Introduction to SENGA+ and its capabilities (Work Package: 4)

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1st workshop of the ExCALIBUR Turbulence at the Exascale project (EP/W026686/1)

Imperial College London
29th September 2022

Newcastle University

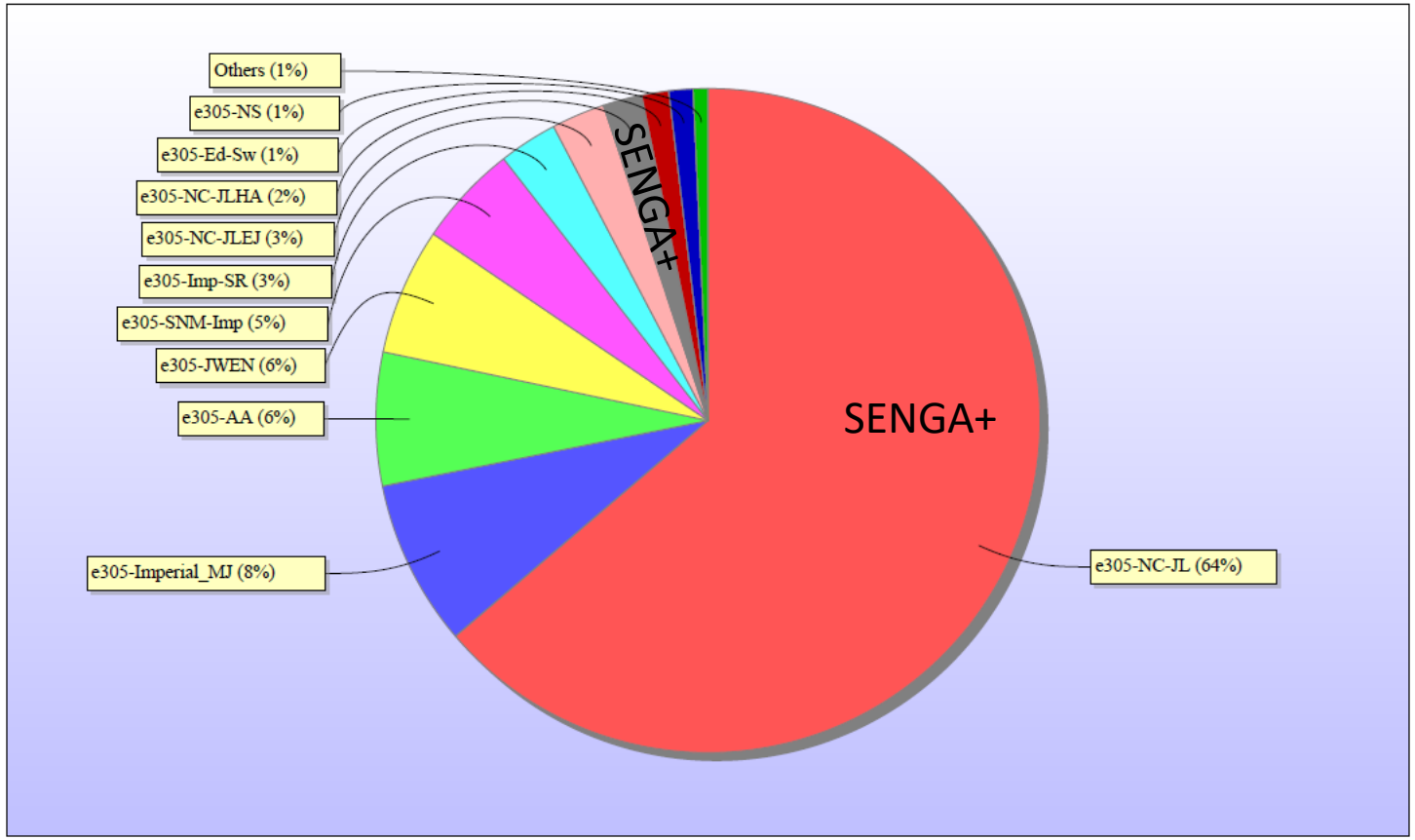
UK CTRF UK CONSORTIUM ON TURBULENT REACTING FLOWS

archer2

UNIVERSITY OF CAMBRIDGE

SENGA+ as the UK community code

Computational time used by UKCTRF groups (Aug 2022):



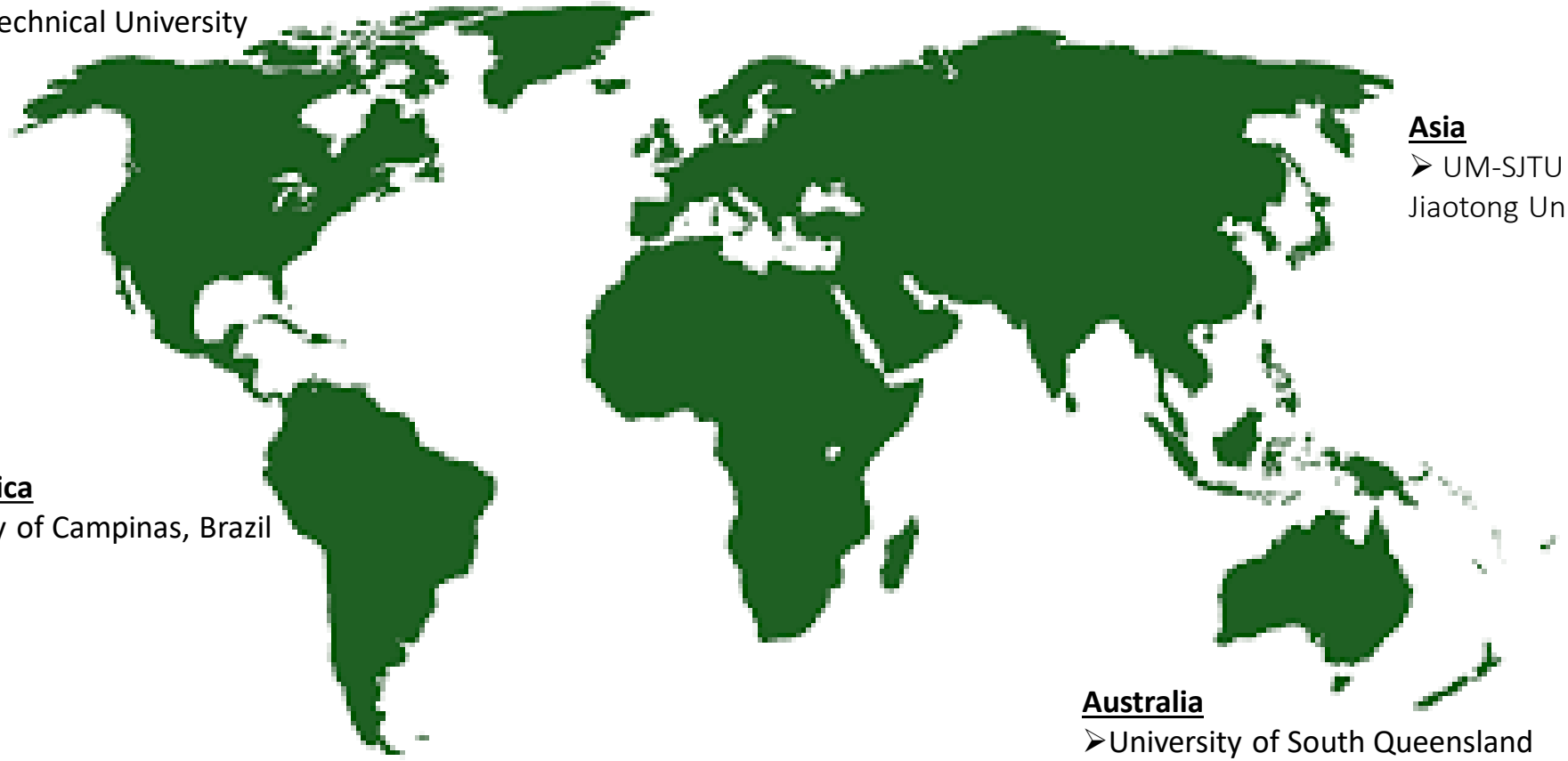
- SENGA/SENGA2 originally developed by Prof. R.S. Cant at Cambridge
- New functionalities (e.g. ignition modelling, multiphase, new boundary condition, flame-shock interaction, complex configuration, conjugate heat transfer) added by Prof. N. Chakraborty at Newcastle
- 66% of the UKCTRF computational time in the last allocation cycle was used by SENGA+ users

International users of SENGA+

UK
- Cambridge University
- Cranfield University
- Liverpool John Moores
- Newcastle University
- Daresbury Laboratory

Europe
- Universität der Bundeswehr München
- University of Eindhoven

North America
- Ontario Technical University



Asia
- UM-SJTU joint institute, Shanghai Jiaotong University

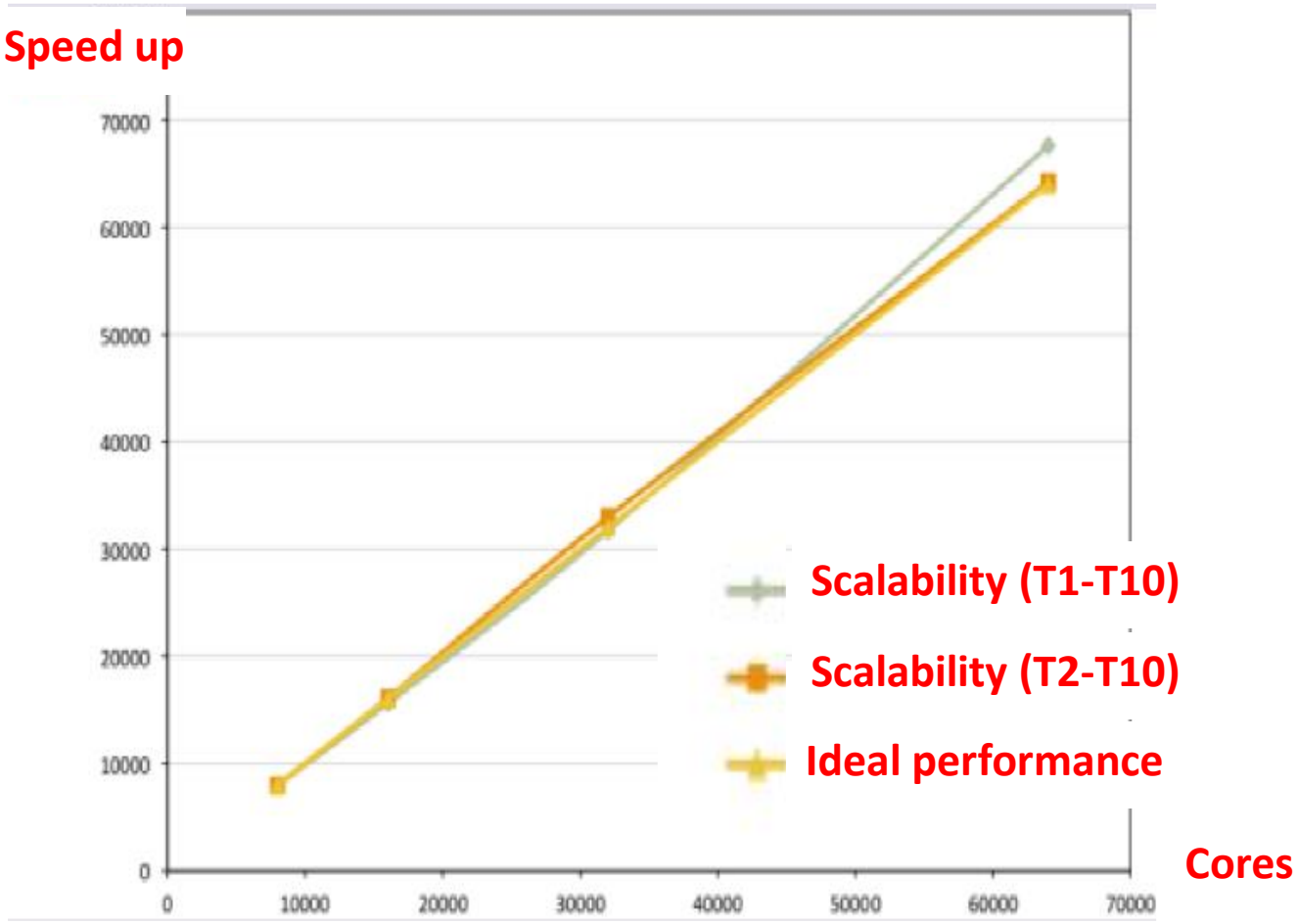
South America
- University of Campinas, Brazil

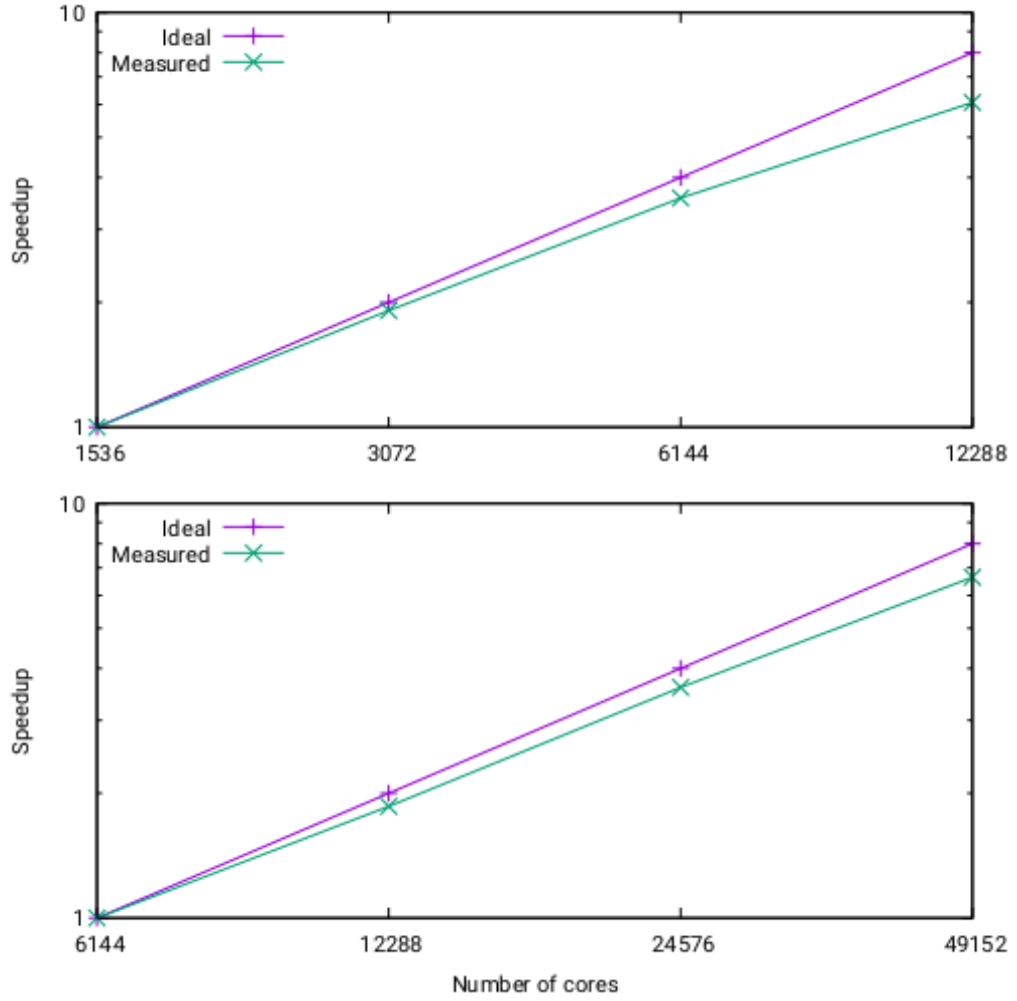
Australia
- University of South Queensland

An introduction to SENGA+

- SENGA+ is a high-fidelity turbulent reacting flow solver, principally used for Direct Numerical Simulations (DNS) of turbulent reacting flows.
- Flagship code of the UK Consortium on Turbulent Reacting Flows (UKCTRF: www.ukctrf.com)
- Solves the governing equations of mass, momentum, energy and species for compressible turbulent reacting flows in 3D using a high-order finite-difference framework. Time stepping uses an explicit RK method with optional implicit operator-splitting method for stiff chemical mechanisms.
- Capable of simulating single-phase or multi-phase (e.g. droplet-laden or particle-laden) combustion processes. The dispersed phase is accounted for by Lagrangian tracking.
- Parallelised using Message Passing Interface (MPI). Recent implementation of HDF5 i/o.
- Chemical reaction mechanism and molecular transport scheme can be chosen depending on the need.

