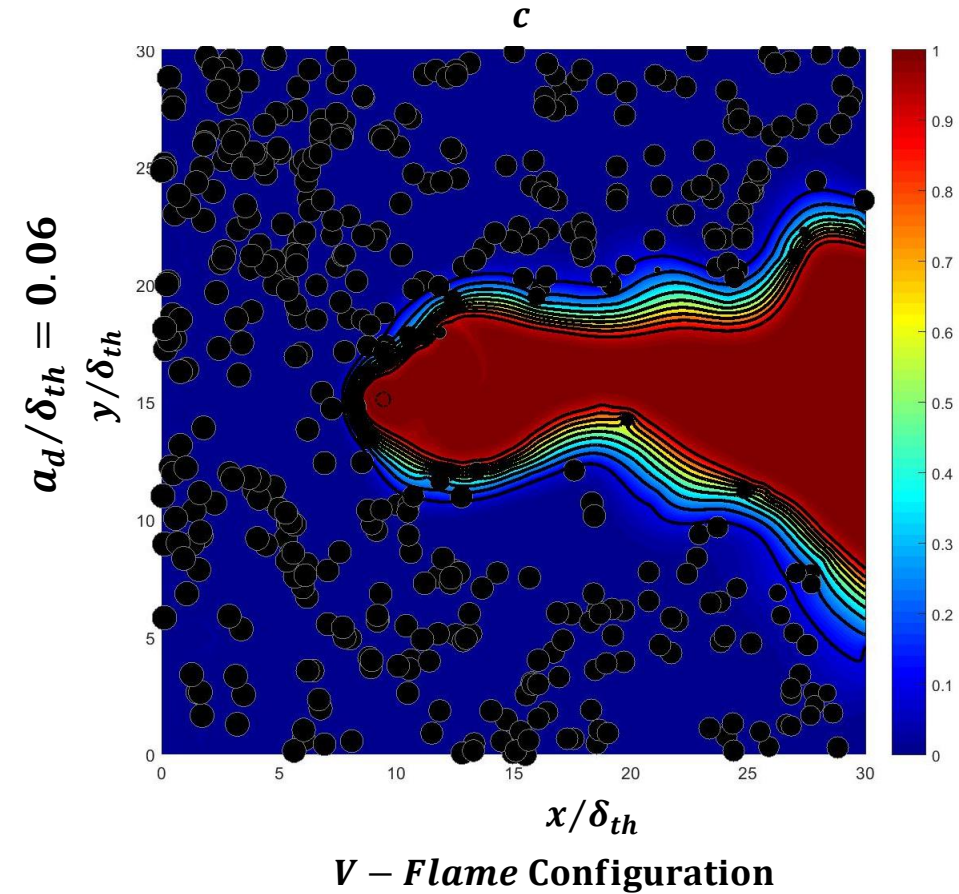
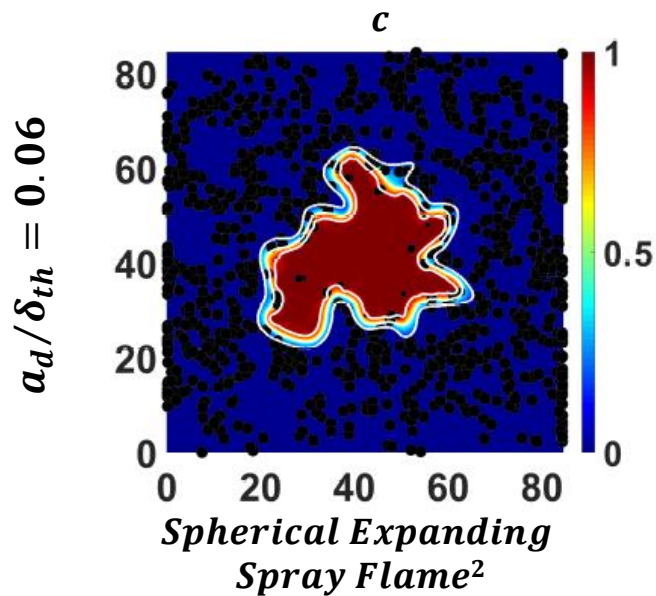
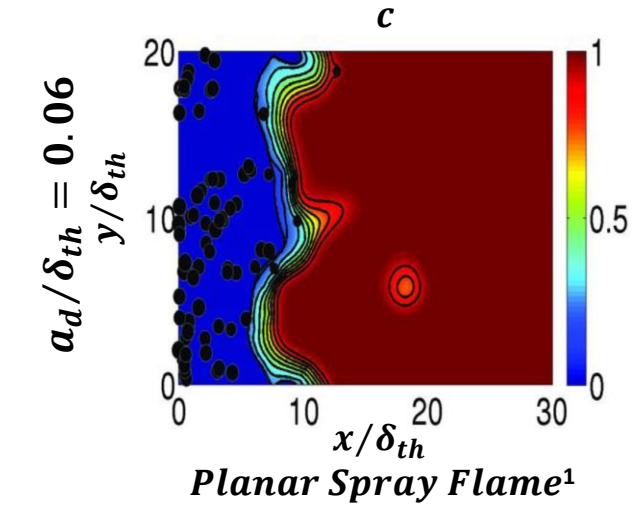


