Influences of configuration on flame propagation in turbulent droplet-laden mixtures

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UK CTRF UK CONSORTIUM ON TURBULENT REACTING FLOWS

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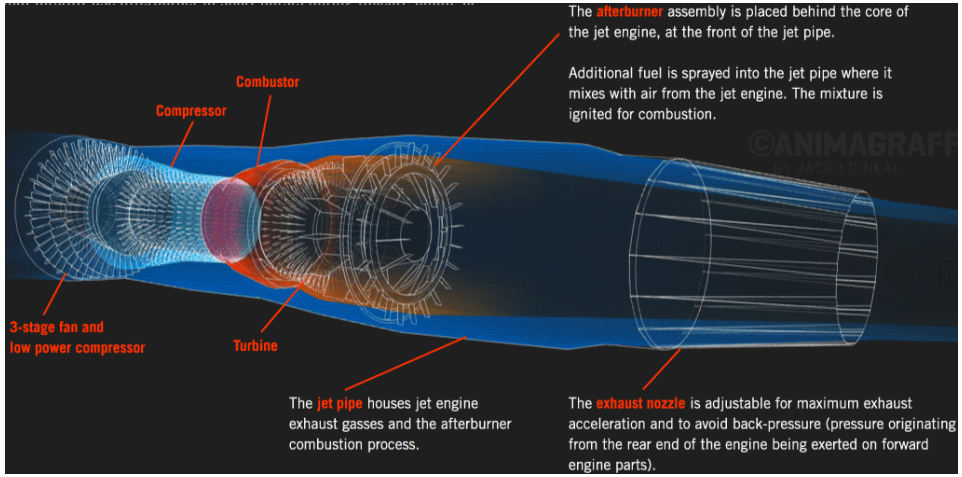
Introduction: Motivation

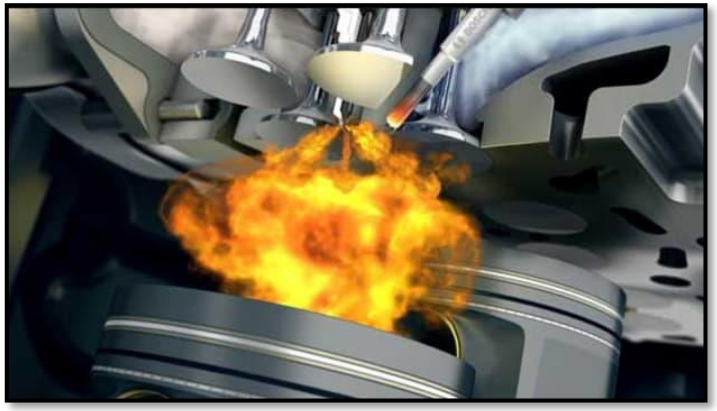


Combustion of droplet-laden mixtures :

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

Includes the critical processes:

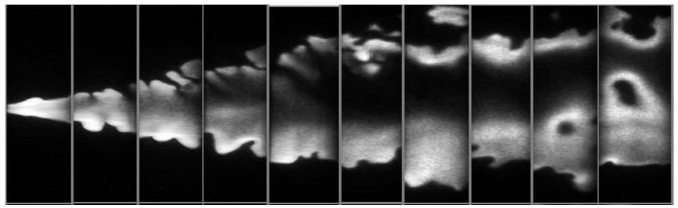
* evaporation of liquid droplets
* mixing of fuel vapour with the surrounding air
* interaction of droplets with the flame and flow field



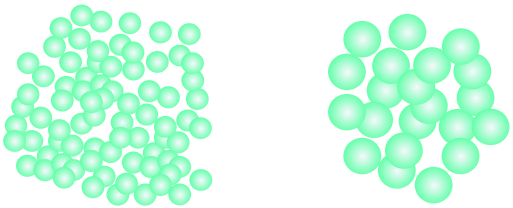
https://www.businessinsider.com/how-a-jet-engine-works-2015-2?utm_source=microsoft&utm_medium=referral&utm_term=windowsapp&r=US&IR=T
https://www.powerandmotoryacht.com/maintenance/diesel-engines-and-cleaner-environment

Introduction: Objectives

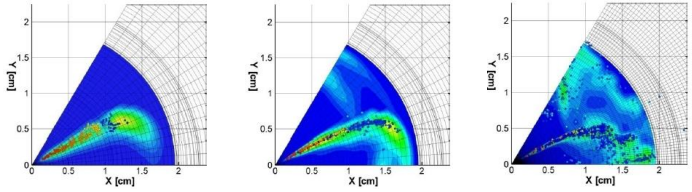
To investigate…



- evolution of the **gaseous reacting mixture composition** within
  (i) unsteady spherically expanding flames, and
  (ii) statistically stationary rod-stabilised V-flames,



- influences of **droplet diameter** on the **reaction zone structure** and **flame propagation characteristics** for two flame configurations,



- implications of findings in the context of **modelling** of turbulent combustion of droplet-laden mixtures.

P.V. Vena et al., 2007. Mixture fraction gradient effects on heat release in partially premixed, Spring Technical Meeting,Combustion Institute Canadian Section.
K. Jaguś, 2009. Large Eddy Simulation of fuel injection and spray combustion in an engine environment, Brunel University, PhD thesis.

Mathematical Background

Liquid Phase:

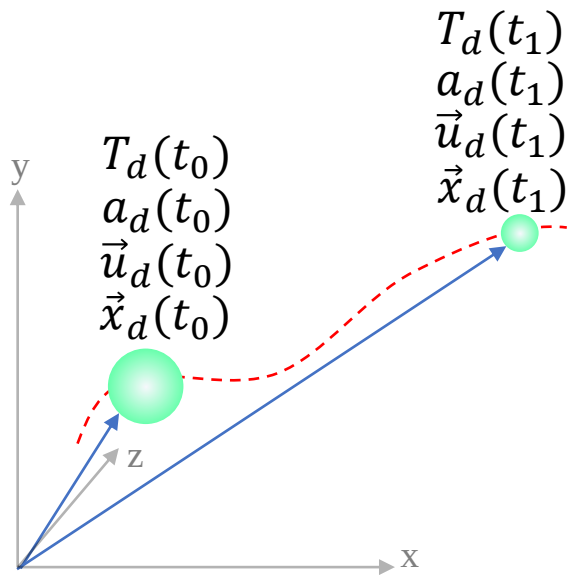
Lagrangian Approach is used for droplets following the approach proposed by Reveillon & Vervisch.

- 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

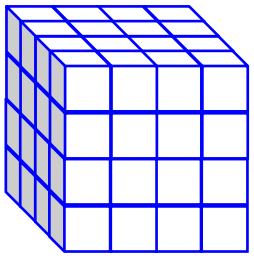


Reveillon, J., and Vervisch, L., 2005. Analysis of weakly turbulent dilute-spray flames and spray combustion regimes, J. Fluid Mech. 537, 317–347.