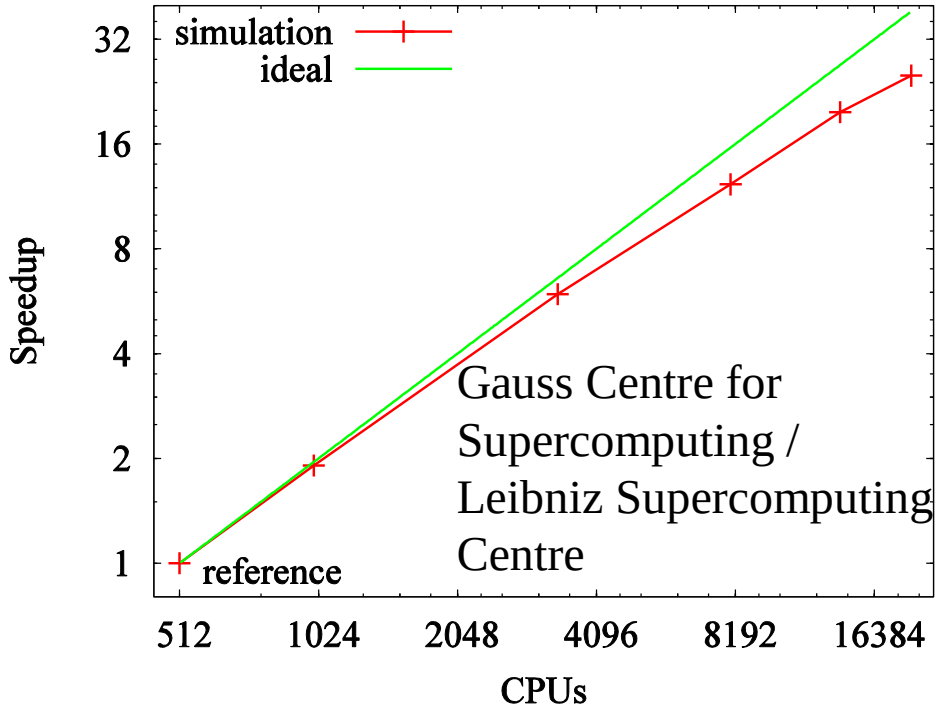
Parallel performance of SENGA+ on ARCHER/2

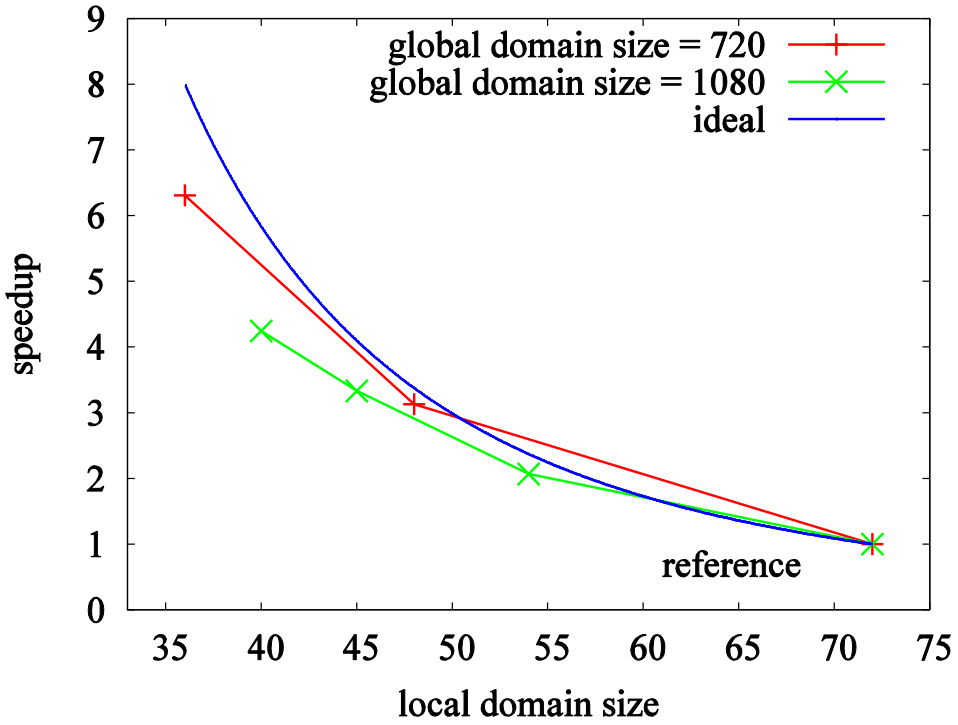




- Scaling exercise was conducted (at Daresbury, Dr J Grasset) using a premixed methane-air flame simulation involving 16 chemical species and 25 reactions

Parallel performance of SENGA+ on international m/c





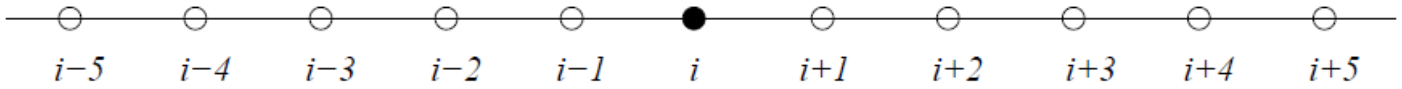
Left: Measured vs. ideal speedup on a domain consisting of 1080^3 mesh points.

Right: speedup relative to the local domain size for a global uniform 720^3 mesh and a global 1080^3 mesh

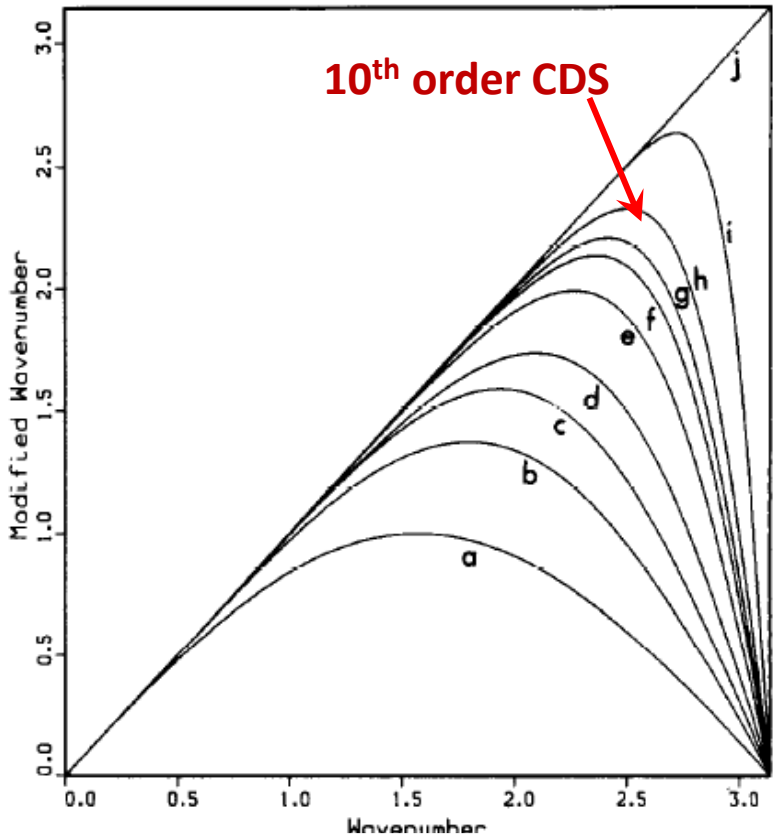
Spatial discretisation in SENGA+

- Spatial discretisation uses a 10^{th} order central difference scheme for the internal grid points. The order of accuracy drops gradually to a 4^{th} order one-sided scheme at the non-periodic boundaries.

- 10^{th} order central difference scheme provides accuracy comparable to a spectral scheme, but with greater flexibility and ease of parallelisation.



- Scheme requires a stencil of 11 points. This implies a halo of 5 points around each parallel subdomain.



Lele, S.K., (1992), Compact finite difference schemes with spectral like resolution, J.Comp. Phys., 103, pp.16-42.

Time advancement in SENGA+

- Explicit time advancement uses a low storage (two registers) 3rd /4th order explicit Runge-Kutta scheme.

$$\frac{\partial \mathbf{U}}{\partial t} = \mathbf{R}(\mathbf{U}, t)$$

$$\mathbf{U} = \{\rho, \rho u, \rho v, \rho w, \rho E, \rho Y_\alpha\}^T$$

For s- stage Runge-Kutta scheme

$$\begin{aligned}
\mathbf{U}^{(i)} &= \mathbf{U}^{(n)} + \delta t \sum_{j=1}^{i-1} a_{ij} \mathbf{R}^{(j)} \\
\mathbf{U}^{(n+1)} &= \mathbf{U}^{(n)} + \delta t \sum_{j=1}^{s} b_j \mathbf{R}^{(j)} \\
t^{(i)} &= t^{(n)} + c_i \delta t \\
\hat{\mathbf{U}}^{(n+1)} &= \mathbf{U}^{(n)} + \delta t \sum_{j=1}^{s} \hat{b}_j \mathbf{R}^{(j)}
\end{aligned}$$

- Adaptive time step size estimated using a PID-type controller.

- For stiff chemistry, the equations are time-advanced using an a semi-implicit additive Runge-Kutta method where a linear system of ODEs is solved using preconditioned Krylov iteration as implemented in the VODPK package.

Byrne, G. D. Pragmatic Experiments with Krylov Methods in the Stiff ODE Setting, Computational Ordinary Preferential Equations, J. Cash and I. Gladwell, eds., Oxford Univ. Press, Oxford (1992) 323-356.

Multi-phase flow (1)

Liquid (Dispersed) Phase:

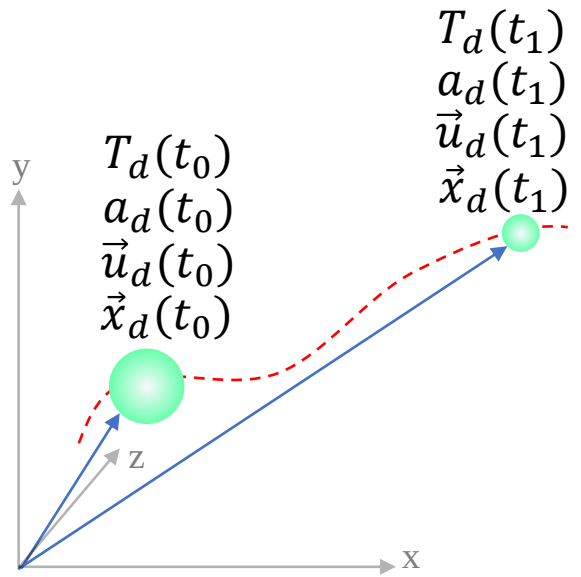
Lagrangian Approach is used for sub-grid spherical droplets following the approach:

- Position: $\frac{d\vec{x}_d}{dt} = \vec{u}_d$
- Velocity: $\frac{d\vec{u}_d}{dt} = \frac{\vec{u}(\vec{x}_d,t)-\vec{u}_d}{\tau_d^u}$
- Diameter: $\frac{da_d^2}{dt} = \frac{a_d^2}{\tau_d^p}$
- Temperature: $\frac{dT_d}{dt} = \frac{\hat{T}(\vec{x}_d,t)-T_d-B_d L_v/C_p^g}{\tau_d^T}$

L_v is the latent heat of vaporization
B_d is the Spalding mass transfer number
C_p^g is the gaseous specific heats at constant pressure

Relaxation time scales associated with droplet:

- Velocity, τ_d^u
- Diameter, τ_d^p
- Temperature, τ_d^T

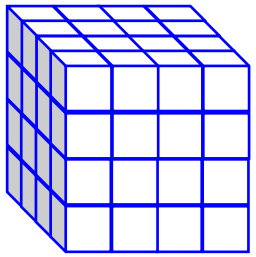


Reveillon, J., Vervisch, L.: Spray vaporization in non-premixed turbulent combustion modelling: a single droplet model. Combust. Flame 121, 75–90 (2000).

Multi-phase flow (2)

Gaseous Phase:

Eulerian Approach is used to solve for gas phase combustion.



$\vec{u}(x,y,z,t)$
$e(x,y,z,t)$
$Y_F(x,y,z,t)$
$Y_O(x,y,z,t)$

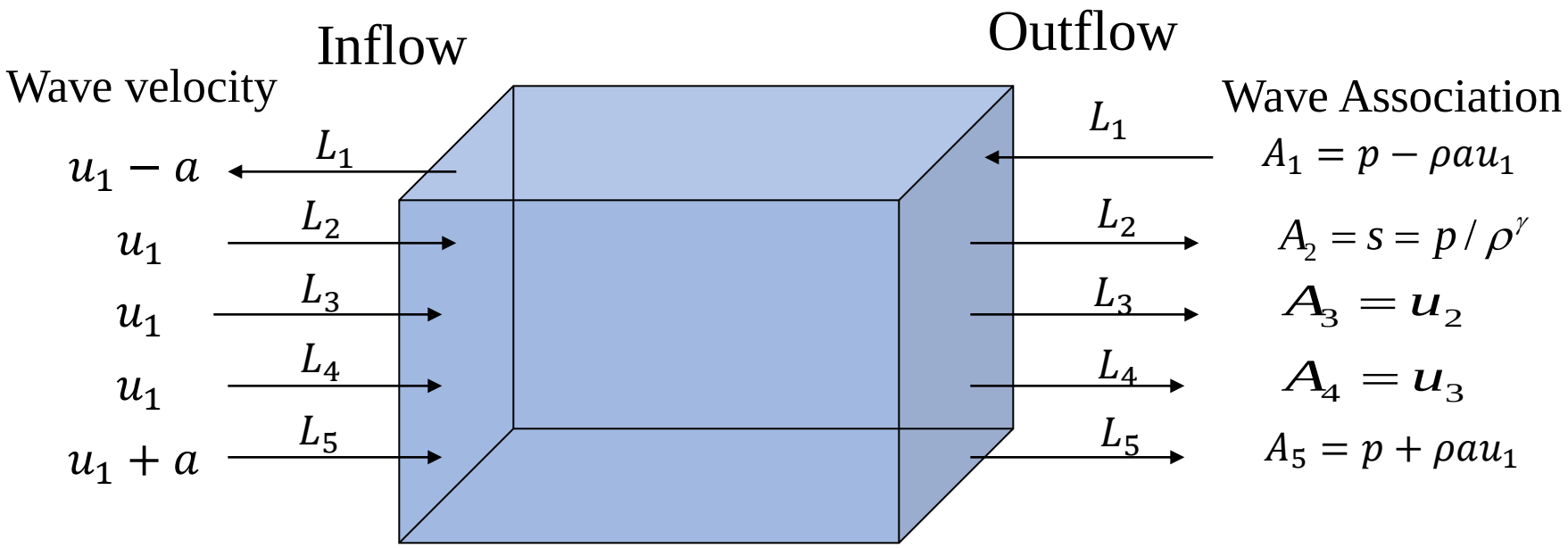
Coupling between two phases:

$$\frac{\partial \rho\psi}{\partial t}+\frac{\partial \rho u_j\psi}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\Gamma_\psi\frac{\partial \psi_1}{\partial x_j}\right)+\dot{w}_\psi+\dot{S}_g+\dot{S}_\psi$$

$\psi_1=\{1,u_i,\hat{T},Y_F,Y_O\}$ for $\psi=\{1,u_j,e,Y_F,Y_O\}$
$\Gamma_\psi=\rho\nu/\sigma_\psi$ for $\psi=\{1,u_i,Y_F,Y_O\}$ and $\Gamma_\psi=\lambda$ for $\psi=e$
$\dot{w}_\psi$ is chemical reaction rate,
$\dot{S}_g$ is an appropriate source/sink term and
$\dot{S}_\psi$ is ***source term due to droplet evaporation***, which is tri-linearly interpolated from the droplet's sub-grid position, $\vec{x}_d$, to the eight surrounding nodes.

