Influences of droplet diameter and overall equivalence ratio on the flame structure for spherically expanding flames propagating in fuel droplet-mist: A Direct Numerical Simulaton Analysis

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Imperial College London

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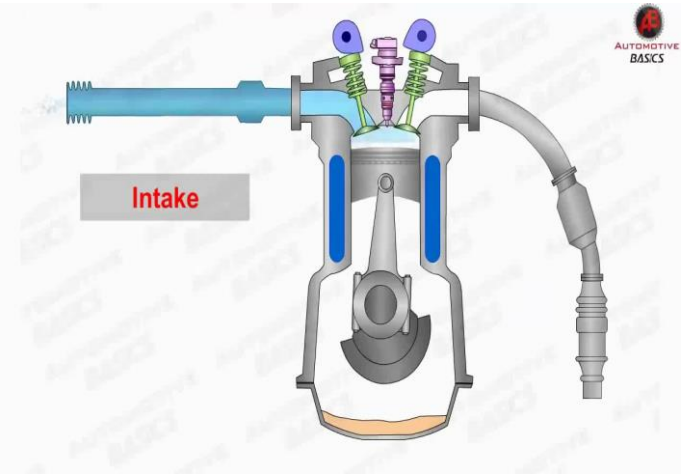
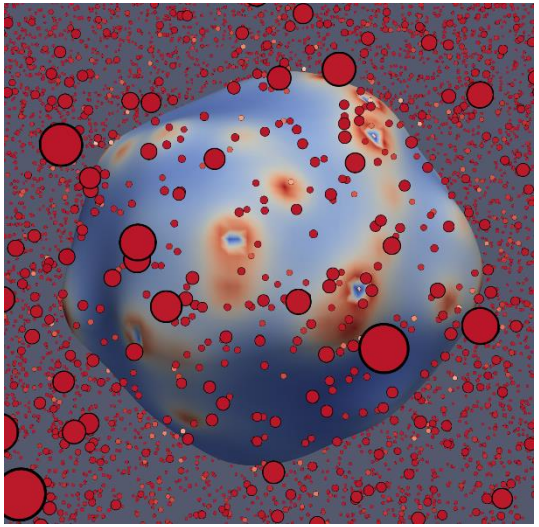
Introduction: Motivation



Significant practical relevance of:

- 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.youtube.com/watch?v=BzgaTDb7E88

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Introduction: Objectives

- **to demonstrate and explain the influences of droplet size and the overall equivalence ratio on**
  - ✓ **the flame structure and wrinkling**
  - ✓ **the evolution of flame surface area and**
  - ✓ **the evolution of burned gas volume**
  - ✓ **displacement and consumption speeds**

  in spherically expanding *laminar* and *turbulent* n-heptane spray flames.

- **to compare the results obtained from spray flames with the corresponding gaseous premixed flames.**

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Mathematical Background

Liquid Phase:

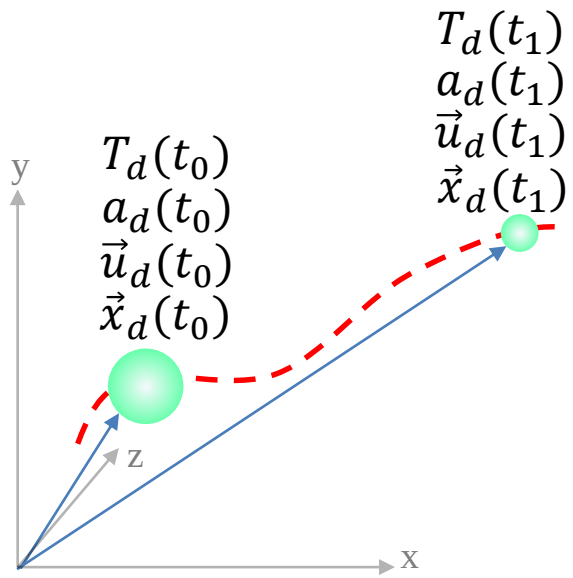
Lagrangian Approach is used for droplets following the approach proposed by Reveillon & Vervisch.