Flame surface area
normalised with its initial
value A/A_0

PDF of ϕ_g in the region
corresponding to
 $0.01 \leq c \leq 0.99$

Normalised volume
 $V_b/(4\pi r_0^3/3)$ of the
region with $c \geq 0.99$

Influence of flame configuration



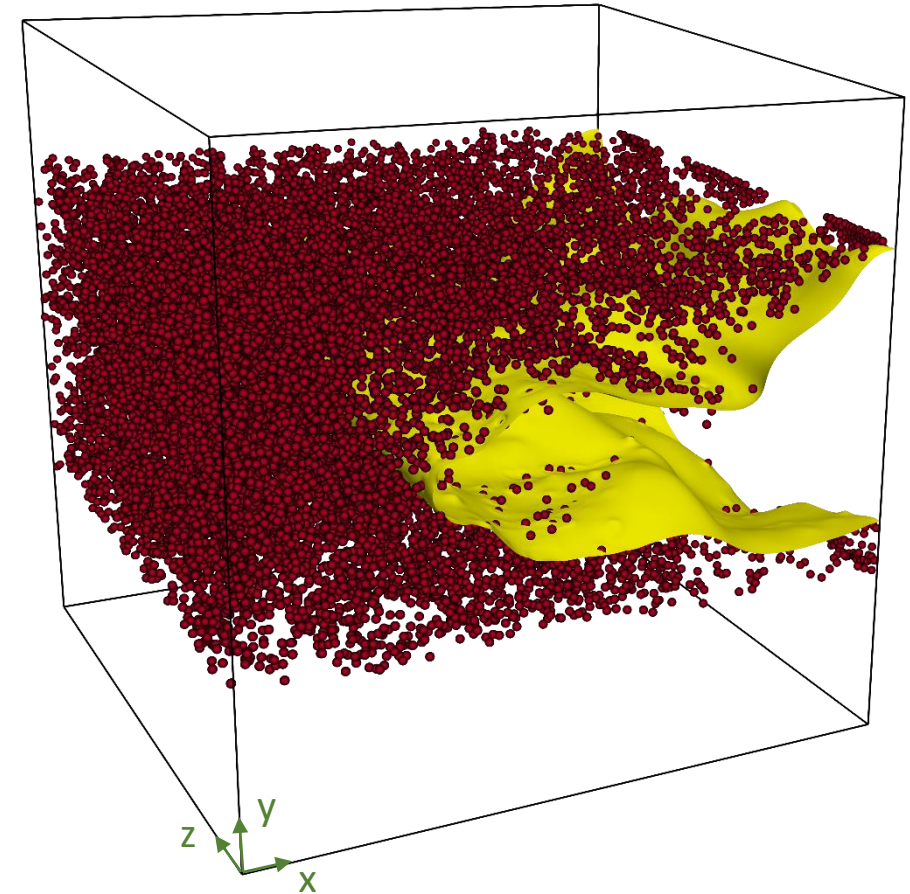
¹D.H. Wacks, N. Chakraborty, and E. Mastorakos, “Statistical Analysis of Turbulent Flame-Droplet Interaction: A Direct Numerical Simulation Study,” Flow, Turbul. Combust. 96, 573 (2016).

²G. Ozel Erol, J.Hasslberger, M. Klein, and N. Chakraborty, “A direct numerical simulation analysis of spherically expanding turbulent flames in fuel droplet-mists for an overall equivalence ratio of unity”, Physics of Fluids, 30,(2018)

Influence of flame configuration

Simulation Parameters

- *Domain:* $(63.3\delta_z)^3$ (where $\delta_z = \alpha_{T0}/S_{b(\phi_g=1)}$ is the Zel'dovich flame thickness)
- *Grid number:* $(384)^3$
- Equivalence ratio: $\phi_d = 1.0$
- Initial rms: $u'/S_{b(\phi_g=1)} = 2.0$
- Longitudinal integral length-scale: $L_{11}/\delta_{th} = 2.5$
- mean inlet velocity of $\bar{u}_{mean}/S_{b,st} = 5$.
- Holder position (x,y): $(120\Delta x, 192\Delta y)$
- Heat release parameter: $\tau = \frac{T_{ad(\phi_g=1)} - T_0}{T_0} = 6.4$
- Droplet diameter: $a_d/\delta_{th} = 0.04, 0.05$ and 0.06