Ideal gas law is considered for gaseous reacting mixtures

Boundary conditions in SENGA+



Wave amplitude variations into and out of the inflow and outflow boundary

For non-reflecting boundary incoming $L_i = 0$

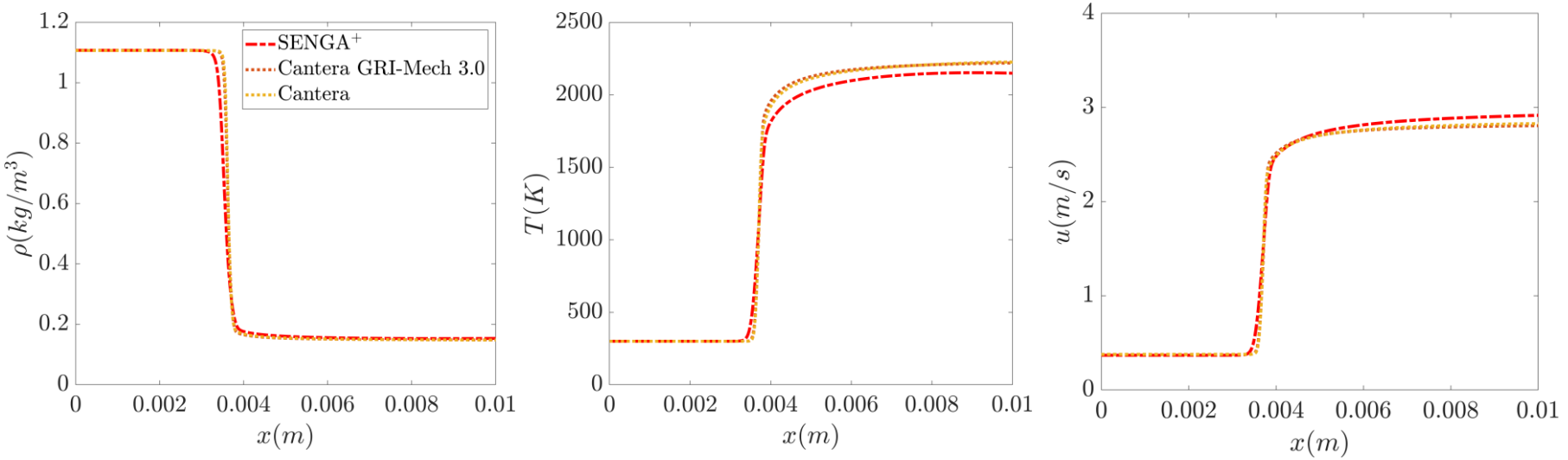
For partially non-reflecting boundary incoming $L_i = \mathrm{K}\ (p\text{-}p_{req})$

Boundary conditions in SENGA+

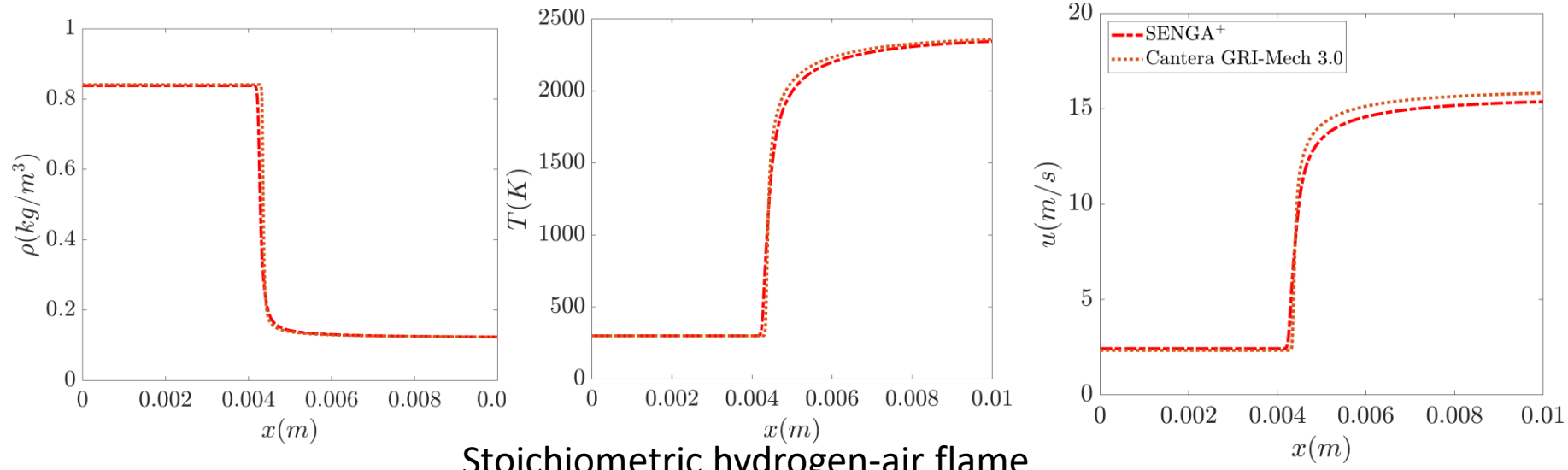
- Boundary conditions specified using the Navier Stokes Characteristics Boundary Conditions (NSCBC) formulation by Poinsot & Lele (1992)
- Incoming wave amplitude variations are specified from BC information
- Outgoing wave amplitude variations are evaluated from internal information

- SENGA+ has BCs for partially non-reflecting outflow, reflecting or non-reflecting inflow, isothermal or adiabatic walls and periodic boundaries.
- Ongoing work includes implementation of improved NSCBC boundary conditions, conjugate heat transfer and immersed boundary methods.