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

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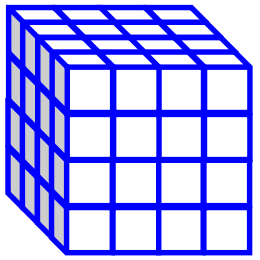
Mathematical Background

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:

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

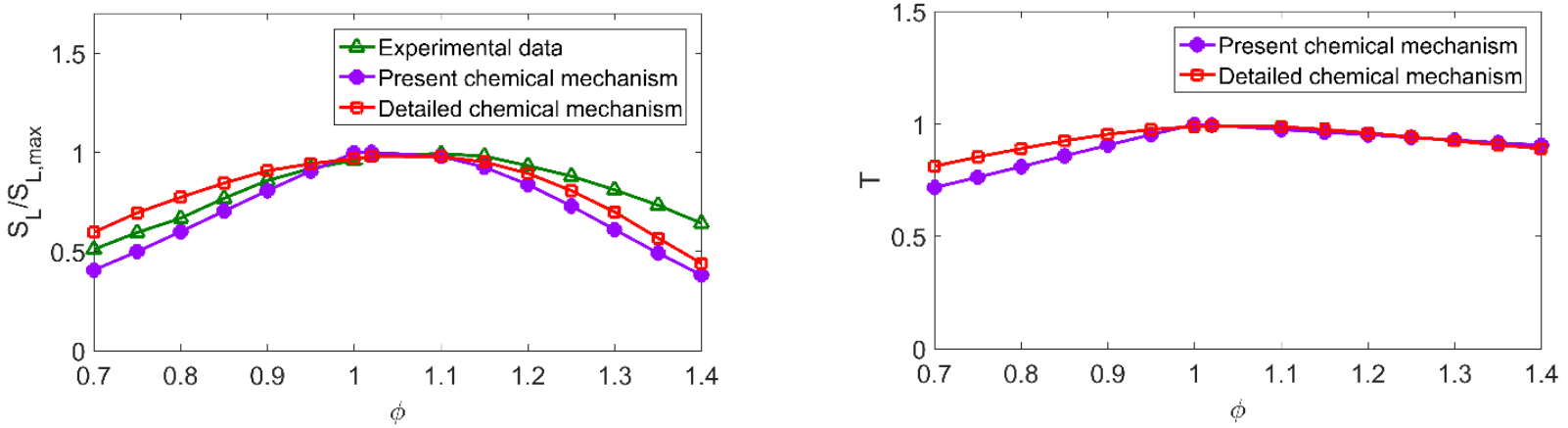
$\psi_1 = \{1, u_j, \hat{T}, Y_F, Y_O\}$ for $\psi = \{1, u_j, e, Y_F, Y_O\}$
$\Gamma_\psi = \rho\nu/\sigma_\psi$ for $\psi = \{1, u_j, Y_F, Y_O\}$ and $\Gamma_\psi = \lambda$ for $\psi = e$
$\dot{w}_\psi$ is chemical reaction rate,
$\dot{S}_g$ is an appropriate source/sink term and
$\dot{S}_\psi$ is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

- 10th order central difference scheme
- Time advancement: Explicit low-storage 3rd order Runge-Kutta scheme.
- A modified single-step Arrhenius-type irreversible chemical reaction:
- Droplets are treated as sub-grid point sources.



Variation of the (a) normalised laminar burning velocity $S_{b(\phi_g)}/\left\{S_{b(\phi_g)}\right\}_{max}$ 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).

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Mathematical Background

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.