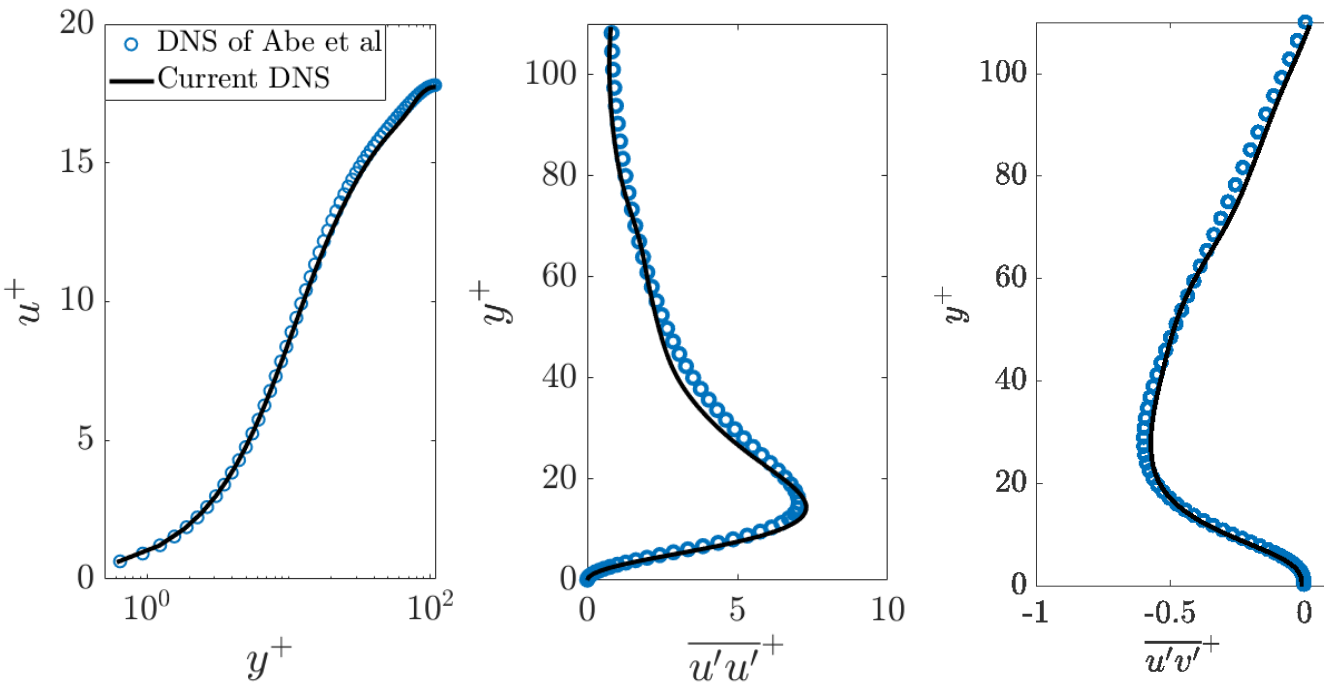
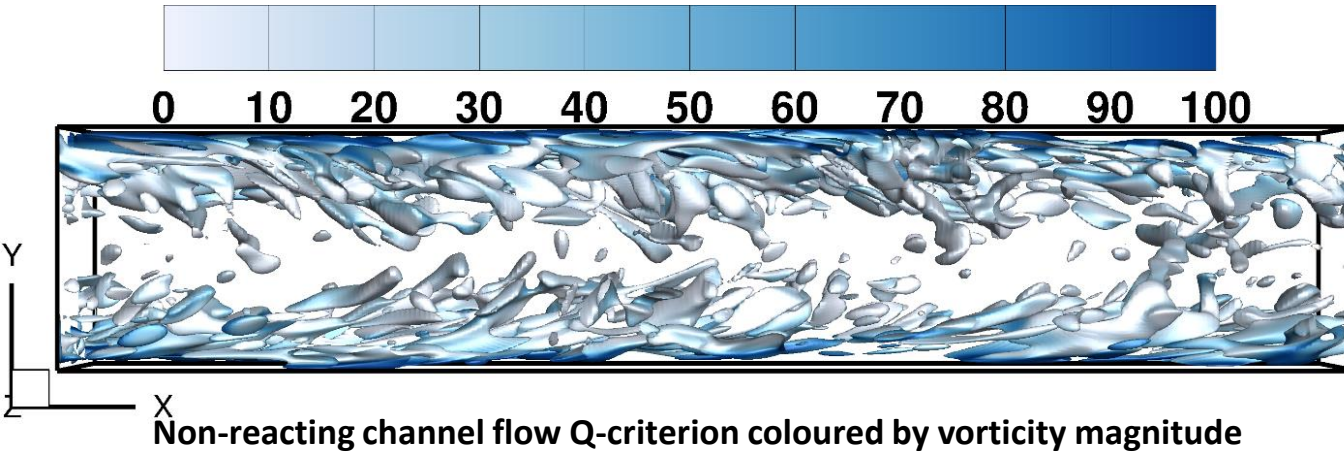


Reaction progress variable isosurfaces at $c = 0.7$ for $a_d/\delta_{th} = 0.06$ initial droplet diameter, at $t = 1t_{flow}$.

Flame-wall interaction

- Flame wall interaction in a fully developed boundary layer channel flow is investigated.
- Some basic definitions used in these flows are:
- Wall shear stress $\tau_{wall} = \mu \overline{\frac{\partial u}{\partial y}} \Big|_{y=0}$.
- Wall friction velocity $u_{\tau} = \sqrt{\frac{\tau_{wall}}{\rho}}$.
- Reynolds number based on wall friction $Re_{\tau} = \frac{\rho u_{\tau} h}{\mu}$.
- Non-dimensional distance from the wall $y^{+} = \frac{u_{\tau} y}{\nu_{wall}}$.

