Effect of turbulence intensity and mixture composition on the localised forced ignition of turbulent homogeneous and inhomogeneous mixtures

C. Turquand d'Auzay[†], V. Papapostolou[†], N. Chakraborty[†], S. Ahmed[‡]

[†] Newcastle University - School of Engineering
[‡] Qatar University - Department of Mechanical and Industrial Engineering - College of Engineering

UKCTRF 2018

12th September 2018

Outline

Outline

Motivation

Why forced ignition ?

- Ignition of flammable mixture with a **spark** or a **laser**
- Initiates combustion and influences subsequent burning
- Significant role in transportation
  - Spark-ignition engine (homogeneous mixture)
  - Direct-injection engines (*in*homogeneous mixtures)
  - Gas-turbine relight (*in*homogeneous mixtures)
- Numerous experimental and numerical investigations[1] [2]

Current investigation of localised forced ignition

- Homogeneous, premixed
- Inhomogeneous, partially premixed

[1] **Mastorakos, E.**, *Progress in Energy Combustion Sciences*, 35 (2009)
[2] **Mastorakos, E.**, *Proceedings of the Combustion Institute*, 36 (2017)

Outline

Computational Framework

Numerical solver

- 3D DNS compressible code SENGA+[1]
- **Mass**, **species**, **momentum** and **energy** equations solved
- Uniformly spaced Cartesian grid
- 10^{th} order in space, 3^{rd} order in time

Spark modelling

- Gaussian in space : $q''' = A_\mathrm{q} \exp(-r^2/2\mathbf{R_{sp}}^2)$
- A_q determined by the volume integral : $\dot{Q} = \int_V q''' dV$
- Heaviside in time : $\dot{Q} = \mathbf{a_{sp}} \rho_0 C_P \tau T_0 \left(\frac{4}{3} \pi \delta_z^3 \right) \left[\frac{H(t) - H(t - t_\mathrm{sp})}{t_\mathrm{sp}} \right]$
- Spark duration : $t_\mathrm{sp} = \mathbf{b_{sp}} t_f$

[1] **Jenkins, K.W., Cant, R.S.**, *Proc. 2nd AFOSR Conf. DNS and LES* (1999)

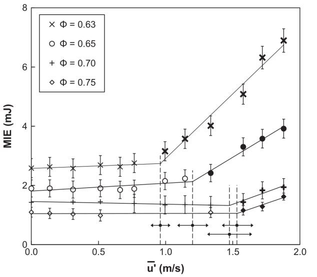
Outline

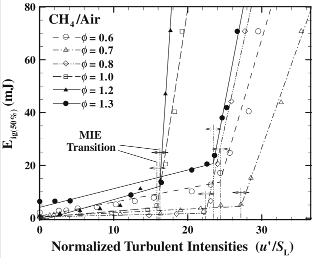
Ignition of homogeneous mixture

Minimum Ignition Energy (MIE)

- Minimum energy deposited to obtain a successful **ignition** or **ignition and subsequent propagation**

(Laser[1])





(Spark[2])

- MIE transition is not yet understood and has yet to be analysed **numerically**

[1] **Cardin, C. et. al.**, *Combustion and Flame*, 160(8) (2013)
[2] **Shy, S.S., Liu, C.C., Shih, W.T.**, *Combustion and Flame*, 157(2) (2010)

Ignition of homogeneous mixture

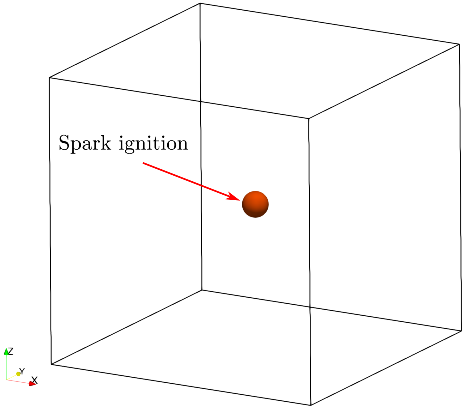
Objectives

- To reproduce numerically Shy *et al.* and Cardin *et al.* experiments for a turbulent homogeneous stoichiometric methane-air mixture
- To understand the effect of turbulence on the early stages of kernel formation and subsequent propagation
- To provide physical insight into the MIE transition