Validation of SENGA+: Chemistry

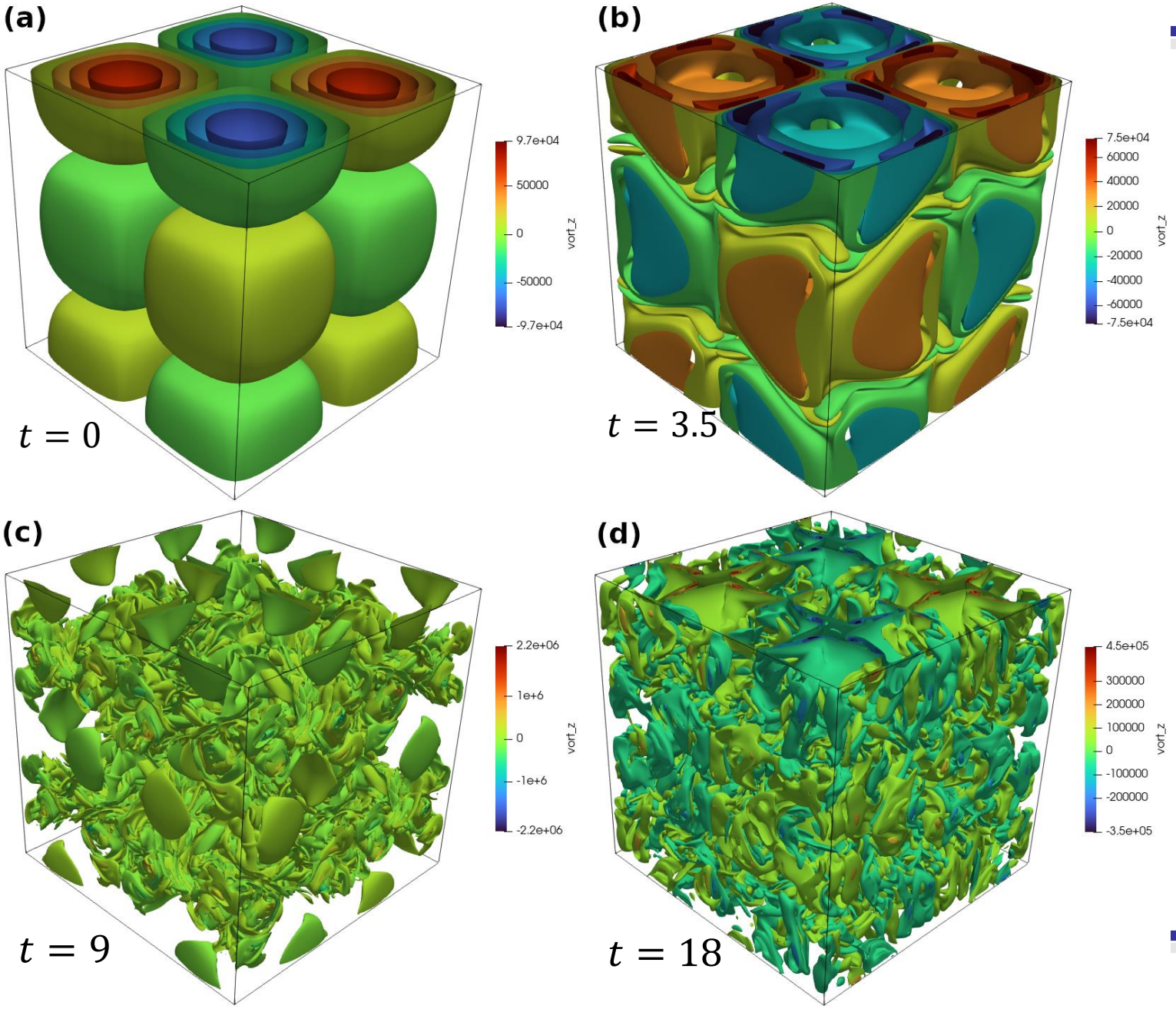


Stoichiometric methane-air flame



Stoichiometric hydrogen-air flame

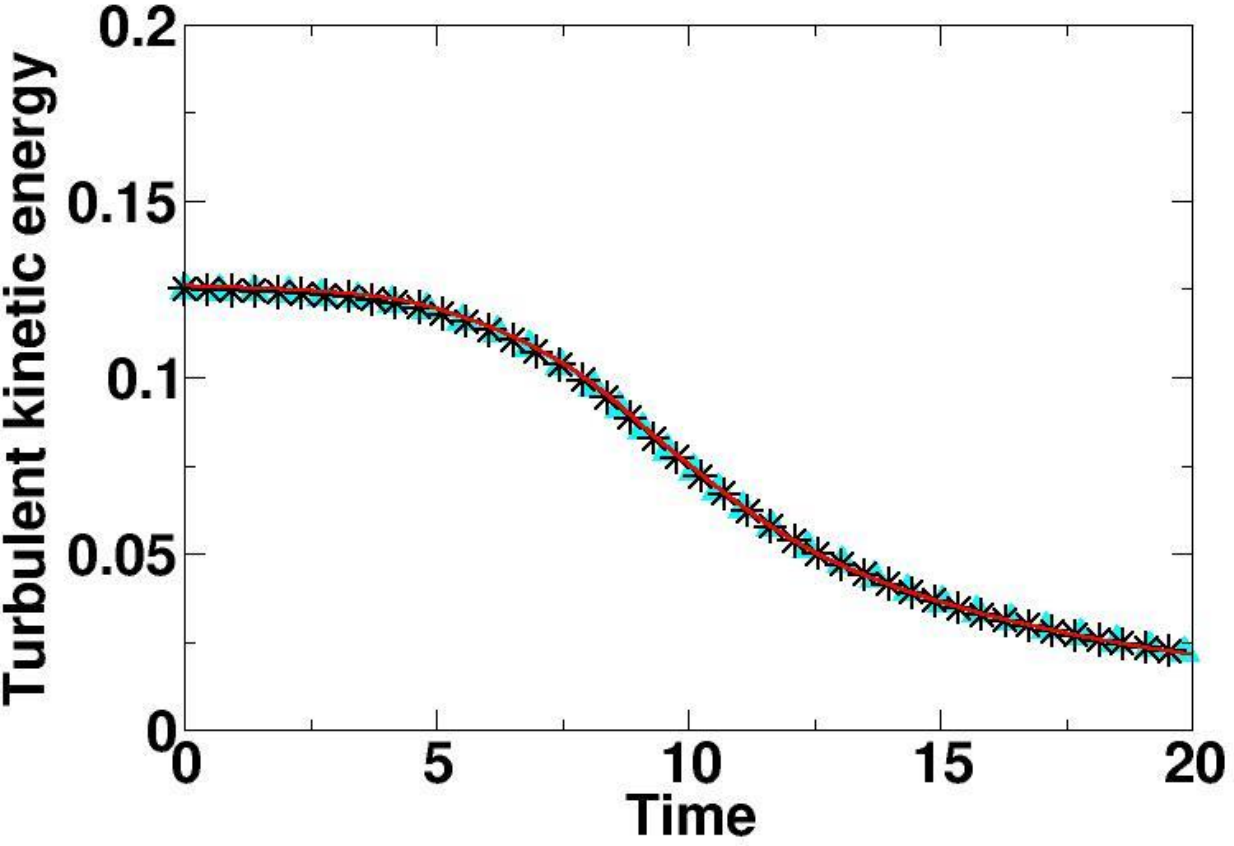
Validation of SENGA+: Turbulence

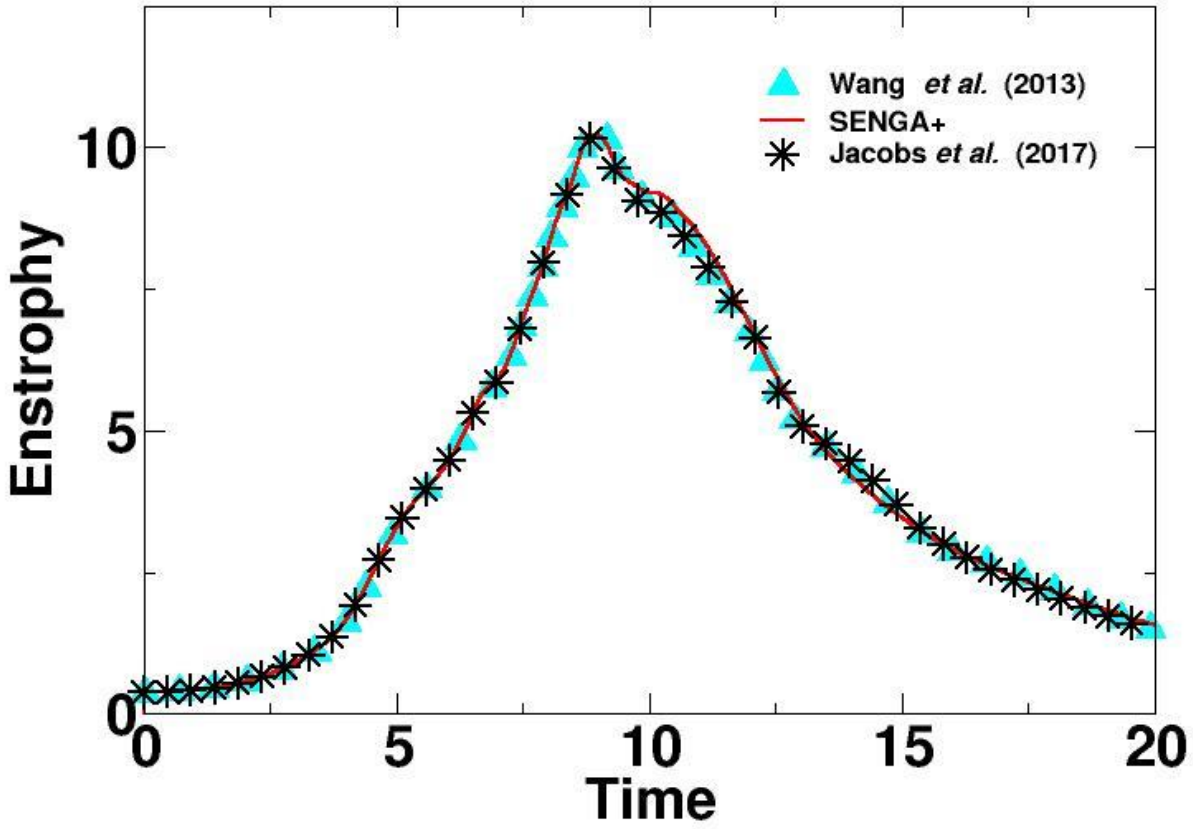


Non-dimensionalised time $t = \dfrac{\hat{t}}{L/U_0}$

Z-vorticity contours

Validation of SENGA+: Turbulence



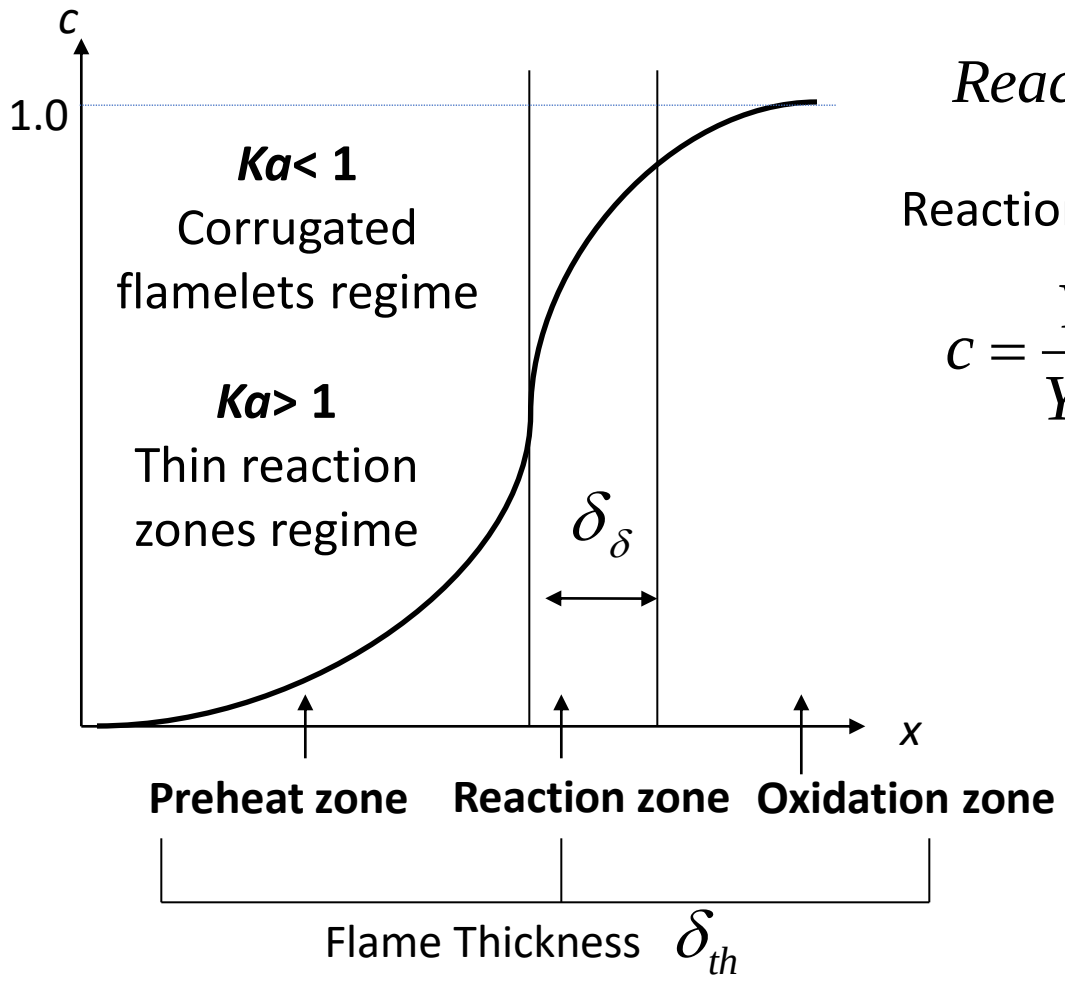


Taylor-Green vortex test case

Jacobs et al., Journal of Computational Science, 18, 12-23 (2017); Wang et al., Int. J. Numer. Methods Fluids, 72 (8), 811-845 (2013)

Turbulent premixed combustion

Premixed Flame Structure



Reaction Mechanism :

$$Reactants \rightarrow Products$$

Reaction progress variable:

$$c = \frac{Y_P - Y_{P0}}{Y_{P\infty} - Y_{P0}}; \quad c = \frac{Y_{R0} - Y_R}{Y_{R0} - Y_{R\infty}}$$

Karlovitz number :

$$Ka = \frac{\delta_{th}^2}{\eta^2} = \frac{v_\eta^{\,2}}{S_L^{\,2}}$$

Damköhler number : $Da = \frac{l\, S_L}{u' \delta_{th}}$

Computational cost of Combustion DNS

Computational cost of DNS of non-reacting incompressible flows:

$$w \sim N_L^{\,3} N_t \sim n_l^3 n_t \,\mathrm{Re}_t^{11/4}$$

Computational cost of DNS of non-reacting compressible flows (for explicit time marching):

$$w \sim N_L^{\,3} N_t \sim n_l^3 n_t \,\mathrm{Re}_t^3 / \mathrm{Ma}$$

Computational cost of DNS of compressible reacting flows:

$$w \sim N_L^{\,3} N_t \sim n_l^3 n_t \,\mathrm{Re}_t^3 / \mathrm{Ma} * (\boldsymbol{Q^3 / Ka^{3/2}})$$

$\boldsymbol{n_l}$: Number of integral eddies within the domain

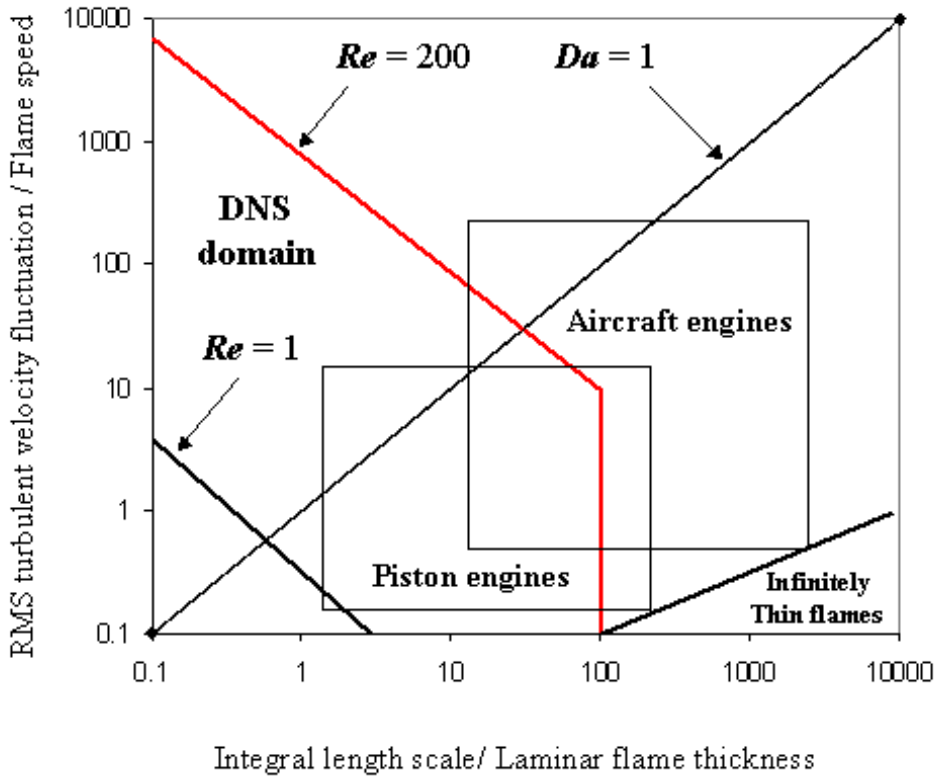
$\boldsymbol{n_t}$: Number of integral eddy turn over times

$\boldsymbol{Q}$: Number of grid points to resolve the flame thickness (Q ~10-20)

$\boldsymbol{Ka}$: Karlovitz number $(Ka \sim \delta_{th}^2 / \eta^2)$

Computational cost of Combustion DNS

Chemistry is modelled in combustion DNS



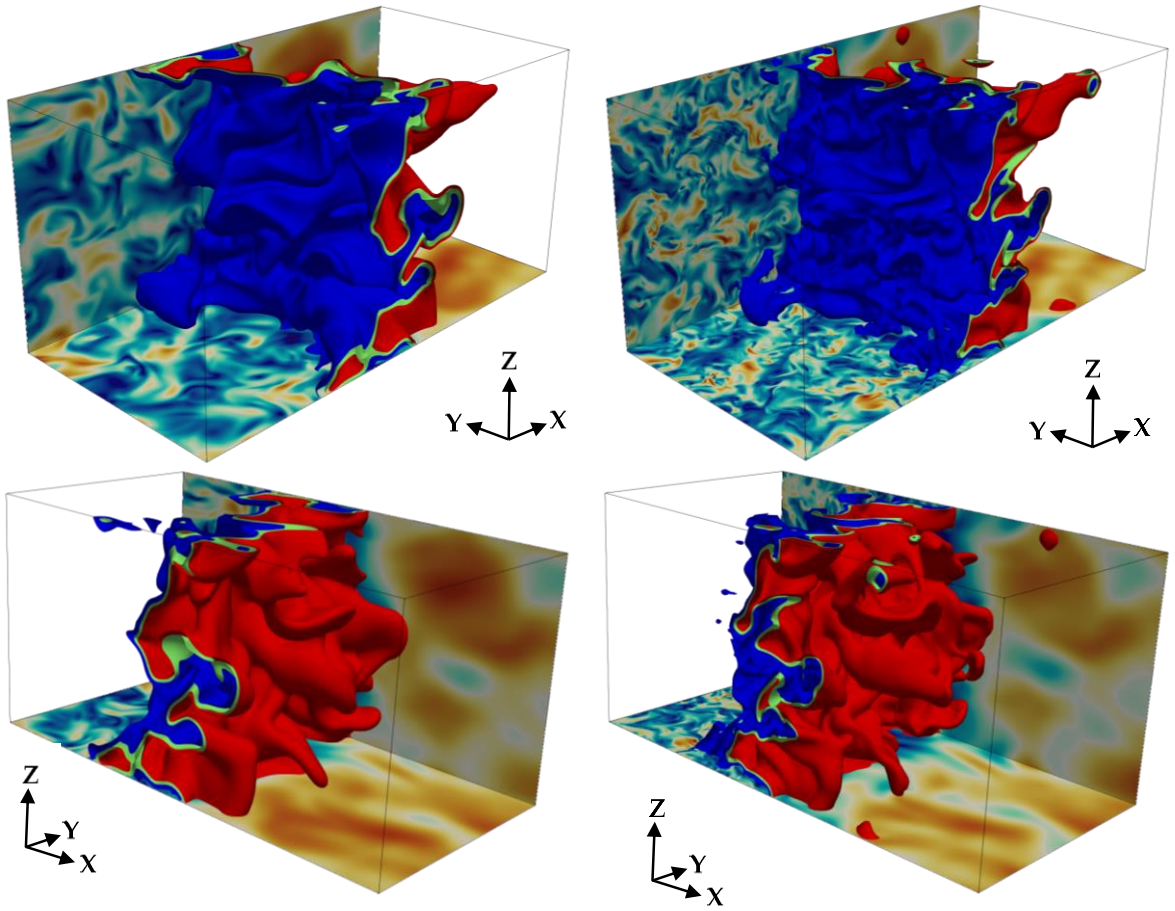
- A skeletal propane-air reaction mechanism involves 27 species and 73 reactions.
- Simulation of a flame would require 1000000 time steps.
- With present algorithms this would take 500 CPU years on a teraflop computer and 1000 terabytes of memory.

The full chemical mechanism of isooctane-air mixture requires more than 800 species and 3500 chemical reactions

Comparison between simple chemistry and detailed chemistry simulations

Simple chemistry CH_4-air

Detailed chemistry CH_4-air



Red isosurface: c = 1.0; Blue isosurfaces: c =0; background: vorticity magnitude

Method	Simple Chemistry and Transport	Detailed Chemistry and Transport
Estimated carbon footprint	~25 $kg\ CO_2$	~$10^3 kg\ CO_2$
CPU cost	$O(10^5)$ CPU hours [32,33]	$O(10^7)$ CPU hours [3]
Data volume	$O(1)$ TB [32,33]	$O(100)$ TB [3]
Parametric variations	Dozens possible [32,33]	Typically, very few (e.g 1-4) [34-37]; more limited in terms of nondimensional numbers, pressure or size of domain.
Data analysis	Straightforward, unambiguous results.	Complex (due to re-evaluation of constitutive laws); Results are not unambiguous due to different possibilities to define reaction progress variable (RPV) [34-36]

Keil et al., Energies, 14,5548,2021; Keil et al., *Energies*, 14, 5695, 2021; Awad et al., Phys. Fluids, 34,055120, 2022

Implications of chemical representation

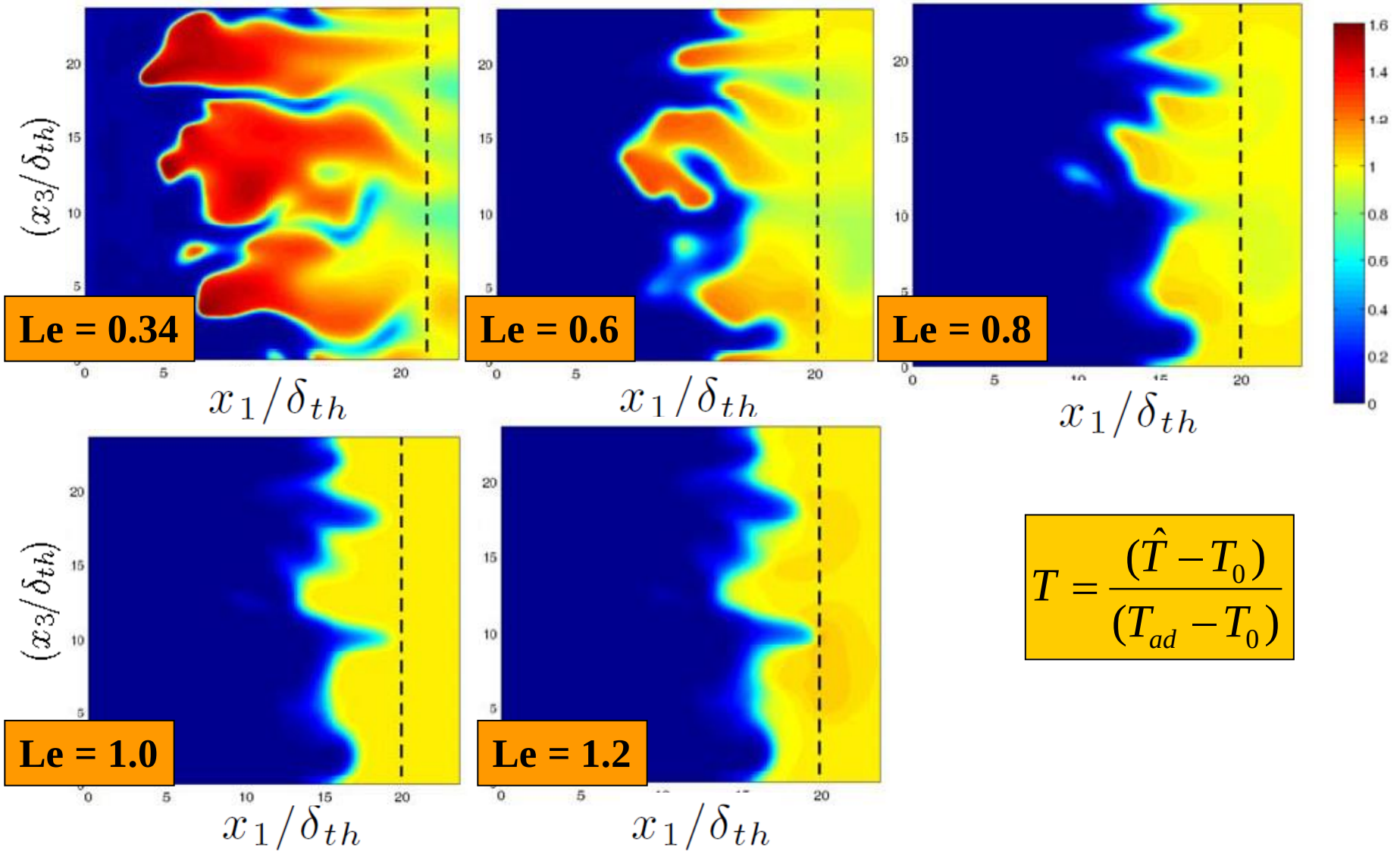
- For typical hydrocarbon and hydrogen flames the CPU cost, data volume and carbon footprint for detailed chemical mechanisms are often 10^2 times of that of the cost for the same problem with simple chemistry.