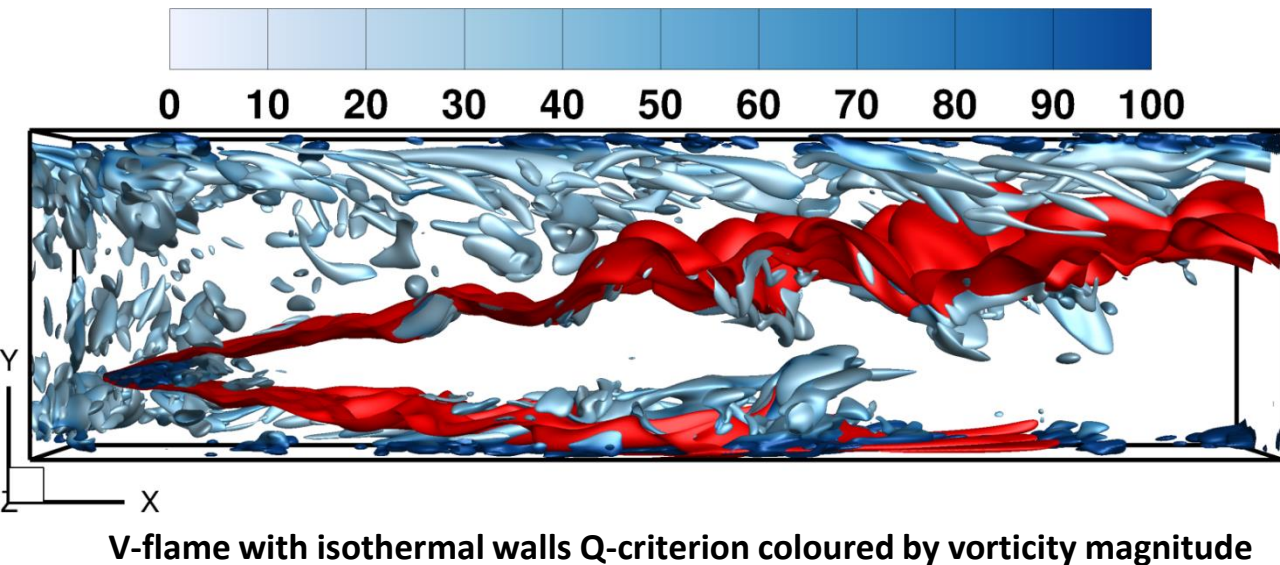
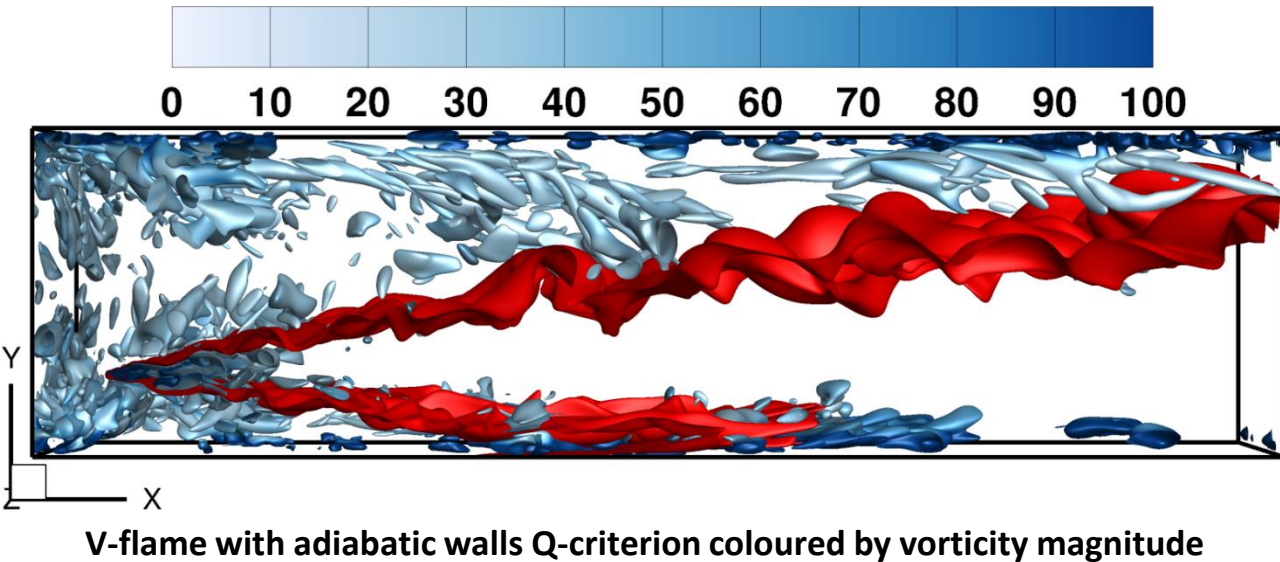
Non-reacting channel flow



Non-reacting channel flow mean velocity and Reynolds stress profiles

- Domain size $10.67h \times 2h \times 4h$.
- $1920 \times 360 \times 720$ (approx. 0.5 billion) grid points.
- $Re_\tau = 110$ for the non-reacting channel.
- $y^+ = 0.6$ at the wall and at least two grid points are in $y^+ \leq 1.0$ region.
- Data validated against DNS of Abe et al.
- Data is recorded in time on the wall normal (y-z) plane.
- Approximately 5 TB of data is generated as inflow conditions for 3 flow through times.