Mathematical Background

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:

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

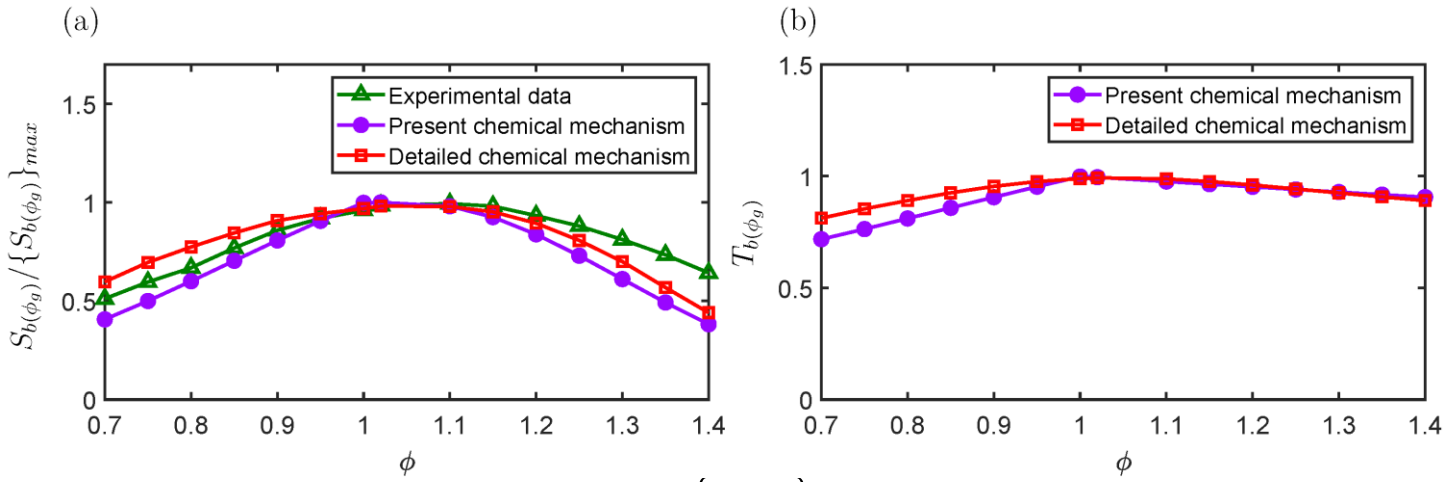
$\psi_1 = \{1, u_j, \hat{T}, Y_F, Y_O\}$ for $\psi = \{1, u_j, e, Y_F, Y_O\}$
$\Gamma_\psi = \rho\nu/\sigma_\psi$ for $\psi = \{1, u_j, Y_F, Y_O\}$ and $\Gamma_\psi = \lambda$ for $\psi = e$
$\dot{w}_\psi$ is chemical reaction rate,
$\dot{S}_g$ is an appropriate source/sink term and
$\dot{S}_\psi$ is ***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.

Mathematical Background

Code:

3D,compressible DNS code, SENGA+

- High order finite difference scheme
- Time advancement: Explicit low-storage 3rd order Runge-Kutta scheme.
- A modified single-step Arrhenius-type irreversible chemical reaction (Tarrazo et al., (2006))
- Droplets are treated as sub-grid point sources.



Variation of the (a) normalised laminar burning velocity $S_{b(\phi_g)}/\{S_{b(\phi_g)}\}_{max}$ and (b) normalised adiabatic flame temperature $T_{b(\phi_g)} = (T_{ad(\phi_g)} - T_0)/(T_{ad(\phi_{g=1})} - T_0)$ with equivalence ratio ϕ_g for n-heptane obtained from modified single step chemistry (Tarrazo *et al.*, 2006), detailed chemical mechanism (Chaos *et al.*, 2007) and experimental (Kumar *et al.*, 2007) data.

Chaos, M. et al.,A high-temperature chemical kinetic model for primary reference fuels. Int. J. Chem. Kinet. 39, (2007).
Kumar, K. et al., Laminar flame speeds of preheated iso-octance/O2/N2 and n-heptane/O2/N2 mixtures, J. Propulsion Power 23, (2007).
Tarrazo, E.Fet al.A simple one-step chemistry model for partially premixed hydrocarbon combustion. Combust. Flame. 147, 32–38 (2006).

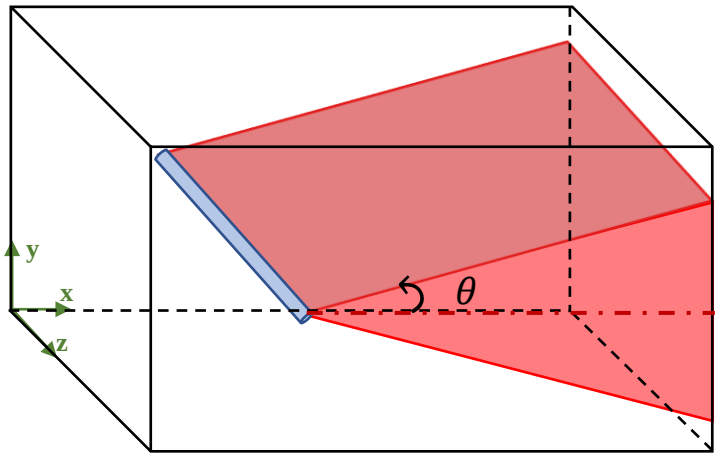
Mathematical Background: V-flame

Reacting flow field initialisation:

1D steady-state laminar spray flame, COSILAB

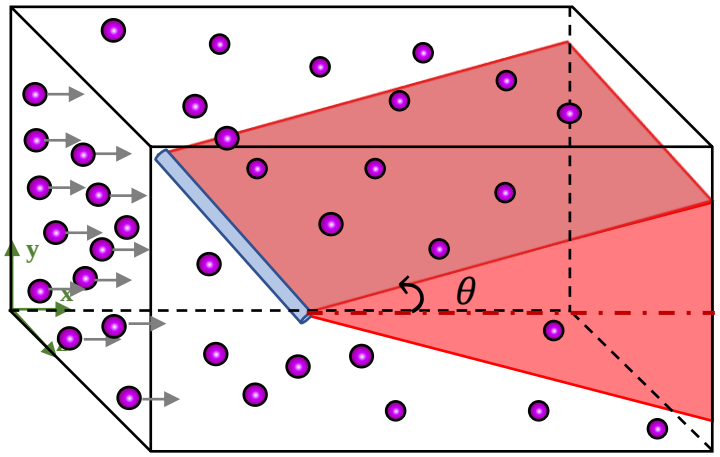
- Generated according to the droplet diameter for an overall equivalence ratio of unity

- 1D profiles are then specified based on the flame angle



Mathematical Background: V-flame

- Fuel is supplied in the form of liquid droplets at the inlet which is placed on the left-hand side of the domain.

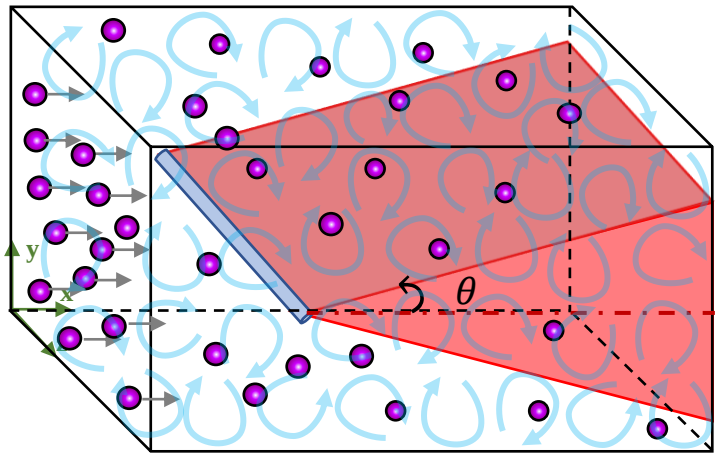


Mathematical Background: V-flame

- Fuel is supplied in the form of liquid droplets at the inlet which is placed on the left-hand side of the domain.

Turbulent flow field initialisation:

- Incompressible homogeneous isotropic velocity field is superimposed on the V-shaped flames propagating into droplet-laden mixtures

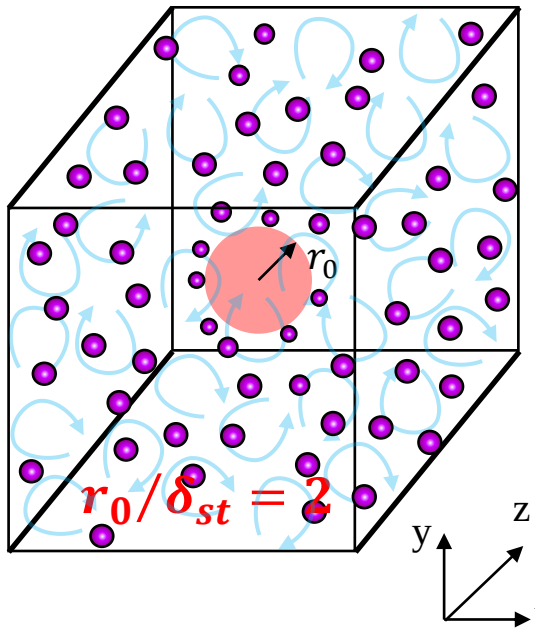


Mathematical Background: Flame kernel

Reacting flow field initialisation:

1D steady-state laminar spray flame, COSILAB

- Generated according to the droplet diameter and overall equivalence ratio
- 1D profiles are then specified in the radial direction from the centre of the domain.