- It is difficult to carry out a large parametric variation with the detailed chemistry because of computational cost but parametric analysis is routinely done using simple chemistry. The cost saved by using a simple chemistry can be used to address turbulent reacting flow problems in relatively complex flow configurations.

- Data analysis for simple chemistry simulations is relatively simple and the comparison with analytical results is relatively straightforward. Key variables such as reaction progress variable cannot be defined uniquely for detailed chemistry.

- Problems where autoignition, preferential diffusion and flameless combustion play key roles cannot be addressed using simple chemistry. However, the standard flame propagation, flame-wall interaction and localised ignition statistics can be captured by simple chemistry.

Lewis number effects on non-dimensional temperature *T* field

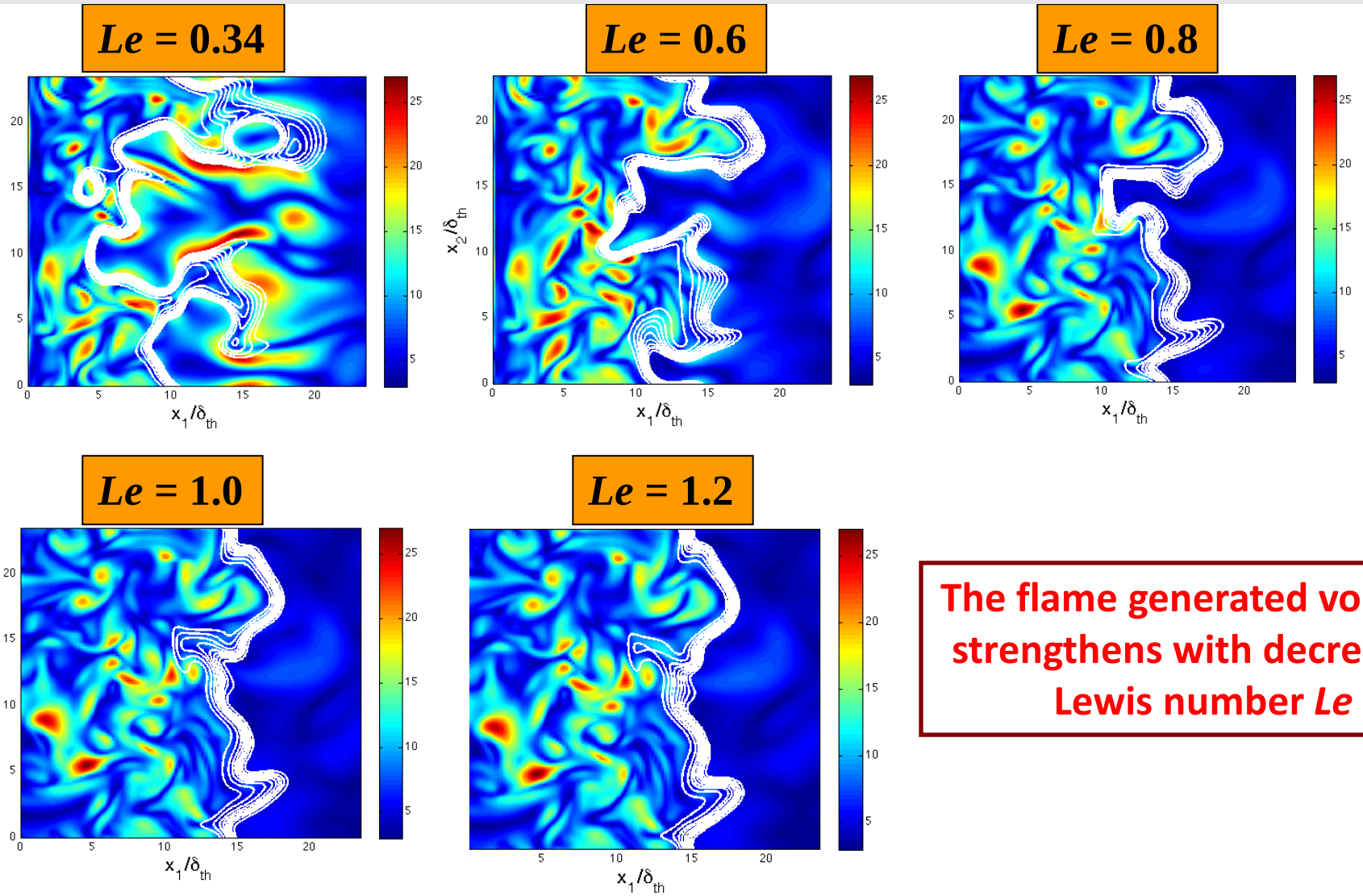


$$T = \frac{(\hat{T} - T_0)}{(T_{ad} - T_0)}$$

Chakraborty and Cant, *Combustion and Flame*, 156, 1427-1444, 2009

Chakraborty and Cant, *Numerical Heat Transfer A*, 55,8,762-779, 2009.

Le effects on distribution of vorticity $\sqrt{\omega_i \omega_i} \times \delta_{th} / S_L$

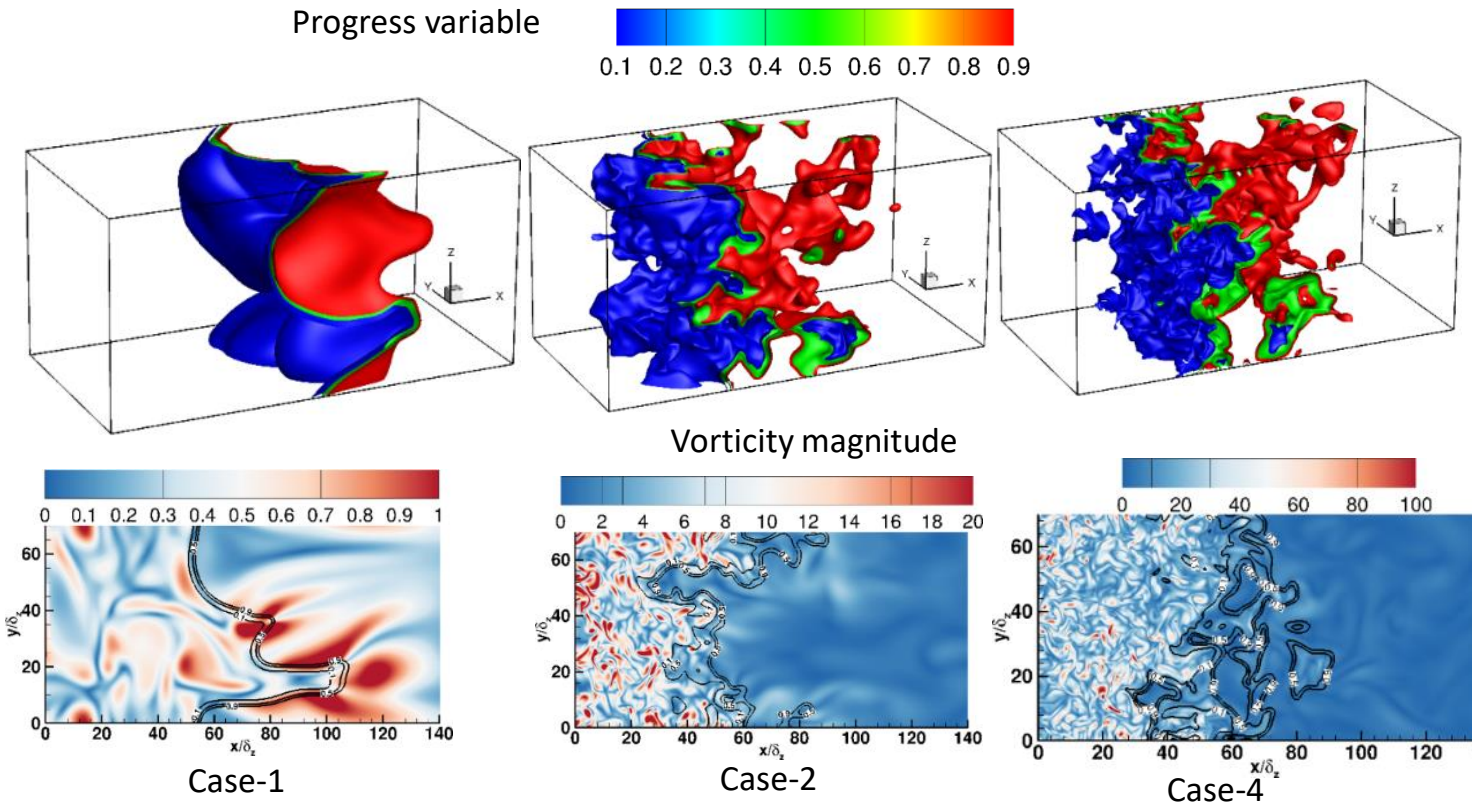


The flame generated vorticity strengthens with decreasing Lewis number *Le*

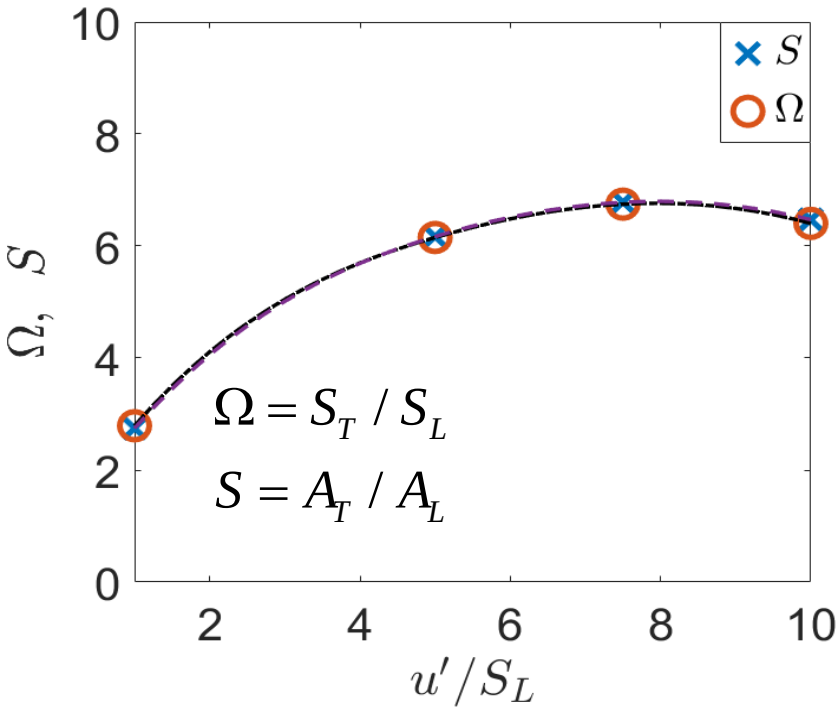
Chakraborty, Eur. J. Mech. Fluids B, 46, 201-220 (2014)

Chakraborty *et al.*, *Phys. Fluids*, 28, 015109, 2016

Flame area & volume-integrated burning rate for statistically planar flames



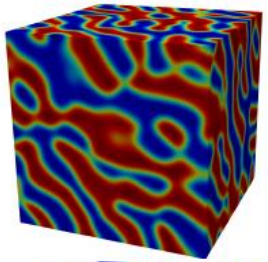
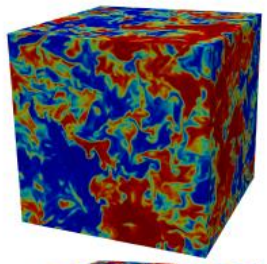
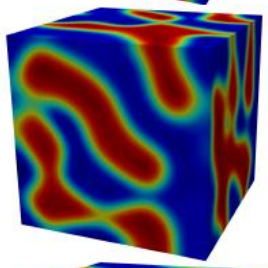
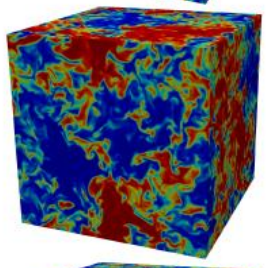
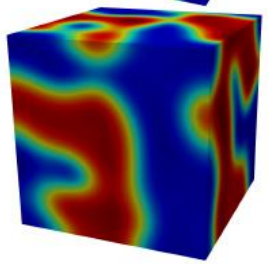
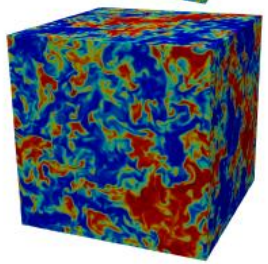
- Turbulent planar flame simulations have been performed.
- Turbulence is forced upstream of the flame using modified Lundgren's forcing.

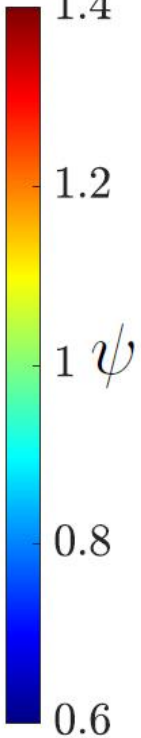


	u'/S_L	Ka	Da	Re_l
Case-1	1	0.577	3	7.56
Case-2	5	6.454	0.6	37.80
Case-3	7.5	11.858	0.4	56.70
Case-4	10	18.257	0.3	75.60

Chakraborty et al., *Phys. Fluids*, 33, 125132, 2021.Kasten et al., *Phys. Fluids* 33, 015111, 2021; Brearley et al., *Fluids*, 5(2), 89, 2020; Brearley et al., *Phys. Fluids*, 31,115109, 2019; Ahmed et al., Combust. Sci. Technol. 191 (2019) 898-920; Ahmed et al., Scientific Reports, 9 (2019) 5092.