V-flame-wall interaction

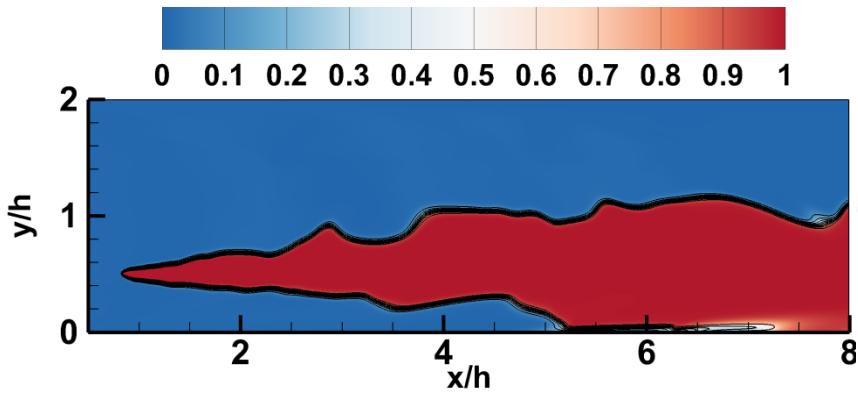


- V-flame is investigated in the $Re_\tau = 110$ channel flow with inert walls.
- Configuration similar to that of Alshaalan & Rutland¹ and Gruber et al.² is used.
- The flame holder is placed in the log layer region of the channel flow at $y^+ = 55$.
- Two wall conditions have been simulated :
 - Isothermal walls
 - Adiabatic walls
- The flame is representative of methane $\phi = 1.0$, $Le = 1.0$ with $S_L/u_\tau = 0.7$.
- Flame behaviour on the bottom wall is different for the two conditions simulated.

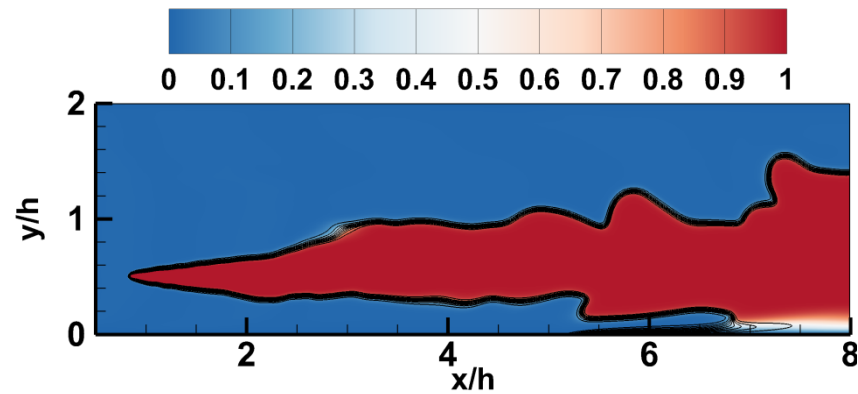
¹TM Alshaalan, CJ Rutland *Symposium (International) on Combustion* 27 (1), 793-799

² A Gruber, R Sankaran, ER Hawkes, JH Chen *Journal of Fluid Mechanics* 658, 5-32