Turbulent flow field initialisation:

- Incompressible homogeneous isotropic velocity field is superimposed on the laminar spherical flames with $r_0/\delta_{st} = 2.0$

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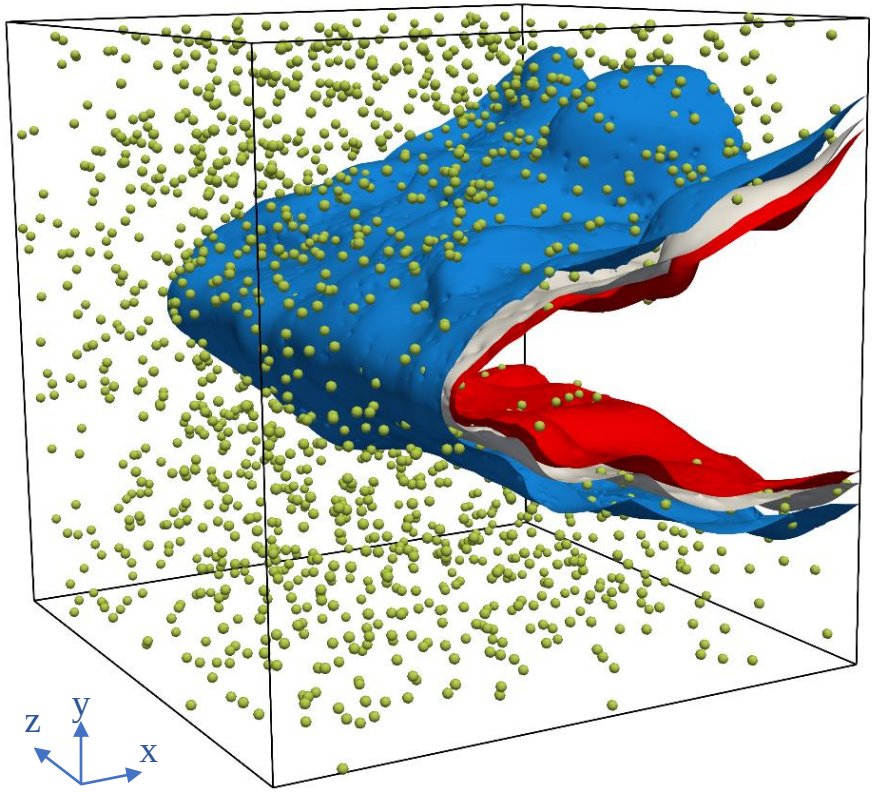
Numerical Implementation: V-flame

Simulation parameters:

- *Domain:* $(30\delta_{st})^3$ (where δ_{st} is the thermal flame thickness of unstrained stoichiometric laminar premixed flame)
- *Grid number:* $(384)^3$
- *Equivalence ratio:* $\phi_{ov} = 1.0$

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

Equivalence ratio: $\phi = \frac{FAR}{FAR_{st}}$



Reaction progress variable iso-surfaces at $c = 0.1, 0.5$ and 0.9 (from blue to red) for $a_d/\delta_{th} = 0.06$ (where a_d and δ_{th} are initial droplet diameter and thermal flame thickness respectively), at $t = 2t_{flow}$.

Numerical Implementation: V-flame

Simulation parameters

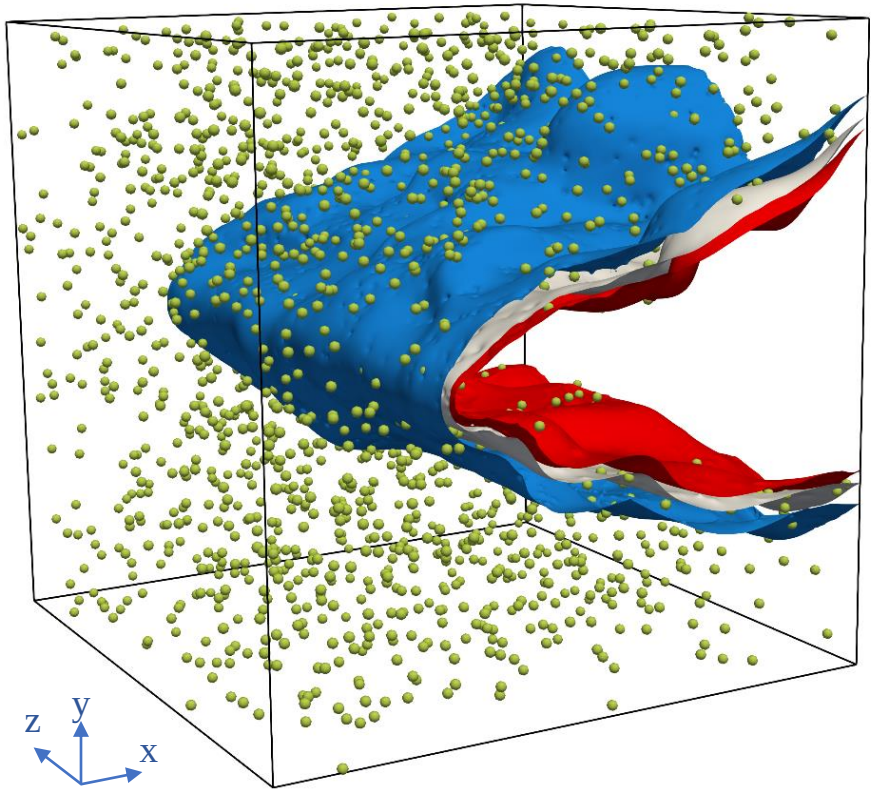
- *Heat release parameter:* $\tau = 6.4$
- *Droplet diameter:* $a_d/\delta_{st} = 0.04$, 0.05 and 0.06

$$\delta_{st} = \frac{(T_{ad(\phi_g=1)} - T_0)}{\max|\nabla \hat{T}|_L}$$

- *Boundary conditions: NSCBC*

x-direction → *inflow and outflow*

y and z directions → *periodic*



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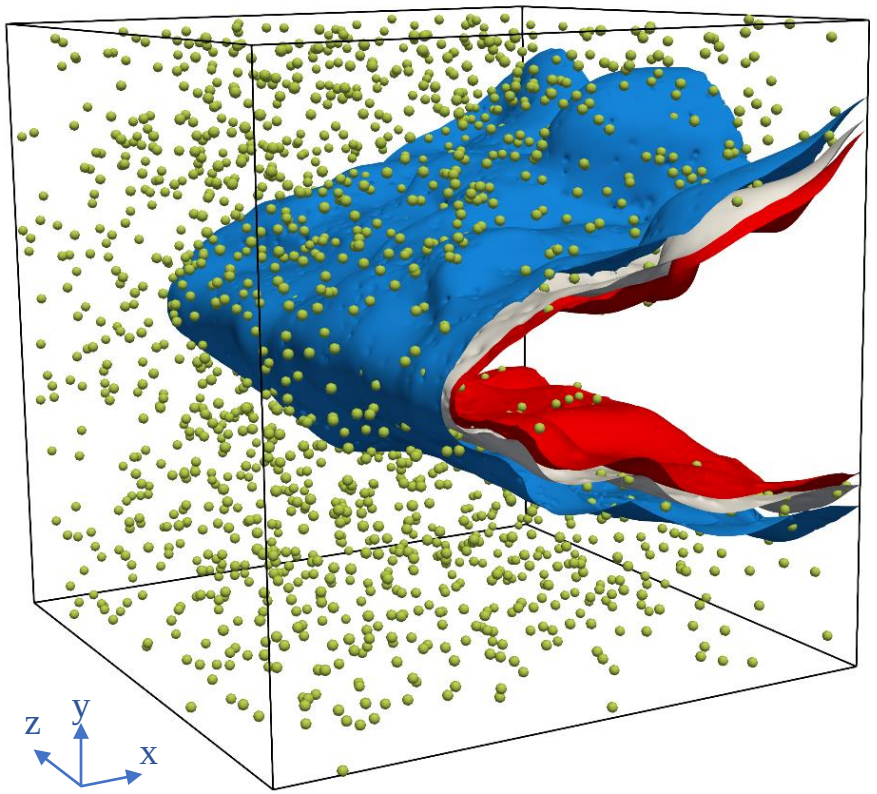
Numerical Implementation: V-flame