Scalar forcing and stratified mixture combustion

ℓ_ψ/ℓ	Initial conditions		Forced turbulence +scalar forcing
0.5		$\rightarrow$ $18T_{turb}$	
1.0		$\rightarrow$ $18T_{turb}$	
1.5		$\rightarrow$ $18T_{turb}$	



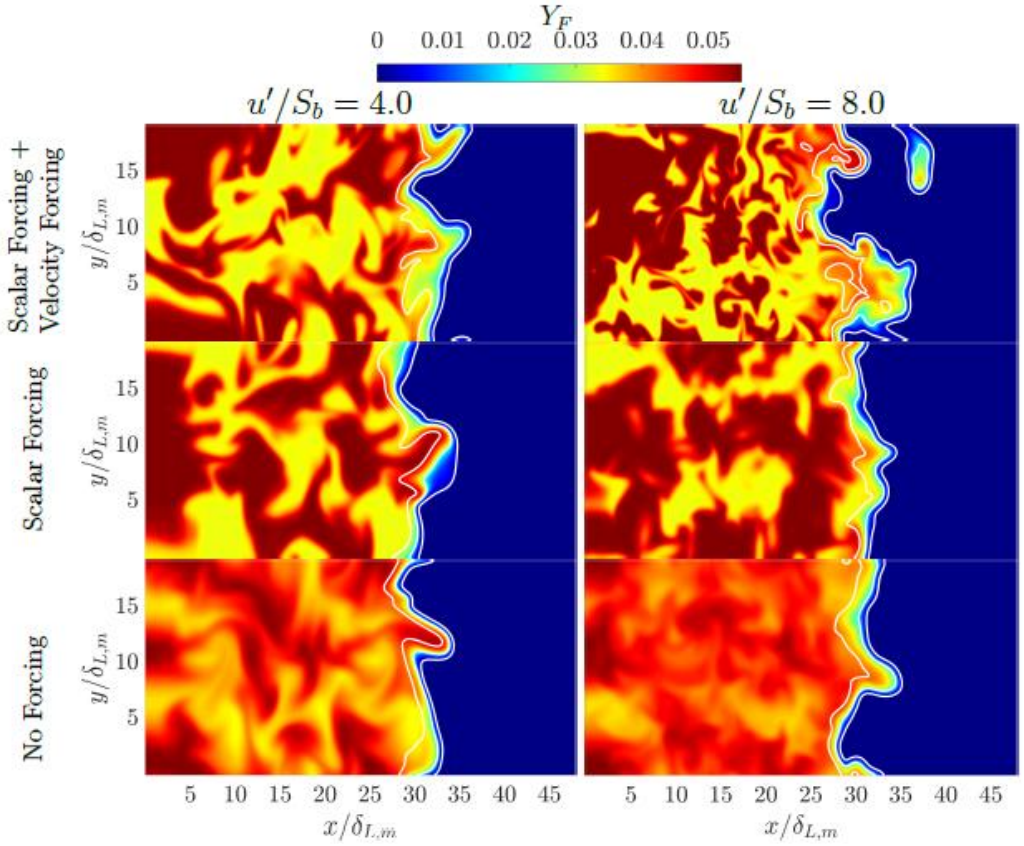
grid: 256^3

$Re_\lambda = 101$

$\langle\psi\rangle = 1.0$

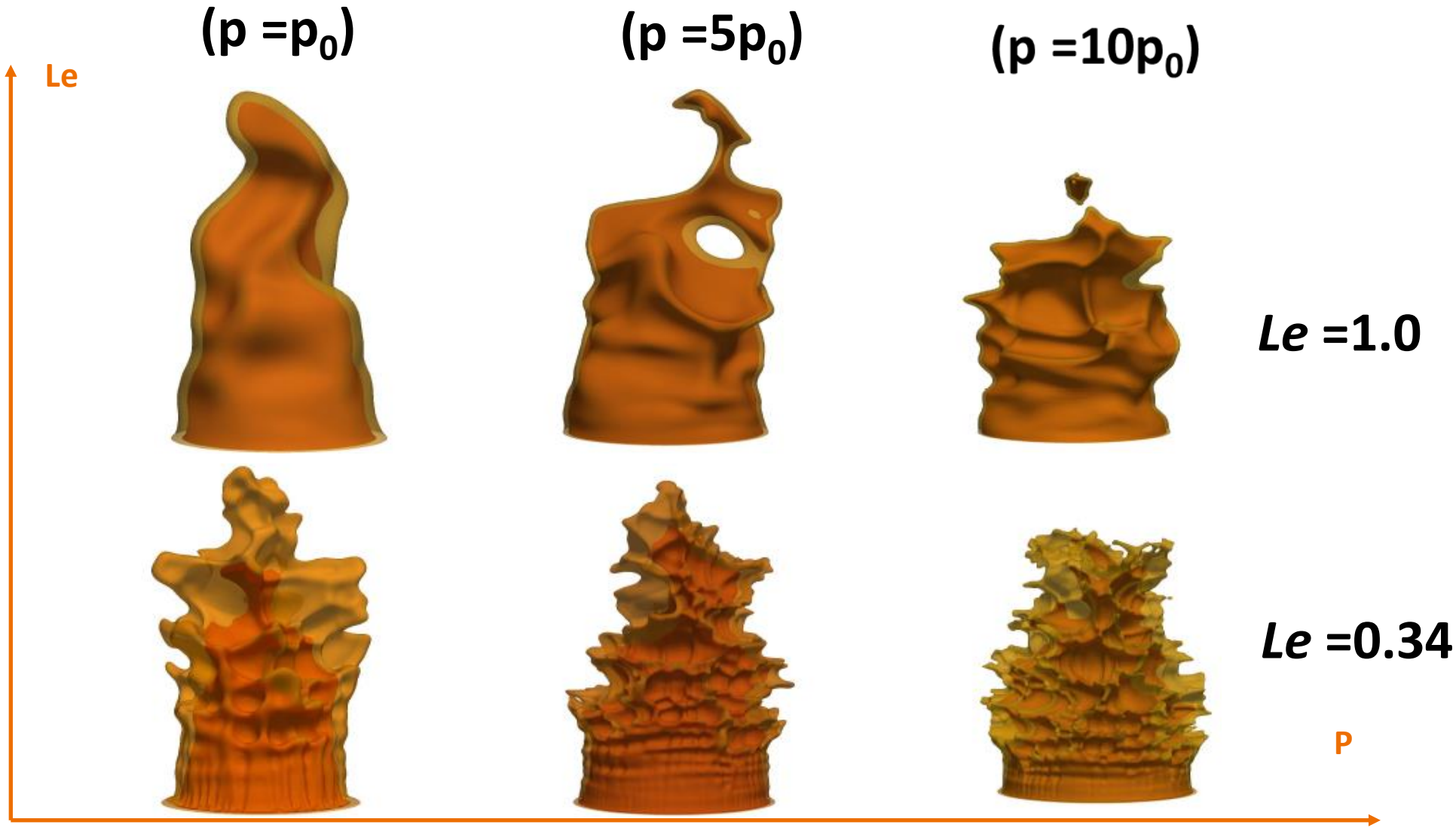
$\psi' = 0.29$

$T_{turb} = \ell/u'$



Brearley et al., *Flow Turb. Combust*. (accepted); Brearley et al., *Flow Turb. Combust*. https://doi.org/10.1007/s10494-021-00314-6 , 2022; Brearley et al., Phys. Fluids, 32, 125111,2020.

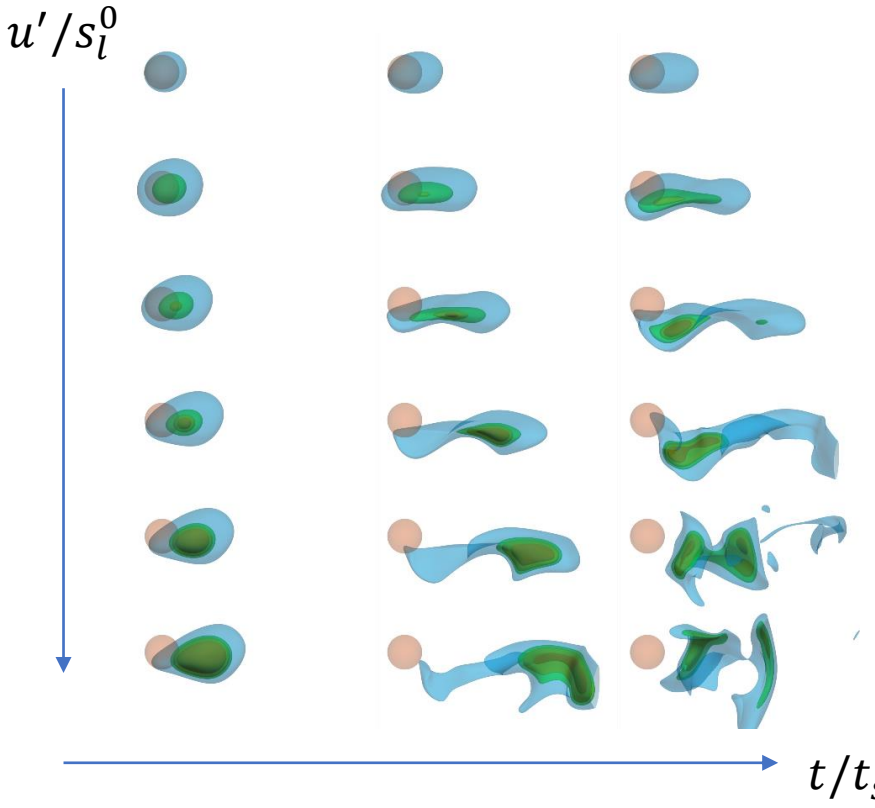
High-pressure turbulent premixed Bunsen flames

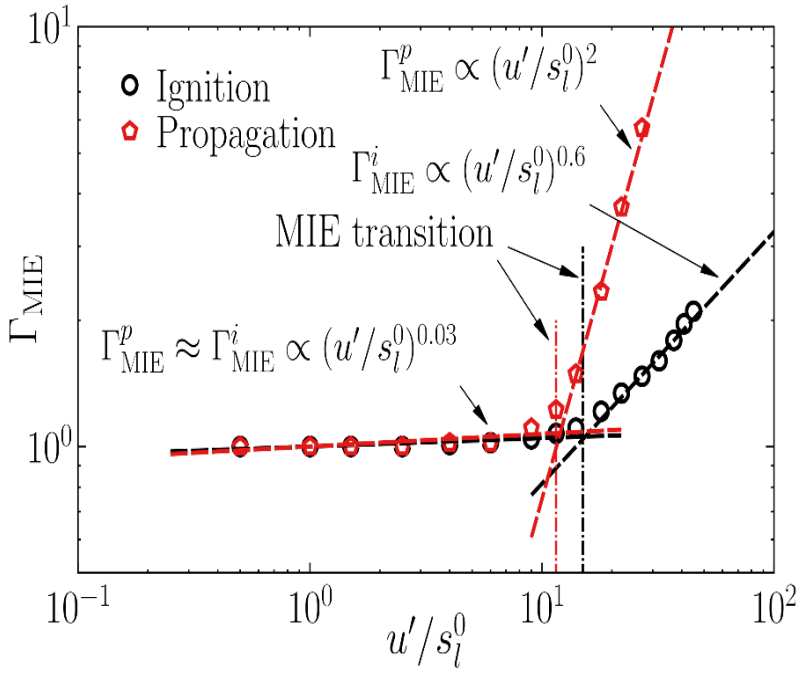


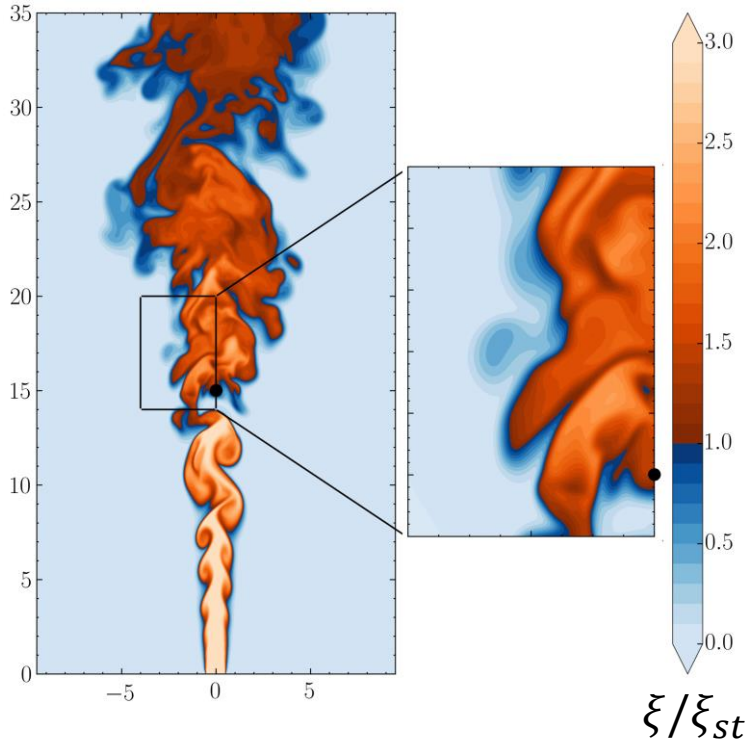
Rasool et al., *Combust. Flame*, https://doi.org/10.1016/j.combustflame.2021.111766 , 2022; Rasool et al. *Combust. Flame*, 231, 111500, 2021;. Keil et al., Flow Turb. Combust., 105, 869–888, 2020; Kasten et al., Combust. Sci. Technol. 192, 2050-2069, 2020; 64.; Keil et al. Combust. Sci. Technol., 192 (11), 2070-2092, 2020. Chakraborty et al., *Proc. Combust. Inst.*, 37, 2231-2239, 2019;

Localised forced ignition

- Applications in Direct Injection (DI) engines and high altitude gas turbine relight
- Fundamental understanding is important for reducing NOx in engines and fire safety
- Reduces the possibility of misfires and improves ignition probability



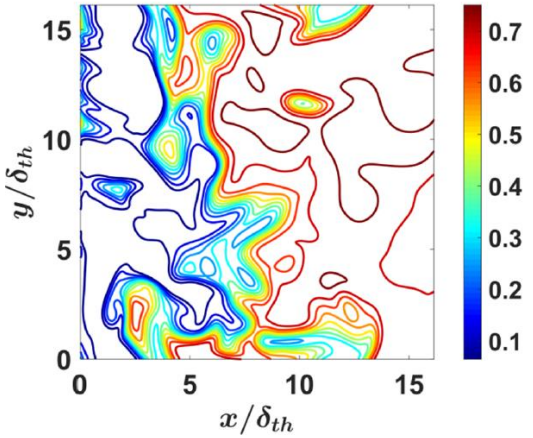




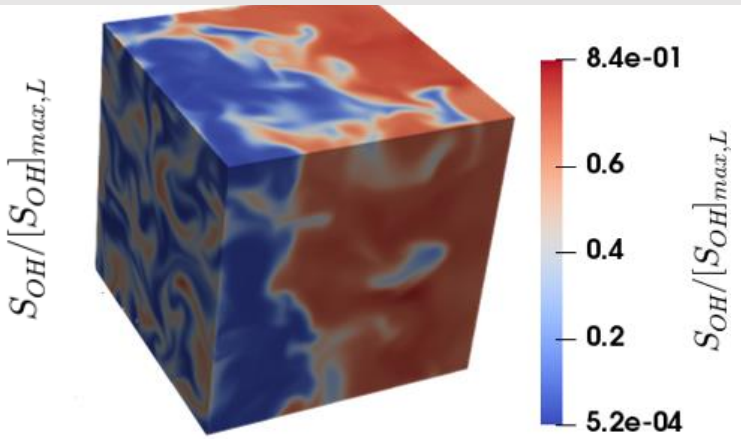
Green lines 10%, 40% and 70% of the maximum reaction rate of fuel

Turquand d'Auzay & Chakraborty, *Proc. Combust. Inst.*, 38, 2775-2782, 2021; Papapostolou et al., Flow Turb. Combust., 107, 367-403,2021; Turquand d'Auzay et al., *Combust. Flame*, 201, 104-117, 2019.