Ignition of homogeneous mixture

Computation set-up

- *Computational domains :*
  $27\delta_{th} \times 27\delta_{th} \times 27\delta_{th} \rightarrow 512^3$ cells
  $37\delta_{th} \times 37\delta_{th} \times 37\delta_{th} \rightarrow 700^3$ cells
- *Chemistry :* Single-step
- *Boundary conditions :*
  NSCBC partially non-reflecting inflow/outflow
- *Initial turbulent field :* Batchelor-Townsend spectrum[1] imposed with Rogallo method[2] with $l_t/\delta_{th} = 4.4$

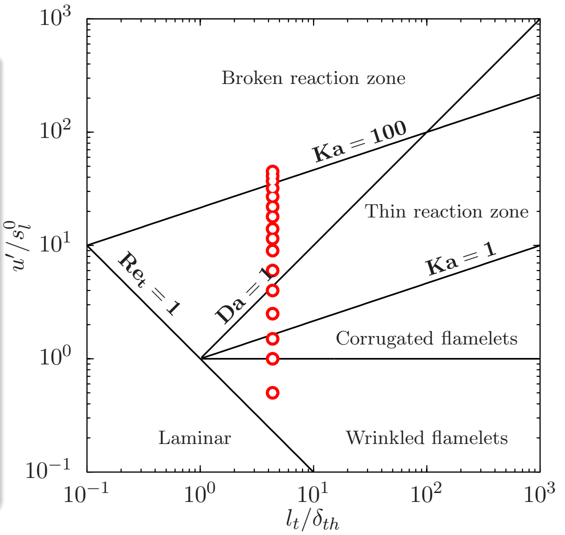


[1] **Batchelor, G.K., Townsend, A.A.**, *Proc. Royal Society London* (1948)
[2] **Rogallo, R.S.**,, *NASA Ames Research Centre* (1990)

Ignition of homogeneous mixture

Simulation parameters

- Binary CH_4-air mixture
  - Equiv. ratio $\phi = 1.0$
  - Heat release $\tau = 3.0$
  - Zel'dovich number $\beta = 6.0$
  - $\mathrm{Sc} = \mathrm{Pr} = 0.7$
- Ignition loc. $L_\mathrm{x}/2, L_\mathrm{y}/2, L_\mathrm{z}/2$
- Ignition radius $R_{sp}/\delta_{th} = 1.2$
- Ignition duration $b_{sp} = 0.2$
- Final time
  - Ignition $t_\mathrm{sim} \approx 1 - 2t_{sp}$
  - Propag. $t_\mathrm{sim} \approx 4 - 10t_{sp}$

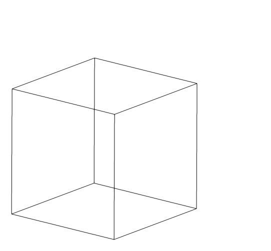


Ignition of homogeneous mixture

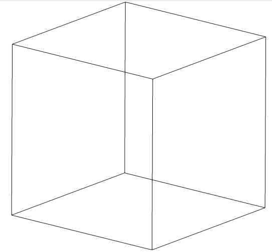
Flame-turbulence interaction

- Iso-surface of $T = (\hat{T} - T_0)/(T_{ad} - T_0) = 0.6$ shown
- Kernel remains perfectly spherical for $u'/s_l^0 = 0.0$
- Kernels get increasingly wrinkled with turbulence

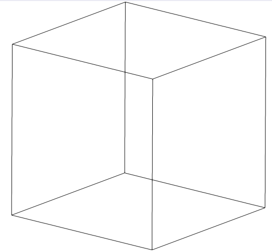
$u'/s_l^0 = 0.0$



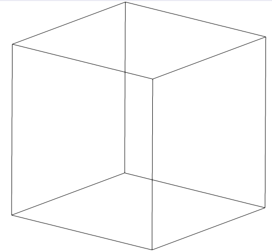
$u'/s_l^0 = 4.0$



$u'/s_l^0 = 9.0$



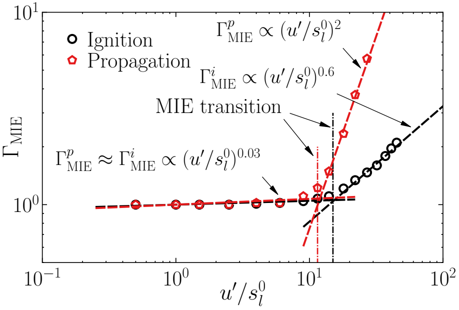
$u'/s_l^0 = 18.0$



Ignition of homogeneous mixture

MIE Transition

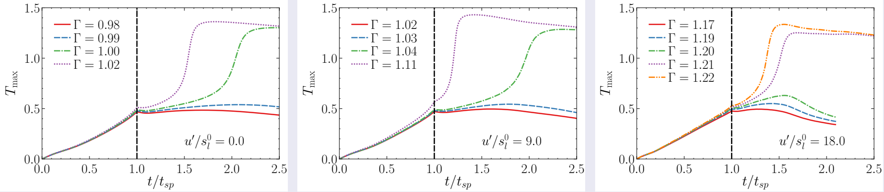
- Good qualitative agreement → Transition is observed
- Quantitative agreement dependent on experimental data