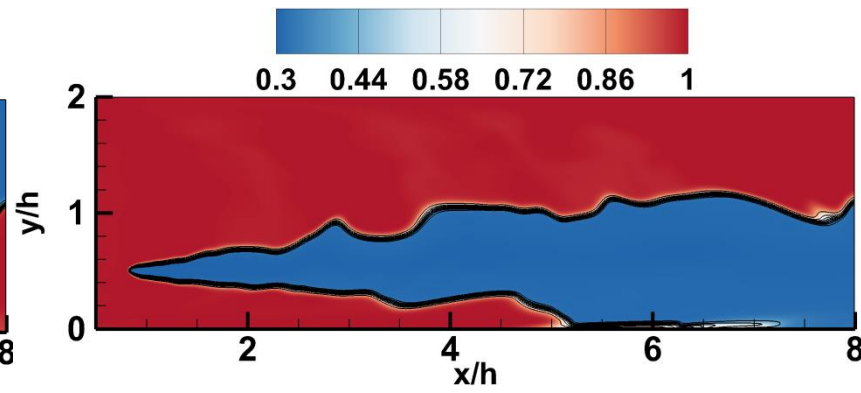
V-flame-wall interaction



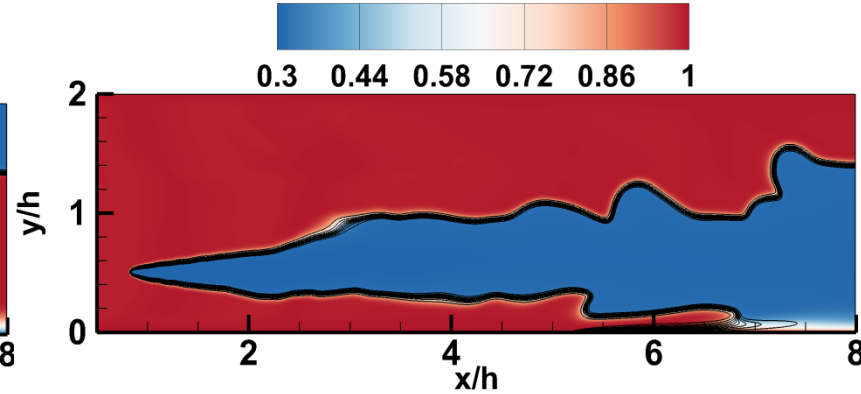
Temperature with adiabatic walls



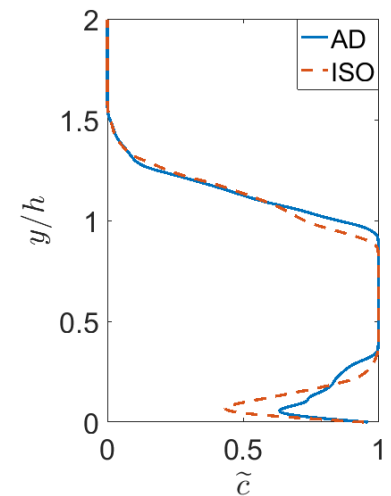
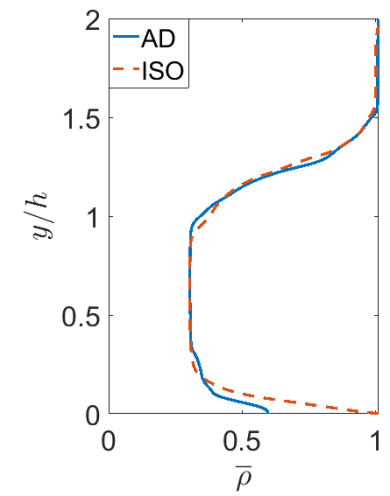
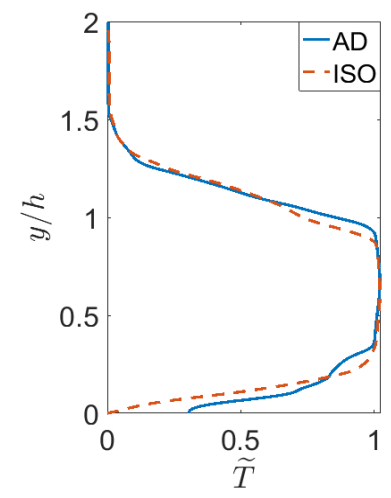
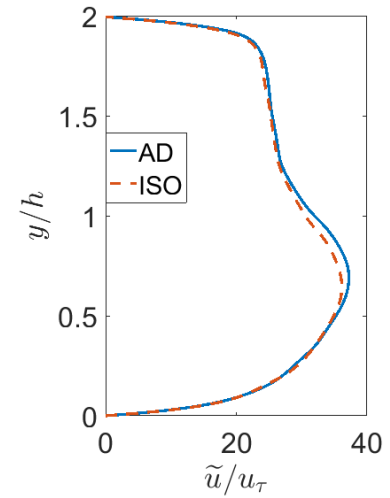
Temperature with isothermal walls



Density with adiabatic walls



Density with isothermal walls



V-flame-wall interaction

- Volume integrated reaction at each y/h :

$$\Omega_{y/h} = \frac{1}{\rho_0 S_L h^2} \int_v \dot{\omega} dv$$

- Volume integrated flame surface at each y/h :