Simulation parameters

- *Holder position (x,y):* $(120\Delta x, 192\ \Delta y)$
- *Holder radius:* $r = 0.3\delta_{st}$
- Y_F, Y_O and T are imposed using a Gaussian weighting function $g(r) = Aexp[-r^2/2\varsigma^2]$ at the flame holder
- *Simulation time:* $t = 2.0t_{flow}$

$$t_{flow} = L_x/u_{mean}$$



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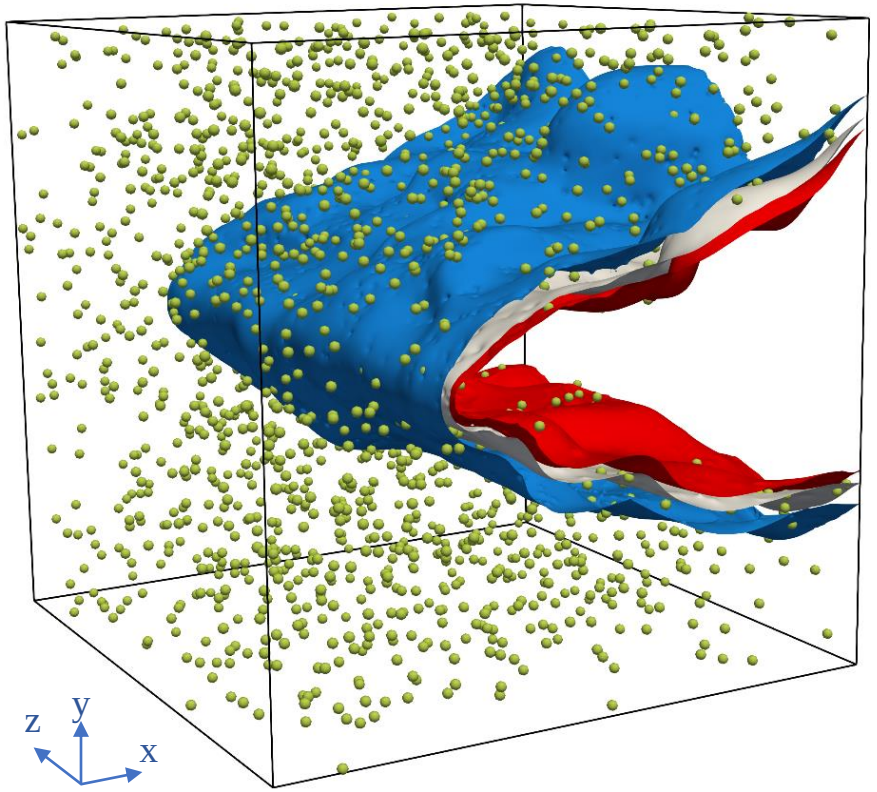
Dunstan, T. D. et al., Geometrical Properties and Turbulent Flame Speed Measurements in Stationary Premixed V-flames Using Direct Numerical Simulation. Flow Turb. Combust. 87, 237-259 (2011).

Numerical Implementation: V-flame

Simulation parameters

- *Initial rms:* $u'/S_{b(\phi_g=1)} = 2.0$
- *Longitudinal integral length-scale:* $L_{11}/\delta_{st} = 2.5$
- *Mean inlet velocity:* $\bar{u}_{mean}/S_{b,st} = 5.0$
- *Turbulent velocity fluctuations at the inlet plane with the help of Taylor's hypothesis*



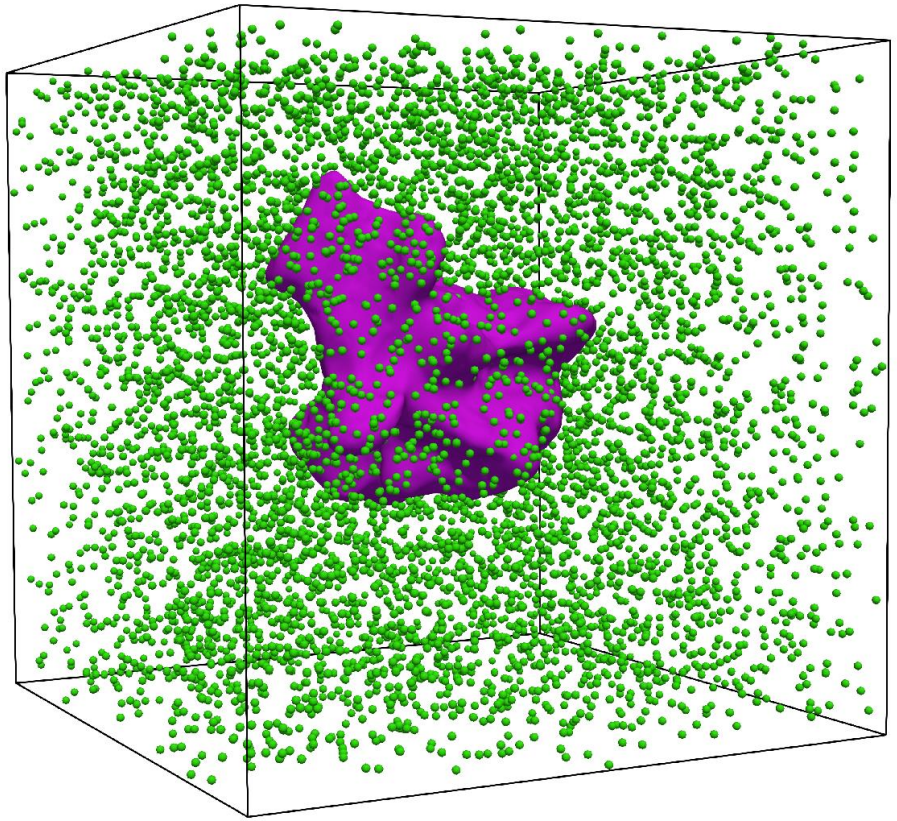
Reaction progress variable iso-surfaces at $c = 0.1, 0.5$ and 0.9 (from blue to red) for $a_d/\delta_{th} = 0.06$ (where a_d and δ_{th} are initial droplet diameter and thermal flame thickness respectively), at $t = 2t_{flow}$.

Chakraborty, N. et al., Unsteady effects of strain rate and curvature on turbulent premixed flames in an inlet-outlet configuration. Combust. Flame 137, 129-147 (2004).