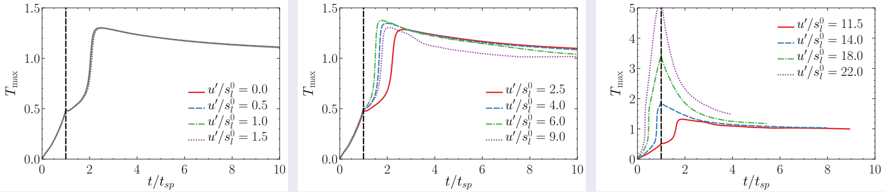
		DNS	Laser	Spark
	$(u'/s_l^0)^p_c$	11.5	7.0 – 10.0	15.0
$\mathbf{\Gamma^p_{MIE}}$	$(u'/s_l^0) \leqslant (u'/s_l^0)^p_c$	0.03	0.01 – 0.1	1.0
	$(u'/s_l^0) \geqslant (u'/s_l^0)^p_c$	2.0	1.4 – 2.1	7 – 16

Ignition of homogeneous mixture

Temporal Evolution - Ignition



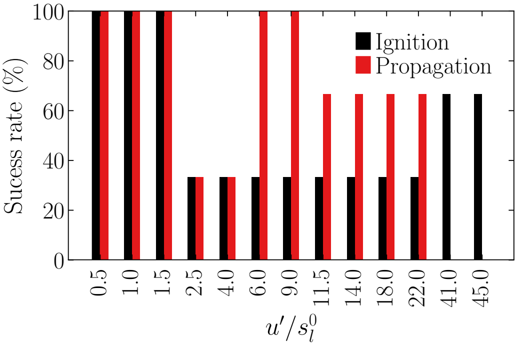
Temporal Evolution - Propagation - $\Gamma = \Gamma^p_{\mathrm{MIE}}$



Ignition of homogeneous mixture

Stochastic behaviour

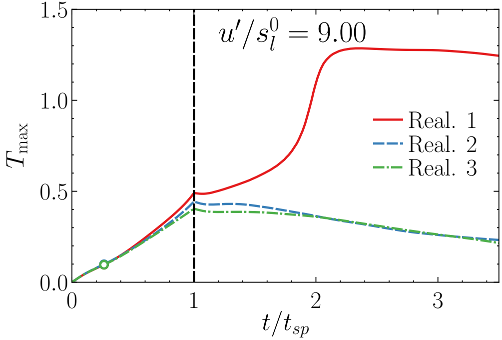
- Success rate very dependent on the initial turbulence
- Measurement of the success rate
  - **3** different initial fields with identical l_t and u'/s_l^0
  - Identical ignition energy
  - Identical spark parameters (radius, duration, location)

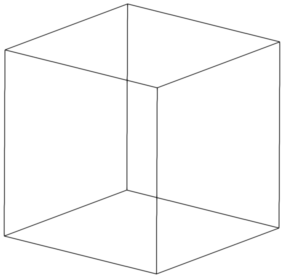


Ignition of homogeneous mixture

Ignition stochasticity

- Analysis of energy balance
- Local spatial fluctuations of curvature increase the normal component of diffusion



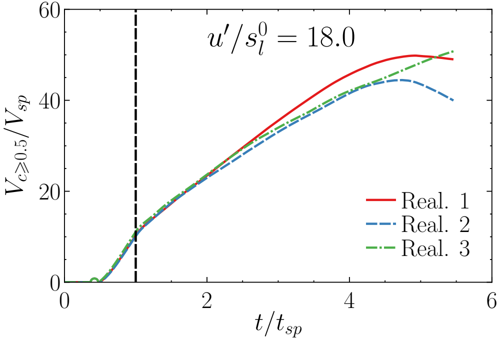


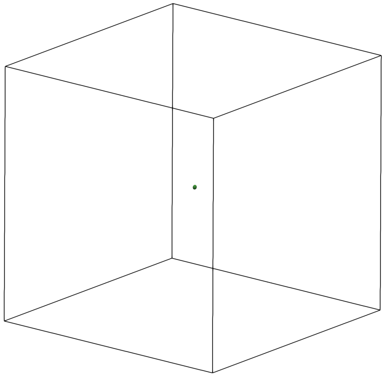
$(T = 0.2)$

Ignition of homogeneous mixture

Propagation stochasticity

- Kernel displaced rapidly due to turbulence
- Propagation dependent on conditions far away from ignitor