MILD combustion

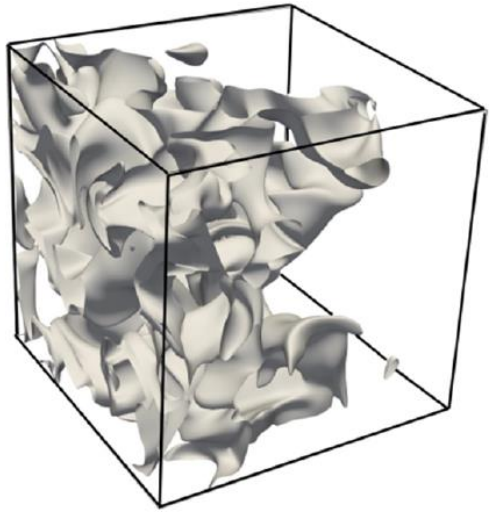


OH-PLIF signal S_{OH}

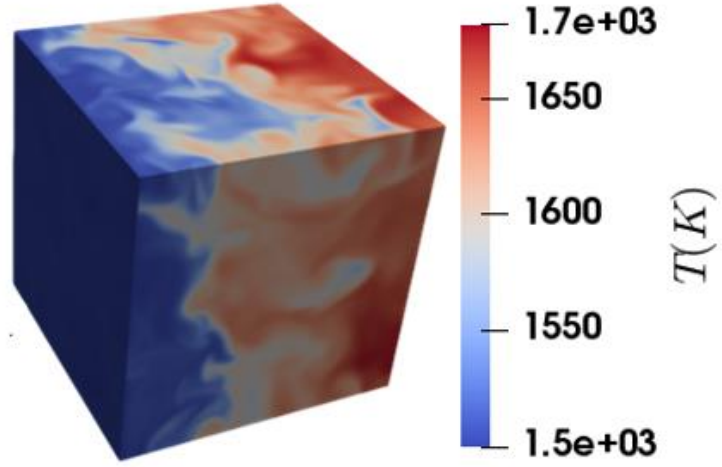


OH-PLIF signal S_{OH}

- Moderate or Intense Low oxygen Dilution (MILD) combustion can potentially improve thermal efficiency and reduce emissions.
- MILD combustion is realised when the initial mixture temperature T_0 is higher than the autoignition temperature T_{ign} and the maximum temperature rise due to combustion is smaller than the autoignition temperature $\Delta T < T_{ign}$.
- It is used in industrial furnaces and gas turbines for the advantages it offers in terms of NOx emission



$c = 0.8$ isosurface



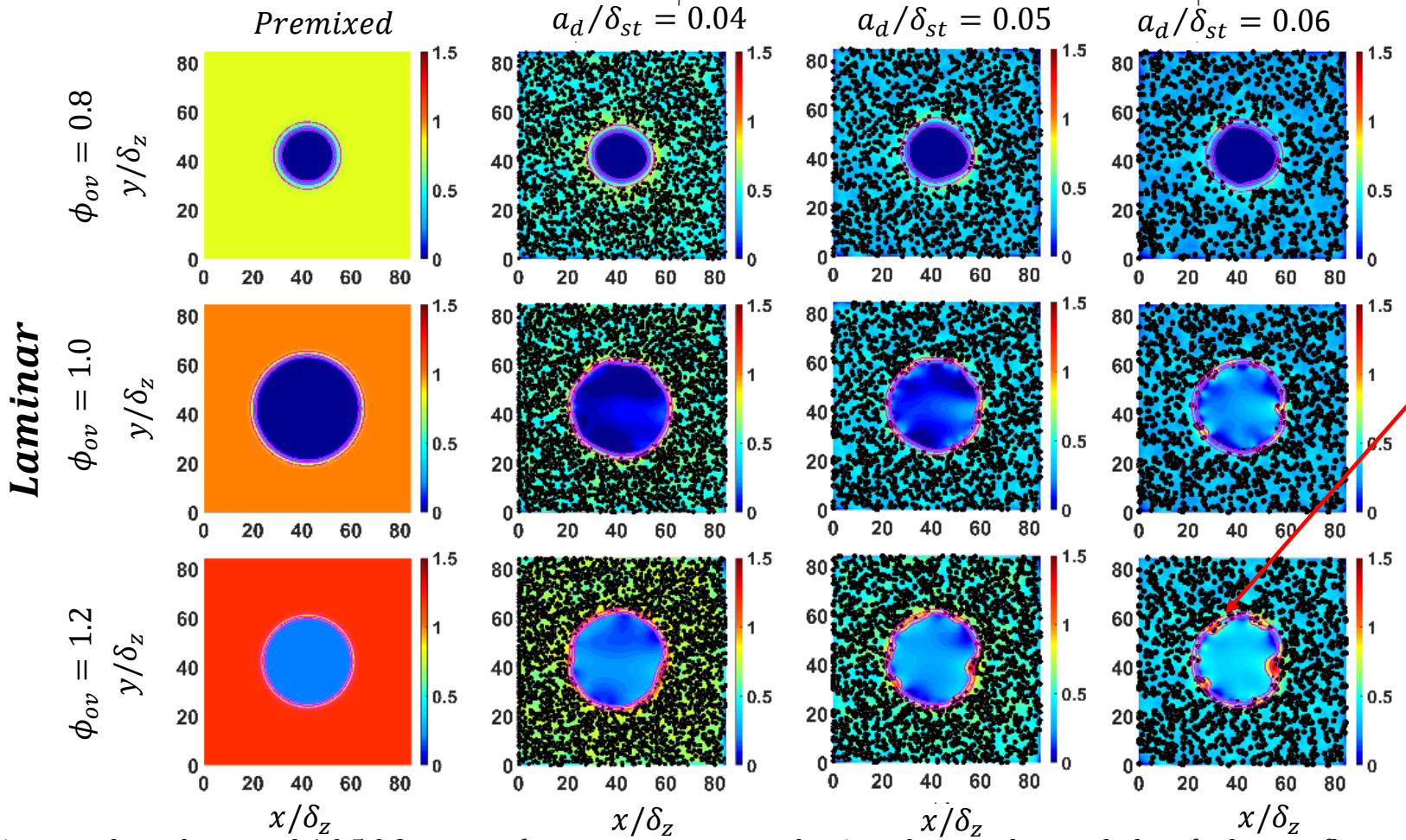
Temperature (K)

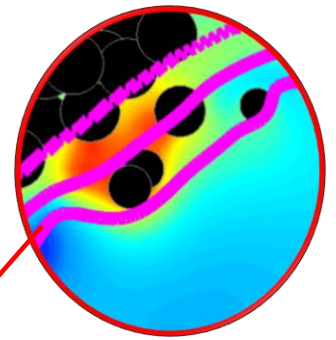
Awad et al., *Energies*, 14, 7677, 2021.

Flame-droplet-turbulence interaction

$\phi_{ov} = \phi_g + \phi_{liq}$

$u'/S_{b(\phi_g=1)} = 4.0$





$$\phi = \frac{(F/A)}{(F/A)_{stoic}}$$

$\phi < 1$: Fuel – lean

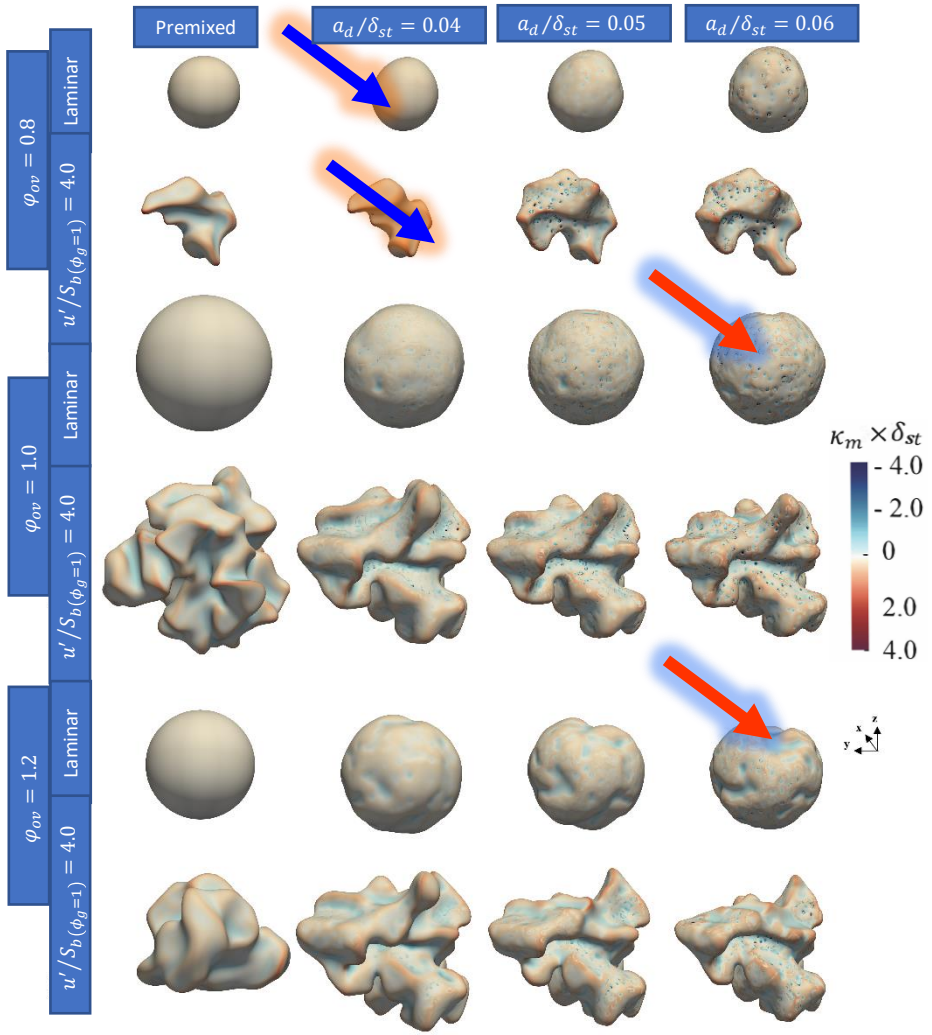
$\phi = 1$: Stoichiometric

$\phi > 1$: Fuel – rich

Distribution of $Y_F/Y_{F,st}$ (magenta lines show c = 0.1,0.5,0.9 contours from outer to inner periphery) on the central *x*-*y* mid-plane for laminar flames with $\phi_{ov} = 0.8, 1.0$ and 1.2. All figures correspond to $t = 2.52\alpha_{T0}/S^2_{b(\phi_g=1)}$

G. Ozel Erol et al., Phys. Fluids., 30, 086104,,(2018) G. Ozel Erol et al., Combust. Sci. Technol.,191, 833-867, (2019)
G. Ozel Erol et al., Flow Turbul. Combust., (2019) https://doi.org/10.1007/s10494-019-00035-x

Droplet-induced flame wrinkling



Instantaneous view of $c = 0.5$ isosurface coloured with local values of $\kappa_m \times \delta_{st}$ for the cases with $\phi_{ov} = 0.8$, $\phi_{ov} = 1.0$ and $\phi_{ov} = 1.2$ at $t = 2.52\alpha_{T0}/S^2_{b(\phi_g=1)}$.

$\phi_{ov} = 0.8, 1.0, 1.2$ and $a_d/\delta_{st} = 0.04, 0.05, 0.06$

Flame normal vector: $\vec{N} = -\nabla c/|\nabla c|$

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

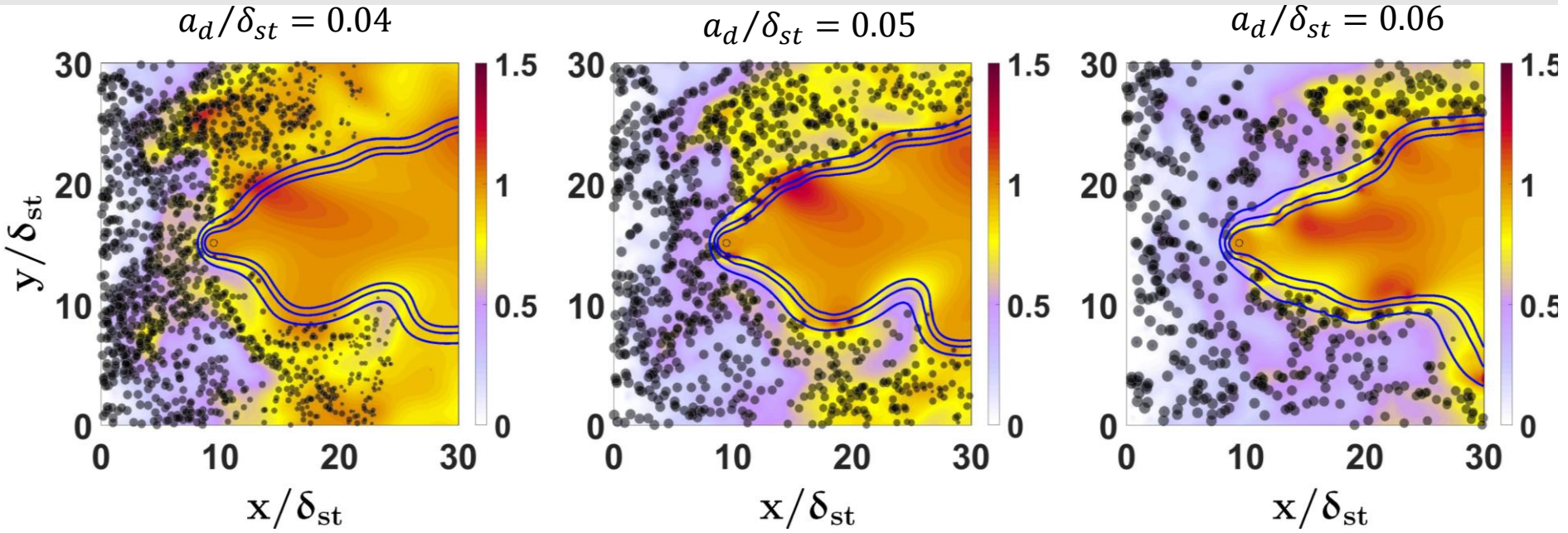
A positive curvature → convex to the reactants

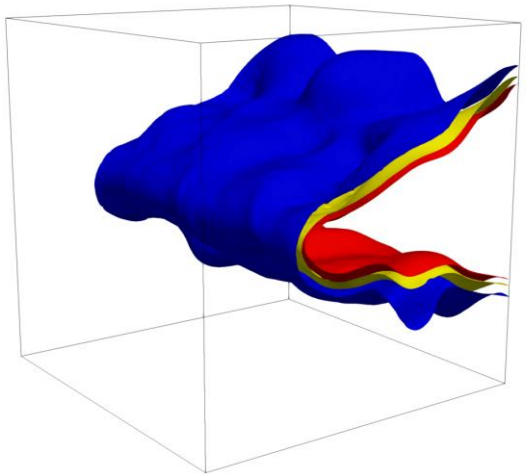
A negative curvature → concave to the reactants

- The droplet case with initial $a_d/\delta_{st} = 0.04$ for $\phi_{ov} = 0.8$ does not show dimples but laminar flame also does not remain spherical.
- Evaporation of clustered droplets creates large distributed dimples for the $\phi_{ov} = 1.2$ cases in contrast to small densely packed dimples in the $\phi_{ov} = 1.0$ cases.

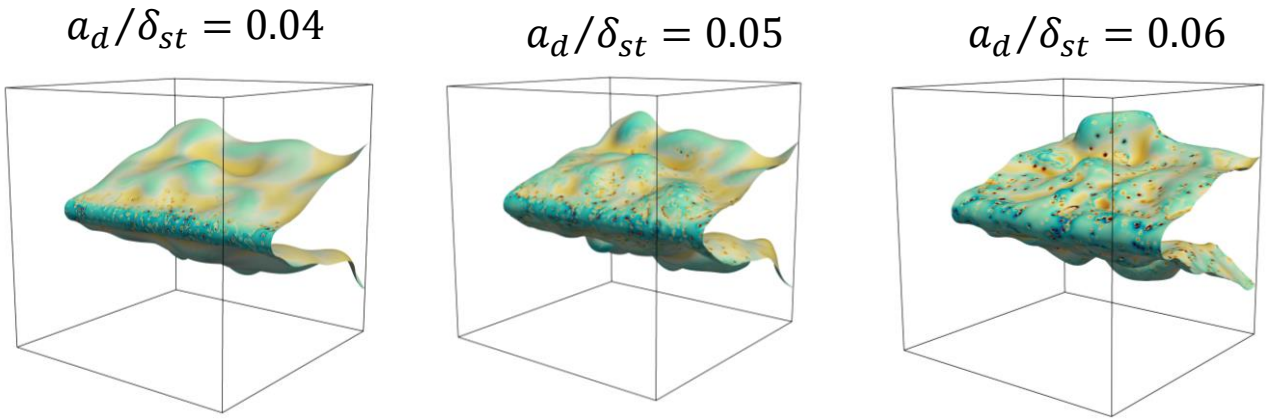
G. Ozel Erol et al., Phys. Fluids., 30, 086104,,(2018) G. Ozel Erol et al., Combust. Sci. Technol.,191, 833-867, (2019)
G. Ozel Erol et al., Flow Turbul. Combust., (2019) https://doi.org/10.1007/s10494-019-00035-x

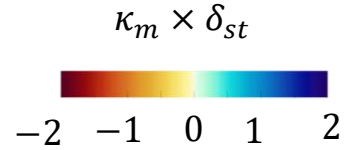
Flame-droplet interaction for laboratory-scale configuration





Instantaneous distributions of gaseous equivalence ratio, ϕ_g on the central x-y mid plane for statistically stationary rod-stabilised V-flames.