$$S_{y/h} = \frac{1}{h^2} \int_v |\nabla c| dv$$

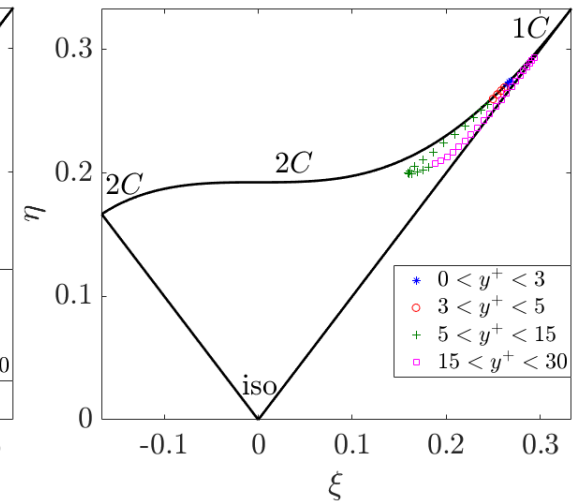
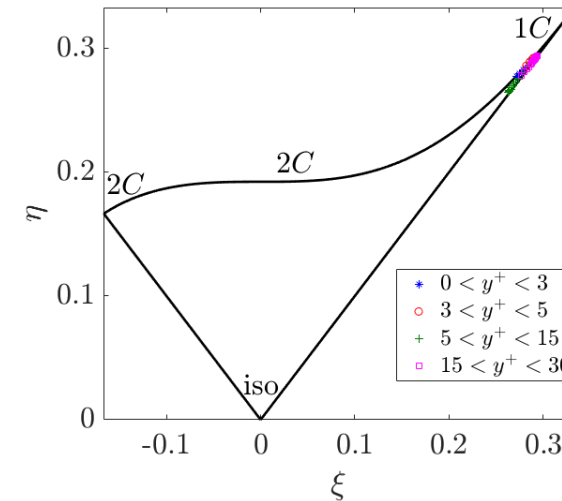
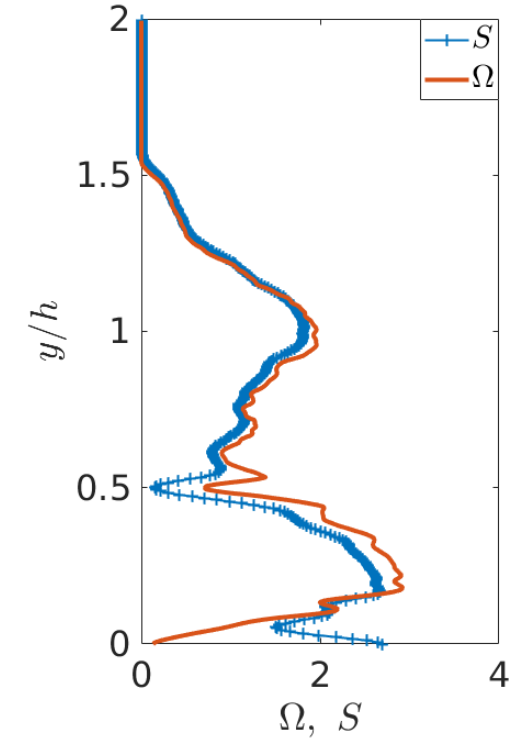
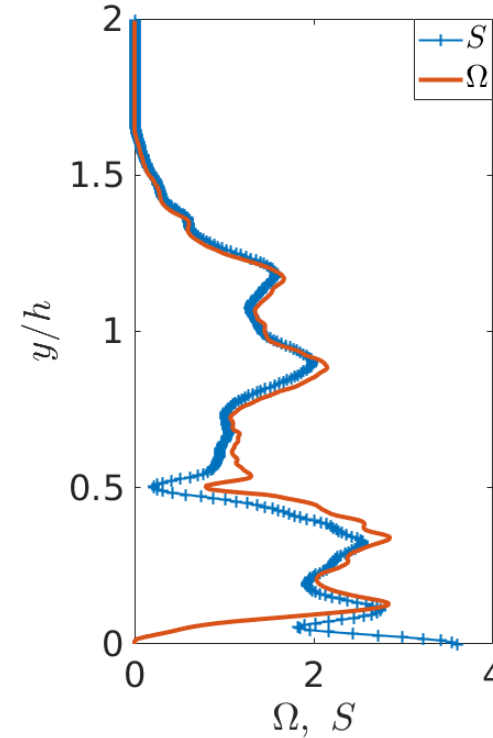
- The anisotropy tensor is defined as :

$$b_{ij} = \frac{\widetilde{u'_i u'_j}}{\widetilde{u'_k u'_k}} - \frac{1}{3} \delta_{ij}$$

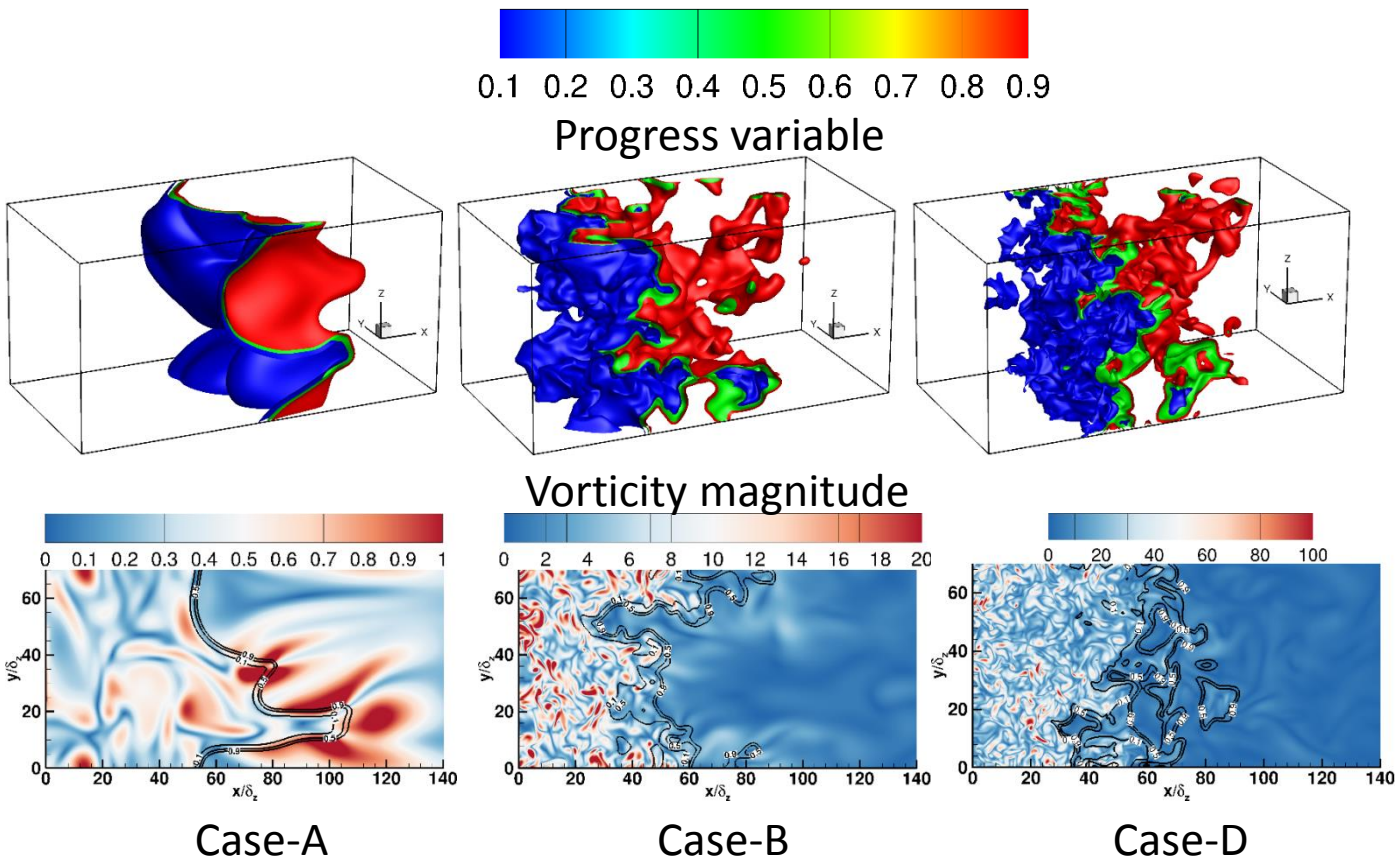
- The second and third invariants of b_{ij} are defined as :