$(T = 0.6)$

Outline

Ignition of inhomogeneous biogas mixtures

Background

- Increased energy demand worlwide and stringent pollution policies
- Necessary to develop engines compatible with several alternative fuels
- Re-use of CO_2 in combustion devices
  - Exhaust Gas Recirculation (EGR) : dilution of fresh gas with exhaust (CO_2)
  - Biogas : mixture of CH_4 and CO_2

Objectives

- Investigate the effects of CO_2 dilution and turbulence on the ignition of a shearless mixing layer
  - Ignition/Propagation success
  - Flame structure

Ignition of inhomogeneous biogas mixtures

Chemistry

- Single-step chemistry can not represent CO_2 dilution
- Westbrook and Dryer 2-step mechanism used instead[1]
  - Constants from CERFACS 2s_CM2 mechanism[2]
  - Pre-exponential adjustment (PEA) for rich mixtures

	A (cgs)	β (cgs)	E_a (cal/mol)
$CH_4 + 1.5\ O_2 \Rightarrow CO + 2\ H_2O$	2.00×10^{15}	0.0	35.0×10^3
$n_{CH_4} = 0.9,\ n_{O_2} = 1.1$			
$CO + 0.5\ O_2 \Rightarrow CO_2$	2.00×10^9	0.0	12.0×10^3
$CO_2 \Rightarrow CO + 0.5\ CO_2$	8.11×10^{10}	0.0	77.194×10^3
$\mathcal{Q} = AT^\beta \exp\left(-E_a/\mathcal{R}_u T\right) \prod_{l=1}^{N} \left[X_l\right]^{n_l}$			

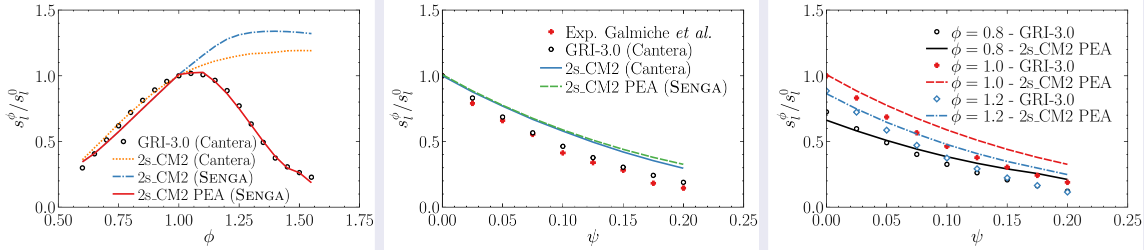
[1] **Westbrook, C.K. and Dryer, F.L.**, *Combustion Sciences and Technology* 27, pp. 31-43 (1981)
[2] **Bibrzycki, J. and Poinsot, T.**, *Work. note ECCOMET WN/CFD/10/17*, CERFACS (2010)

Ignition of inhomogeneous biogas mixtures

Biogas composition

- Global reaction with dilution : $CH_4 + 2\,(O_2 + 3.76N_2) + a\text{Diluent} \Rightarrow \text{Products}$
- Dilution percentage (molar fraction of CO_2) : $\psi = \dfrac{a}{a + 1 + 2 + 7.52} = \dfrac{a}{a + 10.52}$

Chemistry validation



Ignition of inhomogeneous biogas mixtures

Simulation parameters

- *Computational Domain :* $23\delta_{th} \times 23\delta_{th} \times 23\delta_{th}$ (360^3 cells) or $9.25l_t \times 9.25l_t \times 9.25l_t$
- *Boundary conditions :* Periodic in transverse (y/z), NSCBC partially non-reflecting in x-direction
- *Initial turbulent field :* Batchelor-Townsend spectrum[1] imposed with Rogallo method[2], $l_t/\delta_{th} = 2.5$
- *Simulation time :* min. $t/t_{sp} = 10$ and up to $t/t_{sp} = 20$