Mathematical Background: Flame kernel

Simulation parameters

- *Domain:* $(40\delta_{st})^3$
- *Grid number:* $(512)^3$
- *Initial kernel radius:* $r_0/\delta_{st} = 2.0$
- *Initial rms:* $u'/S_{b(\phi_g=1)} = 4.0$
- *Boundary conditions: NSCBC, Partially non-reflecting outflow*



Reaction progress variable, c:

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

Mixture fraction, ξ

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

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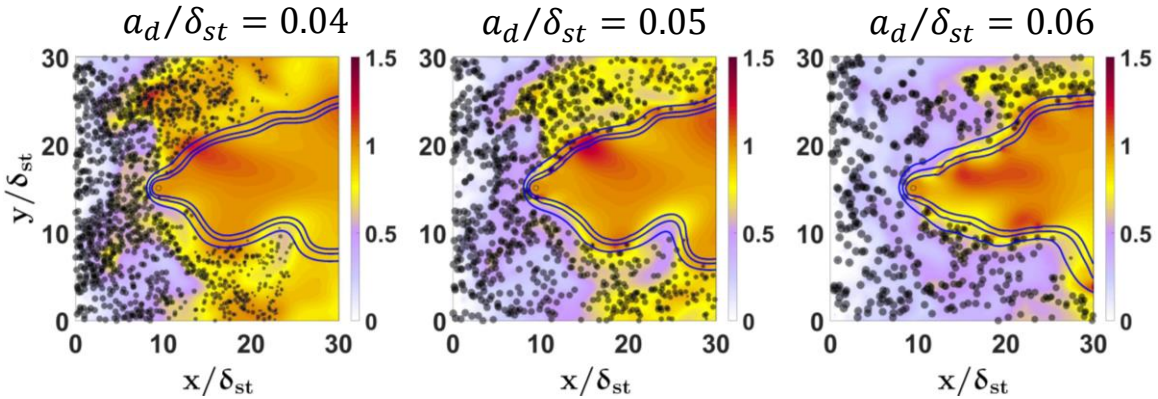
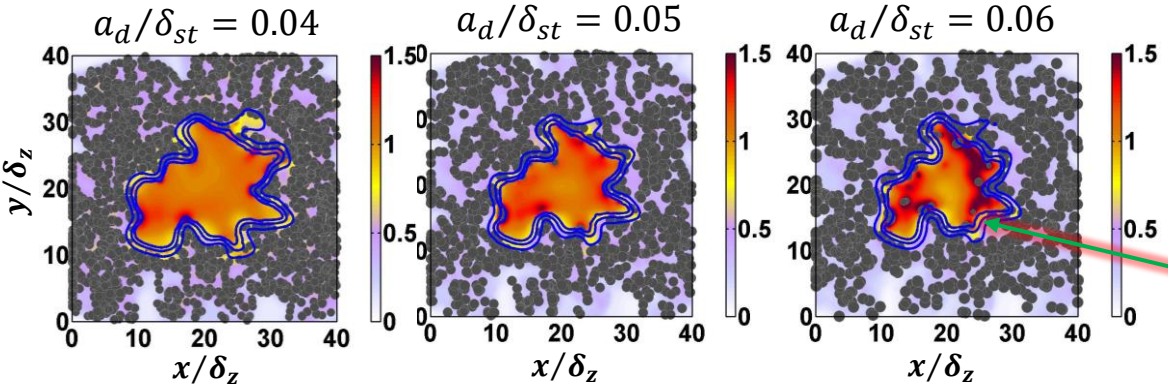
Results: Flame-droplet-turbulence interaction

statistically stationary rod-stabilised V-flames:



unsteady spherically expanding flames:



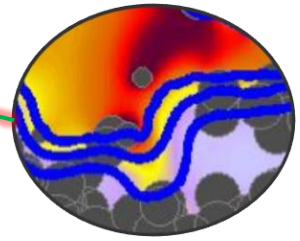
Instantaneous distributions of gaseous equivalence ratio, ϕ_g on the central x-y mid plane for statistically stationary rod-stabilised V-flames (first row) and unsteady spherically expanding flames (second row).

Smaller droplets:

- Mostly complete their evaporation by halfway in the streamwise direction

Larger droplets:

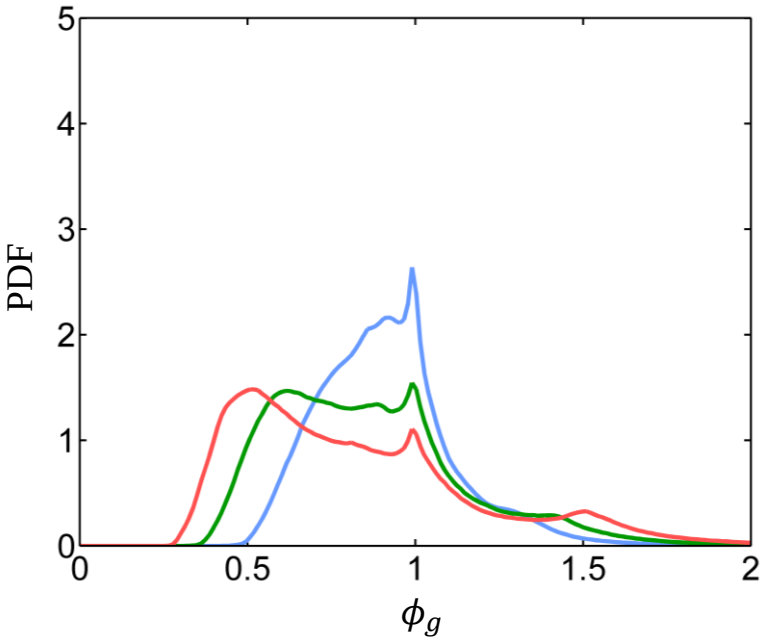
- Survive longer due to their lower evaporation rate
- interact more with the flame than smaller droplets



Results: Gaseous equivalence ratio, ϕ_g

$a_d/\delta_{st} = 0.04$ $a_d/\delta_{st} = 0.05$ $a_d/\delta_{st} = 0.06$

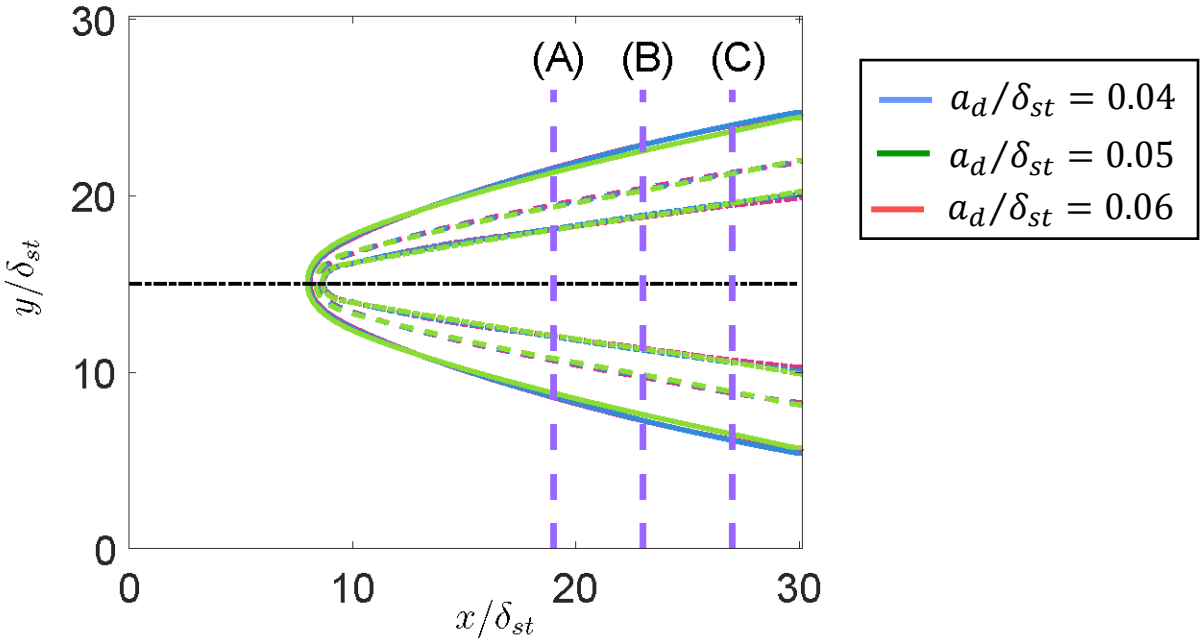
unsteady spherically expanding flames:



PDFs of ϕ_g in the region corresponding to $0.01 \leq c \leq 0.99$ for initial turbulence intensity of $u'/S_{b(\phi_g=1)} = 4.0$

Results: Gaseous equivalence ratio, ϕ_g

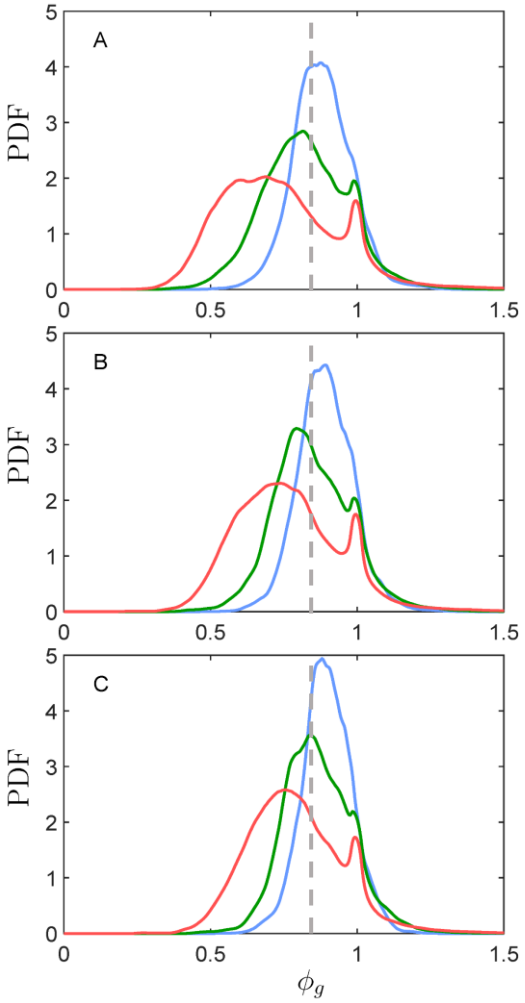
statistically stationary rod-stabilised V-flames:



Contours of $\tilde{c} = 0.1$ (solid line), 0.5 (dashed line) and 0.9 (dotted line) contours.

Distances from the flame holder for A, B and C:

$x_A/\delta_{st} = 9$ $x_B/\delta_{st} = 13$ $x_C/\delta_{st} = 17$



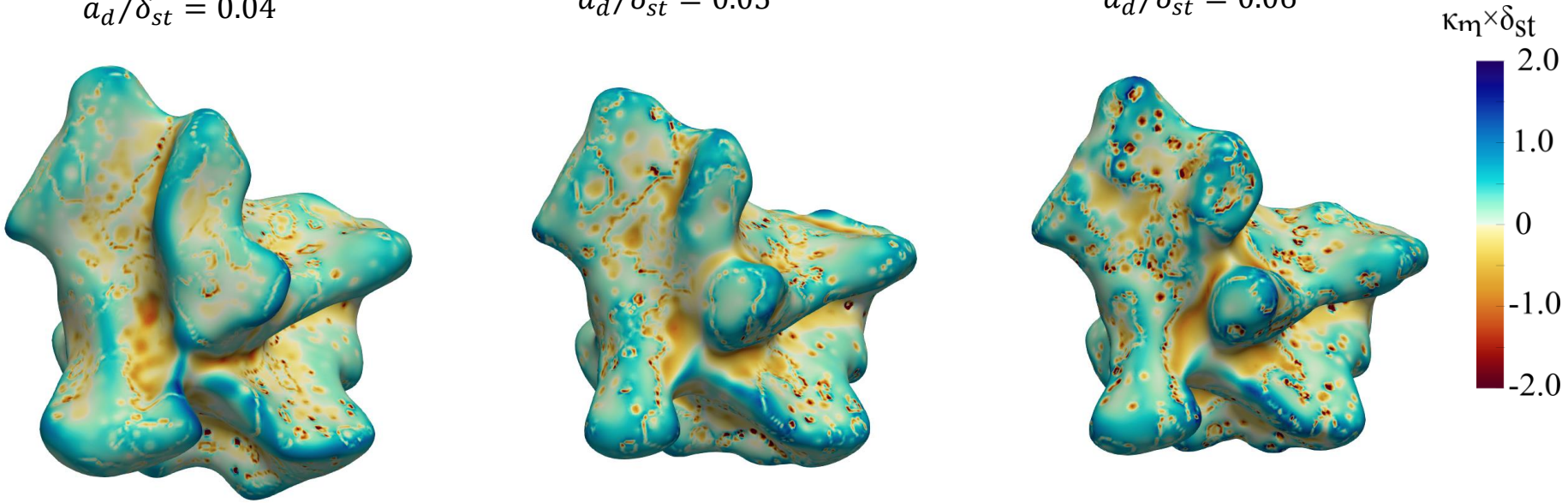
PDFs of ϕ_g in the region corresponding to $0.01 \leq c \leq 0.99$ at different locations A, B and C (top to bottom)

Results: Flame-droplet interaction

unsteady spherically expanding flames:

Local flame curvature: $\kappa_m = 0.5\nabla \cdot \vec{N}$ *Local flame normal:* $\vec{N} = -\nabla c/|\nabla c|$

$a_d/\delta_{st} = 0.04$ $a_d/\delta_{st} = 0.05$ $a_d/\delta_{st} = 0.06$

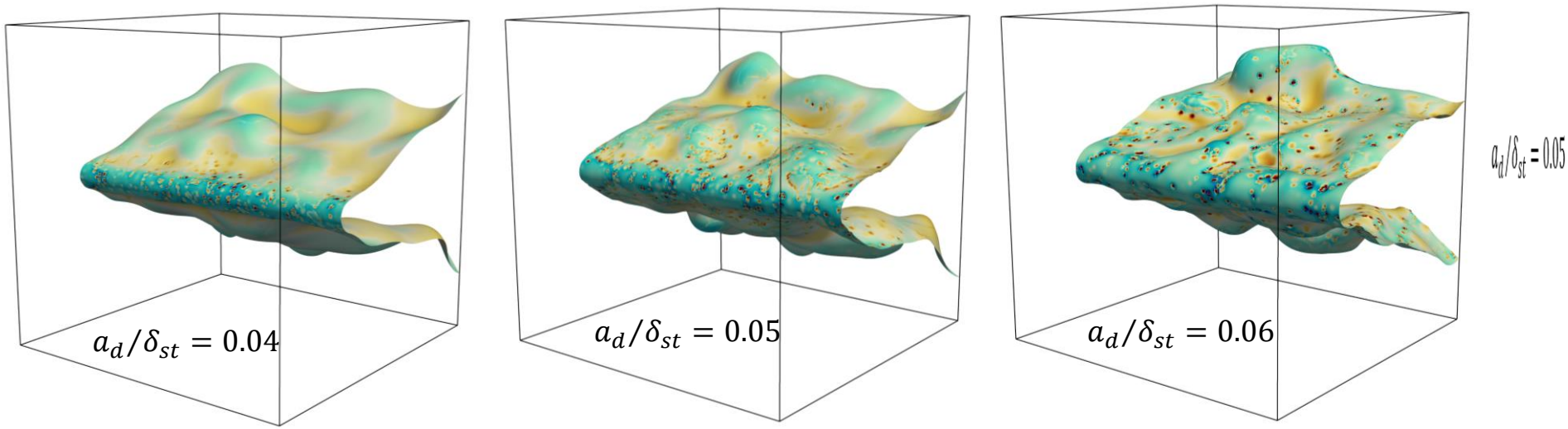


Instantaneous views of $c = 0.5$ isosurface coloured with $\kappa_m \times \delta_{st}$ values for initial $a_d/\delta_{st} = 0.04, 0.05, 0.06$ (left to right) atat $t = 2.52\alpha_{T0}/S^2_{b(\phi_g=1)}$.