$$6\eta^2 = b_{ij} b_{ji}$$

$$6\xi^3 = b_{ij} b_{jk} b_{ki}$$

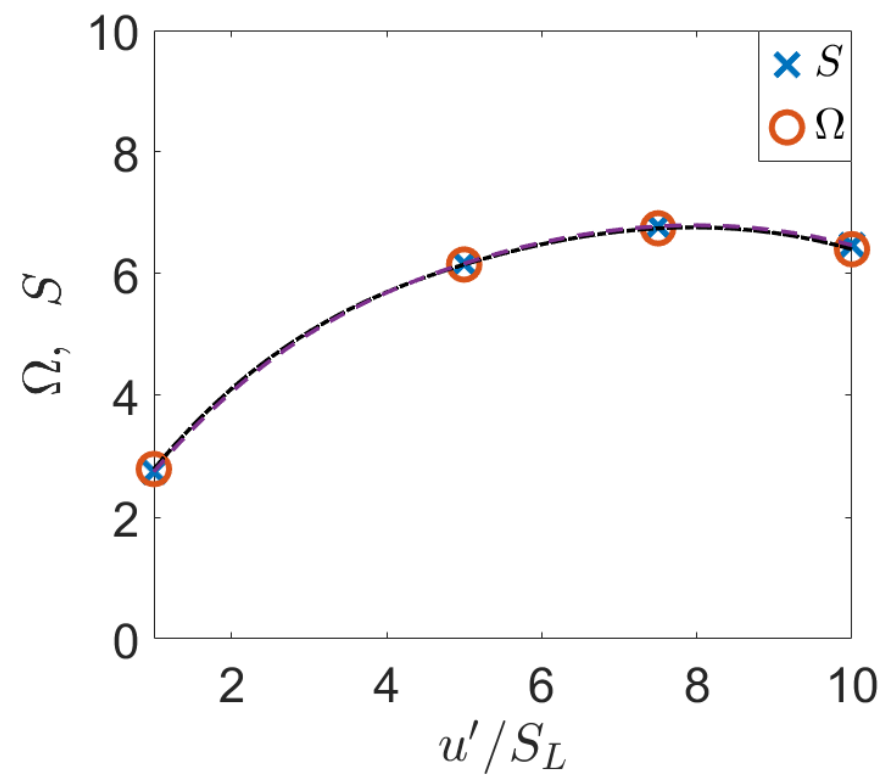


Comparison with planar flames



	u' / S_L	Ka	Da	Re_l
Case-A	1	0.577	3	7.56
Case-B	5	6.454	0.6	37.80
Case-C	7.5	11.858	0.4	56.70
Case-D	10	18.257	0.3	75.60

- Turbulent planar flame simulations have been performed.
- Turbulence is forced upstream of the flame using modified Lundgren’s forcing¹.



¹M Klein, N Chakraborty, S Ketterl *Flow Turbulence Combust* (2017) 99: 955

Conclusions

Droplet flame interaction

- Both **turbulence** and **droplet size** have an important influence on the flame structure.
- **Droplet induced wrinkling** effects are prominent for laminar cases and for small turbulence intensities. It is masked at high turbulence intensities.
- Predominantly fuel-lean **combustion mode** for droplet cases.
- **The growth rate of flame area** decreases with increasing droplet diameter.
- Smaller **burned gas volume** for larger droplet diameters.

Flame-wall interaction

- Changes in the thermal wall boundary conditions have an influence on the flame behaviour.
- The turbulent burning rate and the flame area do not remain proportional to each other in the near wall region.
- Changes in the behaviour of the Reynolds stresses are believed to cause a these changes in the case of adiabatic walls.
- Further investigation of the joint PDFs of reaction rate and Reynolds stress are ongoing to investigate this further.

Acknowledgments

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support from ARCHER (**EP/K025163/1**),
Cirrus(**Tier2 facility**) and
ROCKET the HPC facility at Newcastle University.
20000KAUs used on ARCHER