Spark and mixture set-up

- *Ign. loc. :* $L_x/2, L_y/2, L_z/2$
- *Spark :* $a_{sp} = 3.5$, $R_{sp}/\delta_{th} = 0.5$, $b_{sp} = 0.2$
- *Initial mixture fraction :*
$$\xi = \xi_{st}\left(1 - \mathrm{erf}\left(\frac{x - x_0}{\delta_\theta}\right)\right)$$
- *Mixture composition :* $Y_{o\infty} = 0.233$, $Y_{CH_4\infty} = f(\psi)$, $Y_{CO_2\infty} = g(\psi)$
- *Initial Y_k :* $Y_{CH_4} = Y_{CH_4\infty}\xi$, $Y_{CO_2} = Y_{CO_2\infty}\xi$, $Y_o = Y_{o\infty}(1 - \xi)$

[1] **Batchelor, G.K., Townsend, A.A.**, *Proc. Royal Society London* (1948)
[2] **Rogallo, R.S.**, *NASA Ames Research Centre* (1990)

Ignition of inhomogeneous biogas mixtures

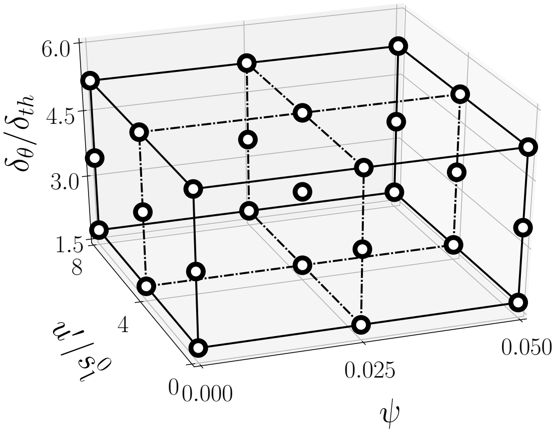
Direct Numerical Simulation dataset

- Turbulence intensity u'/s_l^0

u'/s_l^0	Ka	Da	Re_t
0.0	–	–	–
4.0	5.06	0.63	41.4
8.0	14.3	0.31	82.7

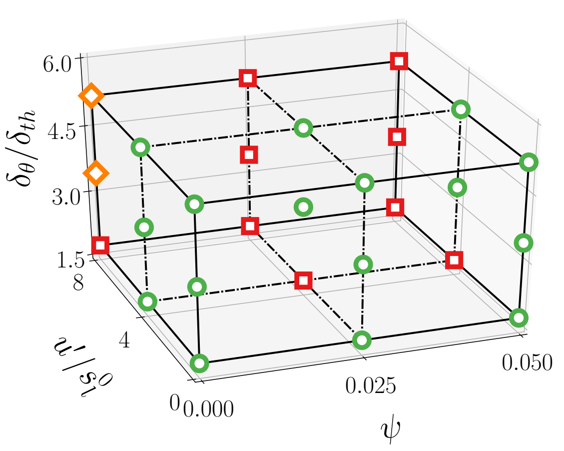
- Initial mixing layer width $\delta_\theta/\delta_{th}$
- Biogas composition ψ

ψ	ξ_{st}	$Y_{CH_4\infty}$	$Y_{CO_2\infty}$
0.000	0.055	1.000	0.000
0.025	0.092	0.574	0.426
0.050	0.128	0.396	0.604



Propagation success

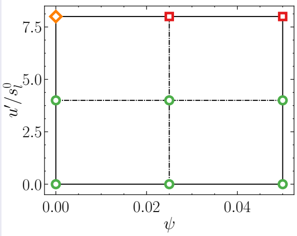
- Measurement of the propagation success by looking at $T_{\max}$ and $V_{c\geqslant 0.9}$
  - No propagation at $t/t_{sp} = 10$: □
  - Propagation up to $t/t_{sp} \leqslant 20$: ◇
  - Propagation at to $t/t_{sp} = 20$: ○
- Conditions for failed propagation :
  - Large turbulence intensity u'/s_l^0
  - Small initial thickness $\delta_\theta/\delta_{th}$, i.e. large initial $\chi = 2D(\nabla\xi)^2$
  - No significant effect of ψ (within the studied range)