Results: Flame-droplet interaction

statistically stationary rod-stabilised V-flames:

Local flame curvature: $\kappa_m = 0.5\nabla \cdot \vec{N}$ *Local flame normal:* $\vec{N} = -\nabla c/|\nabla c|$



Instantaneous views of $c = 0.5$ isosurface coloured with $\kappa_m \times \delta_{st}$ values for initial $a_d/\delta_{st} = 0.04, 0.05, 0.06$ (left to right) at $t = 2.0t_{flow}$

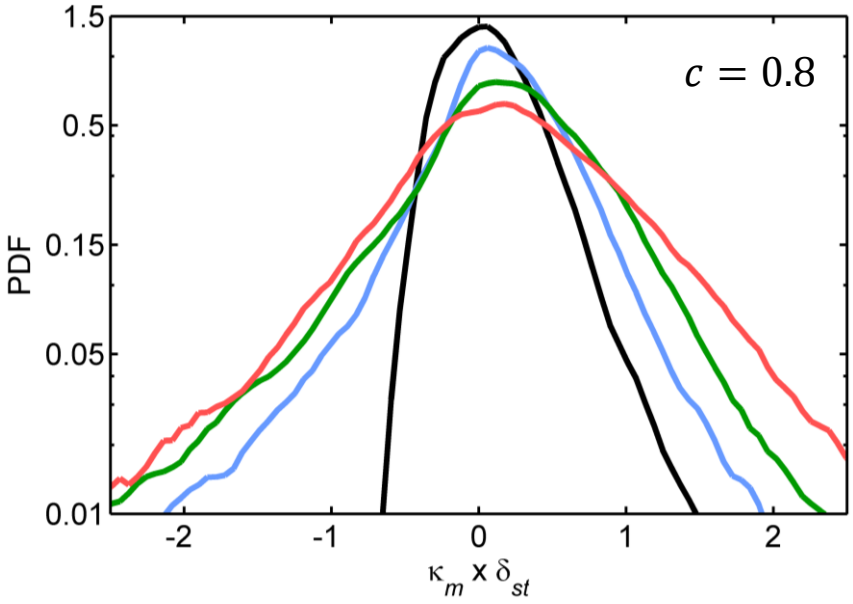
$$t_{flow} = L_x/u_{mean}$$

- A smoother surface for smaller droplets due to their faster evaporation rate ahead of the flame
- The flame surfaces for large droplet cases are significantly disturbed by droplets and exhibit dimples with negative local curvature values.

Results: Flame-droplet interaction

$a_d/\delta_{st} = 0.04$ $a_d/\delta_{st} = 0.05$
$a_d/\delta_{st} = 0.06$ Gaseous premixed

unsteady spherically expanding flames:

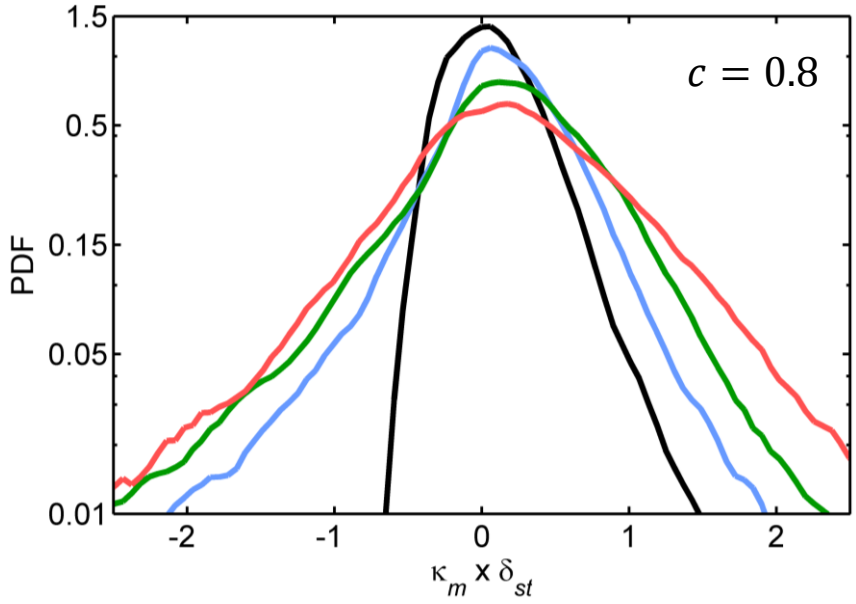


PDFs of $\kappa_m \times \delta_{st}$ of the $c = 0.8$ isosurface for initial turbulence intensity of $u'/S_{b(\phi_g=1)} = 4.0$

Results: Flame-droplet interaction

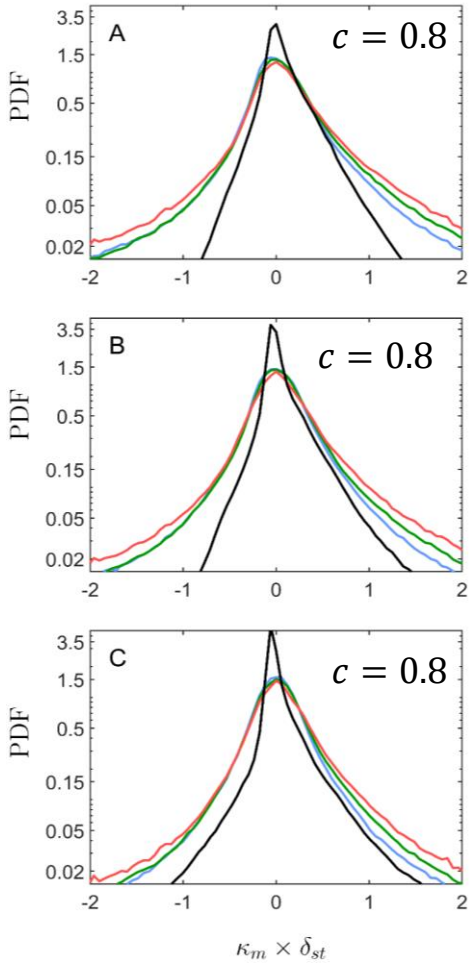
$a_d/\delta_{st} = 0.04$ $a_d/\delta_{st} = 0.05$
$a_d/\delta_{st} = 0.06$ Gaseous premixed

unsteady spherically expanding flames:



PDFs of $\kappa_m \times \delta_{st}$ of the $c = 0.8$ isosurface for initial turbulence intensity of $u'/S_{b(\phi_g=1)} = 4.0$

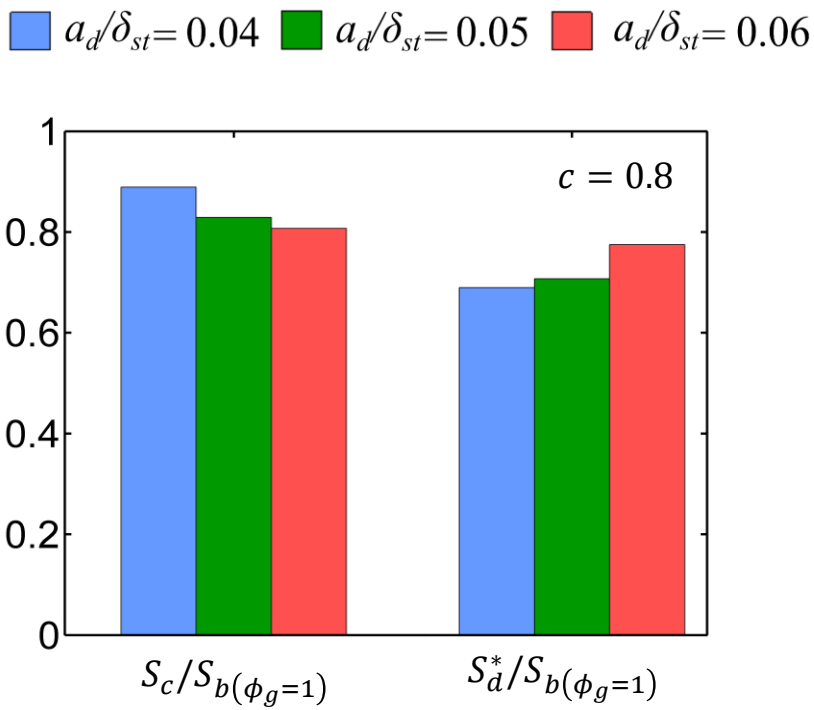
statistically stationary rod-stabilised V-flames:



PDFs of $\kappa_m \times \delta_{st}$ of the $c = 0.8$ isosurface at locations A, B and C (top to bottom)

Results: Flame propagation

unsteady spherically expanding flames:



Mean values of $S_c/S_{b(\phi_g=1)}$ and $S_d^*/S_{b(\phi_g=1)}$ on $c = 0.8$ isosurface along with alternative flame speeds $S_A^*/S_{b(\phi_g=1)}$ and $S_V^*/S_{b(\phi_g=1)}$.

Displacement speed:

$$S_d = \frac{[\nabla \cdot (\rho D \nabla c) + \dot{w}_c + \dot{S}_c + \dot{A}_c]}{\rho |\nabla c|}$$

Density-weighted displacement speed: $S_d^* = \rho\, S_d/\rho_0$

Term associated with droplet evaporation:

$\dot{\boldsymbol{S}}_{\boldsymbol{c}} = -[\boldsymbol{\xi_{st}}/\{\boldsymbol{Y_{O\infty}}\boldsymbol{\xi}^{\boldsymbol{2}}(\boldsymbol{1}-\boldsymbol{\xi_{st}})\}]\left[\boldsymbol{\xi}\dot{\boldsymbol{S}}_{\boldsymbol{O}} + (\boldsymbol{Y_{O\infty}}-\boldsymbol{Y_O})\dot{\boldsymbol{S}}_{\boldsymbol{\xi}}\right]$ for $\xi \le \xi_{st}$;
$\dot{\boldsymbol{S}}_{\boldsymbol{c}} = -[\boldsymbol{1}/\{\boldsymbol{Y_{O\infty}}(\boldsymbol{1}-\boldsymbol{\xi})^{\boldsymbol{2}}\}]\left[(\boldsymbol{1}-\boldsymbol{\xi})\dot{\boldsymbol{S}}_{\boldsymbol{O}} + \boldsymbol{Y_O}\dot{\boldsymbol{S}}_{\boldsymbol{\xi}}\right]$ for $\xi > \xi_{st}$

Term associated with mixture inhomogeneity:

$\dot{\boldsymbol{A}}_{\boldsymbol{c}} = \boldsymbol{2\rho D\nabla\xi\cdot\nabla c/\xi}$ for $\xi \le \xi_{st}$;
$\dot{\boldsymbol{A}}_{\boldsymbol{c}} = \boldsymbol{-2\rho D\nabla\xi\cdot\nabla c/(1-\xi)}$ for $\xi > \xi_{st}$

$$S_c = \rho_0^{-1}\int \dot{w}_c dn$$

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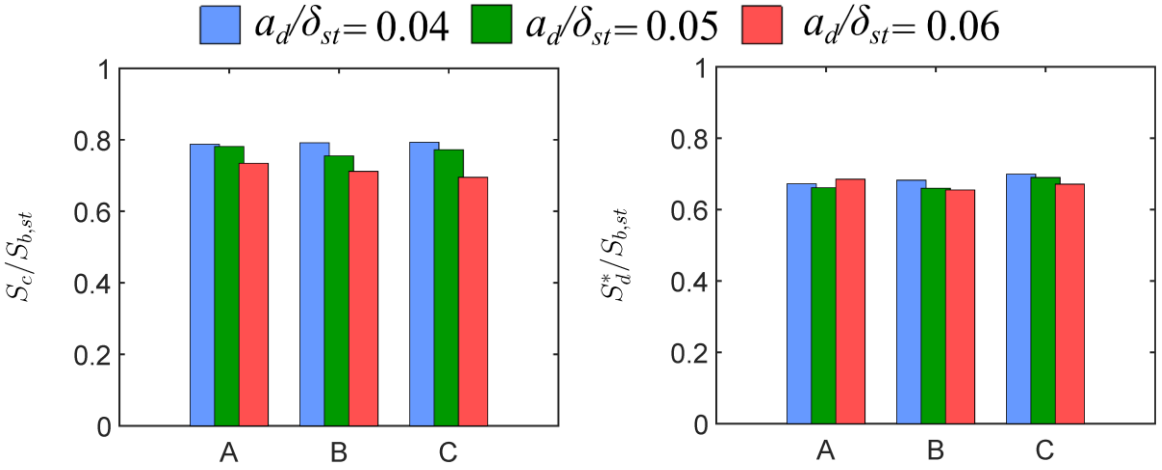
Results: Flame propagation

statistically stationary rod-stabilised V-flames:



The mean values of $S_c/S_{b(\phi_g=1)}$ and $S_d^*/S_{b(\phi_g=1)}$ on the $c = 0.8$ isosurface at locations A-C.

Displacement speed:

$$S_d = \frac{[\nabla \cdot (\rho D \nabla c) + \dot{w}_c + \dot{S}_c + \dot{A}_c]}{\rho |\nabla c|}$$

Density-weighted displacement speed: $S_d^* = \rho\, S_d/\rho_0$

Consumption speed: $S_c = \rho_0^{-1} \int \dot{w}_c dn$

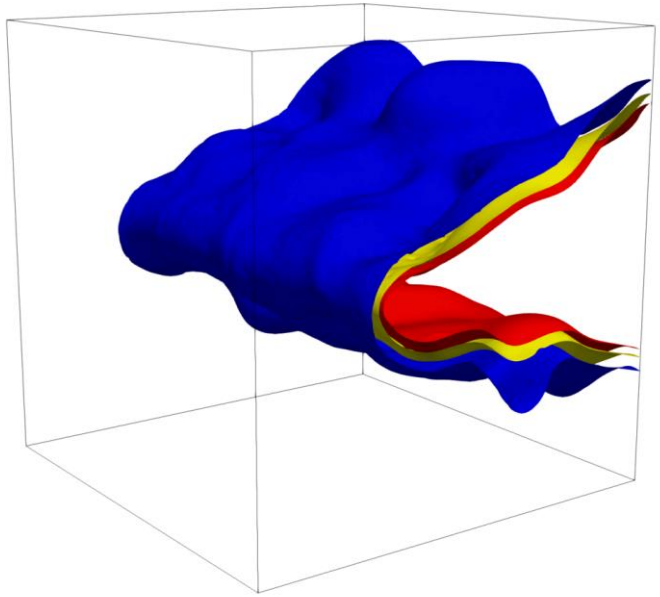
- a_d/δ_{st} ↗ the mean $S_c/S_{b(\phi_g=1)}$ ↘
- $S_d^*/S_{b(\phi_g=1)}$ for a given value of a_d/δ_{st} remain comparable at locations A, B and C

Conclusions

Flame propagation into droplet-laden mixtures has been analysed for two different flame configurations: (i) unsteady spherically expanding flames, and (ii) statistically stationary rod-stabilised V-flames and gives rise to the below observations:

- **Fuel-lean nature** of the gaseous phase combustion,
- Flame-droplet interaction gives rise to dimples on the flame surface,
- The mean values of **consumption speed** decreases with increasing droplet diameter,
- But the mean values of **density weighted displacement speed** remains comparable.

THANK YOU



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