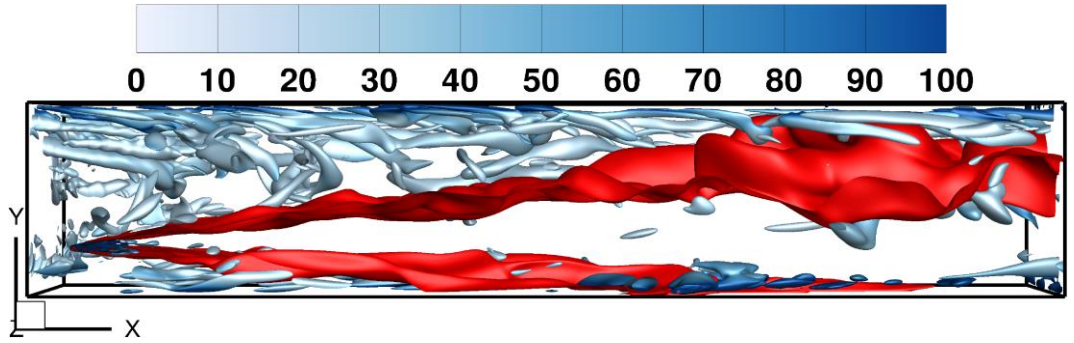




Ozel-Erol et al., *Int. J. Multiphase Flow,* 133, 103455, 2020; Ozel-Erol & Chakraborty, *Fluids*, 6, 1, 2021.

Simulation configurations in turbulent boundary layers

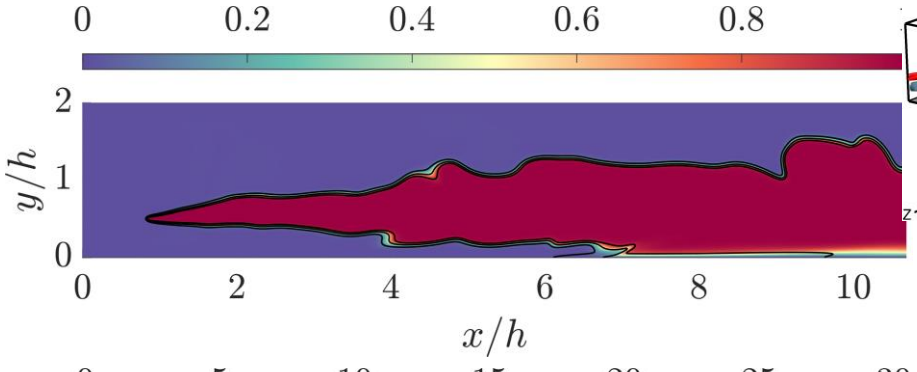
Oblique FWI for V-flames



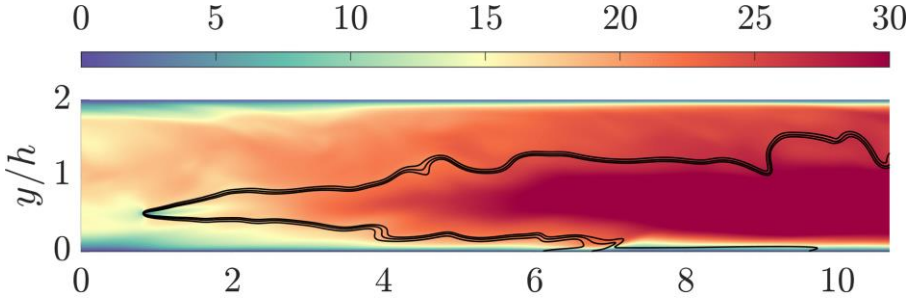
Q-criterion coloured by vorticity magnitude

Non-Dim. Temperature

$$T = \frac{\hat{T} - T_0}{T_{ad} - T_0}$$

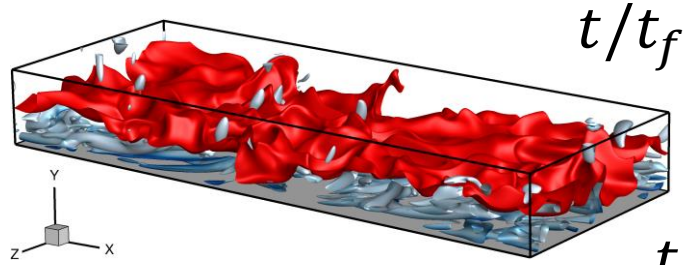


Non-Dim. Streamwise Velocity



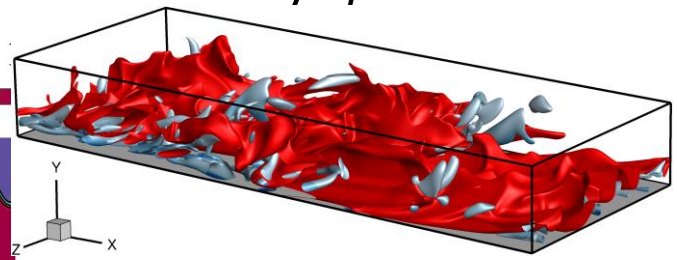
Head-on interaction (HOI)

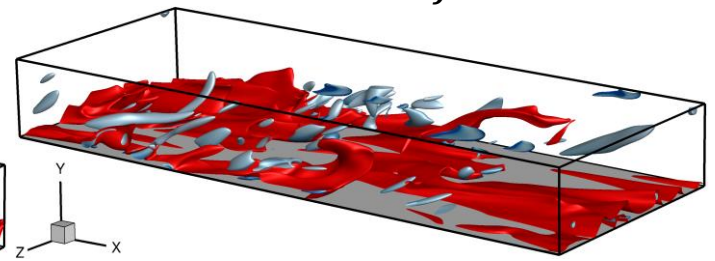
$t/t_f = 5.9$



$t/t_f = 14.6$

$t/t_f = 12.4$

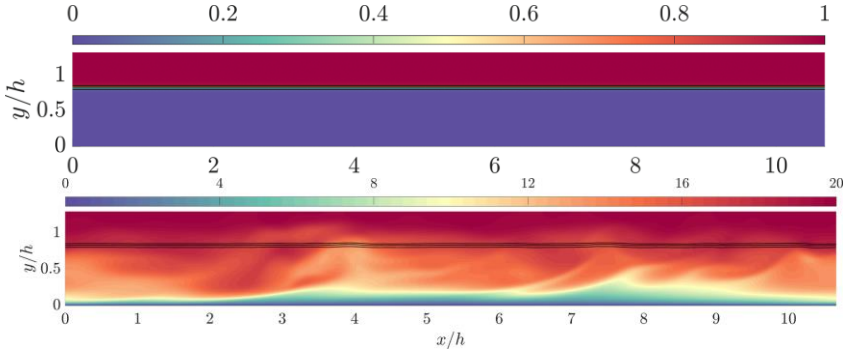




Q-criterion coloured by vorticity magnitude

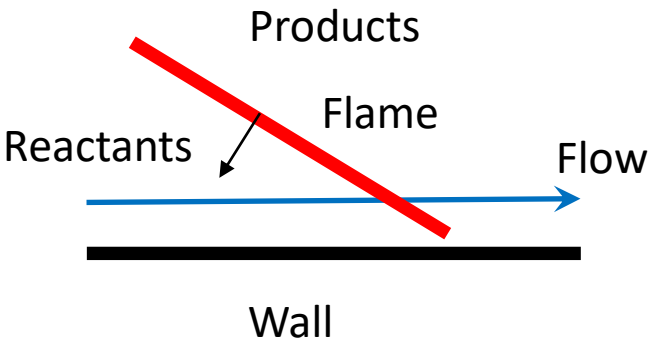
Non-Dim. Temperature

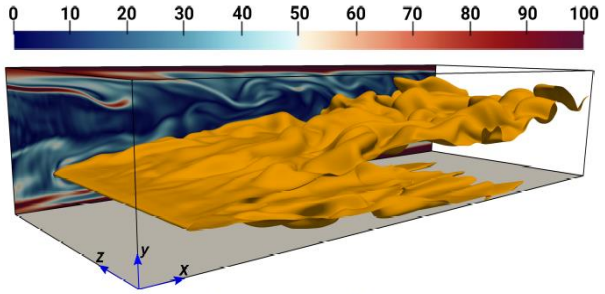
Non-Dim. Streamwise Velocity



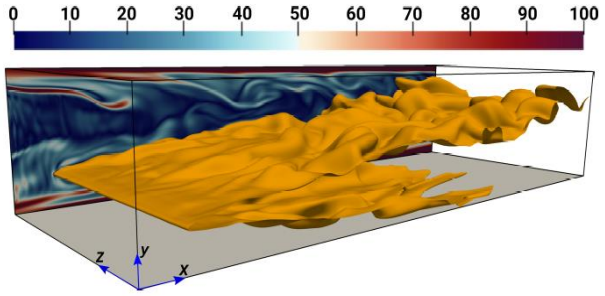
Ahmed, et al., *Int. J. Heat and Fluid Flow* , 92, 108881,(2021); Ahmed, et al., "*Combust. Flame,* 233, 111575 (2021); Ahmed et al., "Flow, Turb. Combust. 106, 701-732 (2021)

Mean shear stress at the wall for different boundary conditions

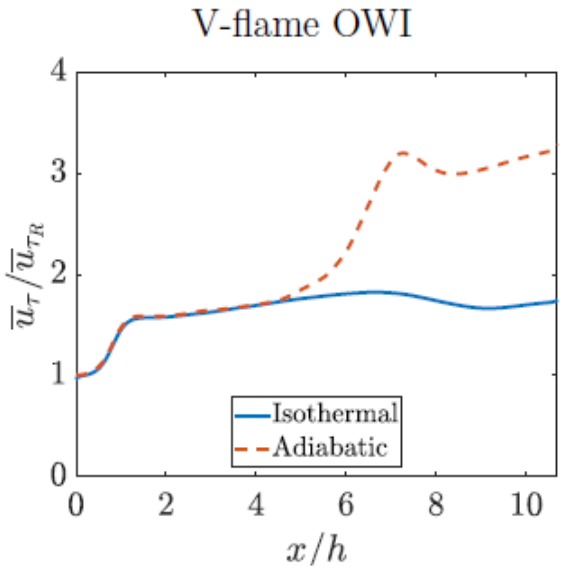


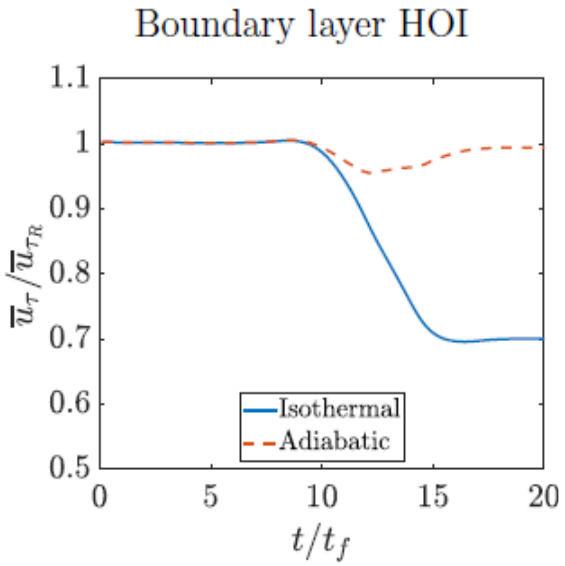


Isothermal Walls



Adiabatic Walls

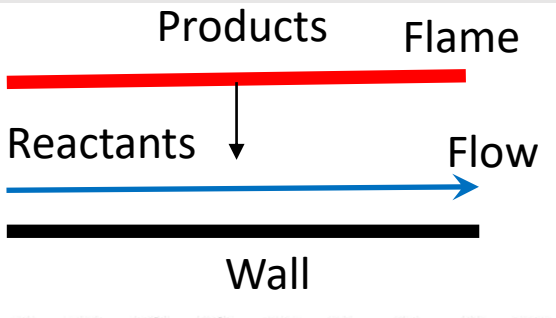


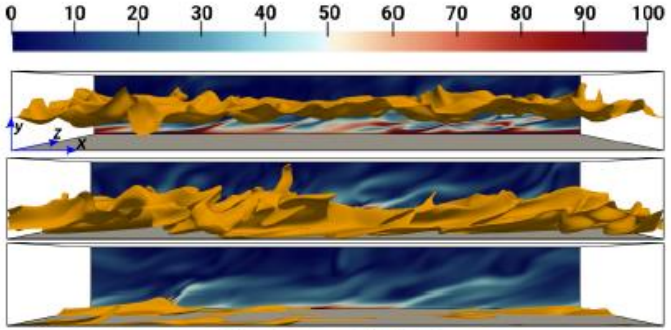


Isothermal

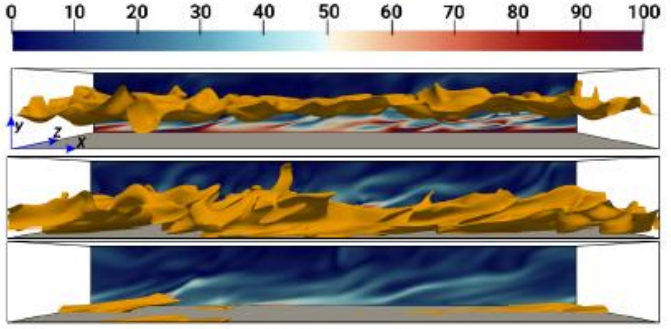
Adiabatic

Wall boundary condition, orientation of mean direction of flame propagation with respect to wall normal, and orientation of flame normal to the background flow direction are important factors for FWI





Isothermal Wall



Adiabatic Wall

Ahmed et al., *Int. J. Heat and Fluid Flow* , 92, 108881,(2021) Ghai et al., Entropy (2022); Ghai et al. Phys. Fluids (2022)

Importance of SENGA+ Work Package

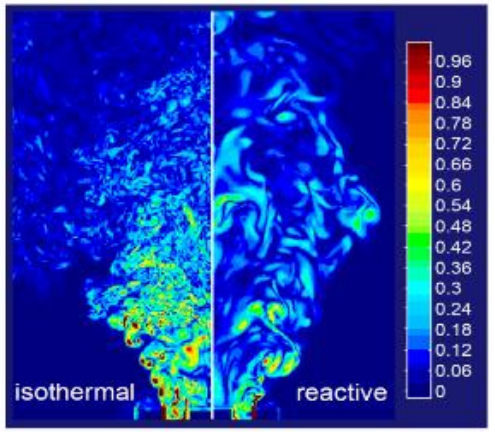
- 81% of the global energy demand is met by combustion but there is a need to move from the conventional fossil fuels to more environmentally friendly high hydrogen content (HHC) fuels (e.g. lean H_2 combustion, NH_3 combustion, NH_3-H_2 blends and e-fuels) to tackle the problems of global warming and also for achieving net-zero targets.
- Hydrogen combustion chemistry is significantly different from hydrocarbon fuels and both atomic and molecular hydrogen induce significant amount of preferential diffusion. Thus, use of HHC fuels often bring challenges (e.g. flashback within turbulent boundary layers in gas turbines). Moreover, the existing combustion models may not perform well at high-pressure HHC fuel combustion where thermo-diffusive and hydrodynamic instabilities interact with each other.

High-fidelity simulations enabled by SENGA+ will help in terms of fundamental physical understanding which in turn will translate into model development for RANS and LES. RANS/LES equipped with accurate models will contribute to the development of next generation combustors.

Work Package & High-priority Use Cases

- Work Package of SENGA+ will have following 4 sub work packages:

(1) Re-Engineering of SENGA+ with OPS
(2) SENGA+ high-level framework
(3) Evaluation and validation of the new SENGA+
(4) High Priority Use Cases



(1) Premixed swirl flames for HHC fuels
(generic configuration for gas turbine combustors but challenging case for simulation and modelling for net-zero hydrogen based combustion)

(2) Turbulent boundary layer flashback for hydrogen-rich fuels
(important from the point of view of safety of operation and structural integrity in gas turbines for net-zero combustion of HHC fuels)

Thank you for your attention

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