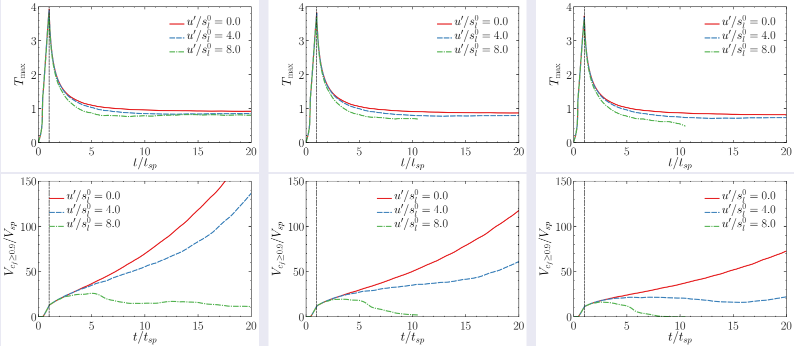
Ignition of inhomogeneous biogas mixtures

Propagation success

- Plane $\delta_\theta/\delta_{th} = 3.45$



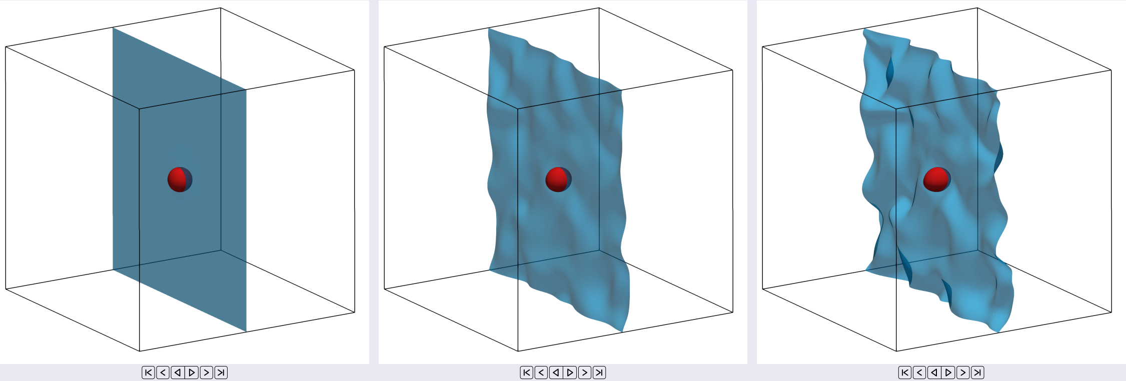
Temporal evolution of $T_{\max}$ and $V_{c\geqslant 0.9}/V_{sp}$



(a) $\psi = 0.0$ **(b)** $\psi = 0.025$ **(c)** $\psi = 0.05$

Ignition of inhomogeneous biogas mixtures

Iso-surfaces of $\xi = \xi_{st}$ and $c = 0.7$



(a) $u'/s_l^0 = 0.0$ **(b)** $u'/s_l^0 = 4.0$ **(c)** $u'/s_l^0 = 8.0$

Outline

Conclusions

Response of spark ignition to turbulence/composition

- Homogeneous mixtures
  - MIE is of particular interest for gas turbine relight, and ICE
  - The transition in MIE observed experimentally has been reproduced numerically (ignition and propagation)
  - Good qualitative/quantitative comparison with experimental results
  - Stochastic behaviour correctly captured
- Inhomegeneous mixtures
  - Dilution does not affect the energy input/max. temperature reached
  - Turbulence intensity remains the key parameter for the success of propagation
  - Dilution has a significant impact on the growth rate of the kernels
  - Shown the formation of edge flames (triple points)

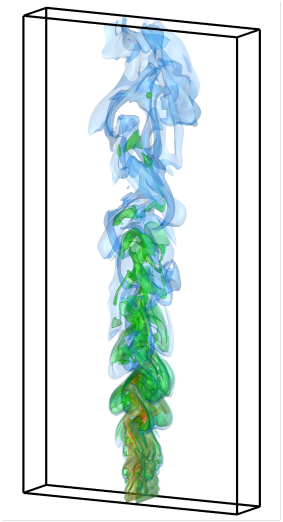
Future work

Kernel ignition

- In-depth analysis of the mixing layer database (in progress)
- Generation of DNS database and analysis of MIE for spray combustion (in progress)

Jet ignition

- New DNS database of biogas jet ignition (in progress)



Acknowledgements

Financial support

- British Council (Newton Grant)
- EPSRC

Computational support

- Rocket HPC (Newcastle)
- Cirrus (EPSRC)
- ARCHER : 10,000 kAUs