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Mathematical Background

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1D steady-state laminar spray flame, COSILAB

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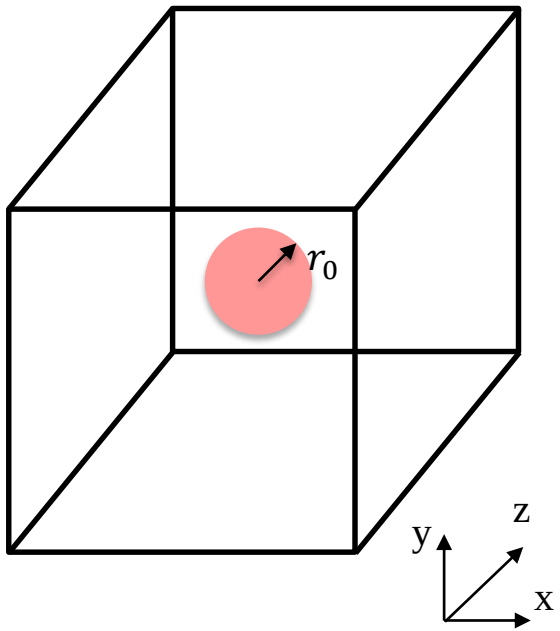

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Mathematical Background

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1D steady-state laminar spray flame, COSILAB

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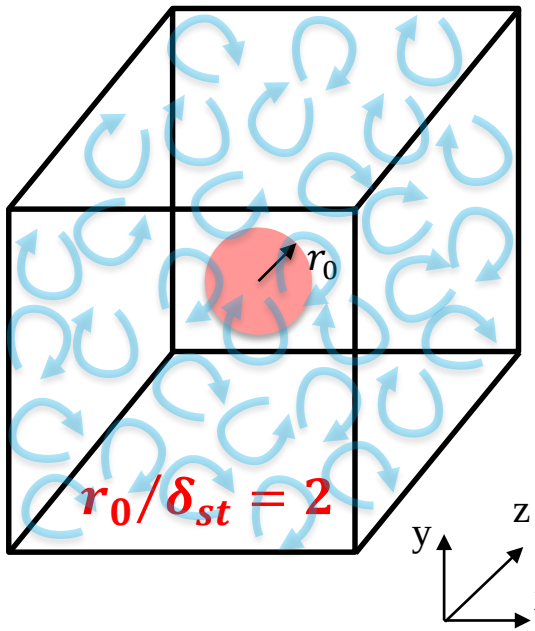

Turbulent flow field initialisation:

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

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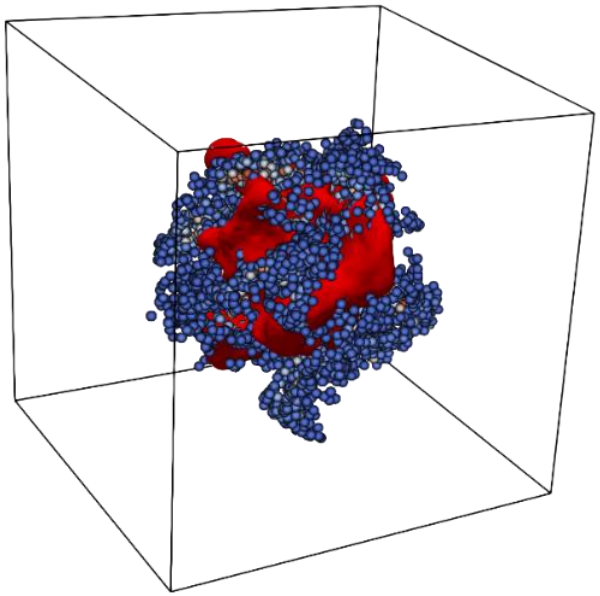
Mathematical Background

Simulation parameters

- 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 kernel radius: $r_0/\delta_{st} = 2.0$
- Equivalence ratio: $\phi_{ov} = 0.8, 1.0$ and 1.2

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



Equivalence ratio:

$$\phi = \frac{FAR}{FAR_{st}}$$

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

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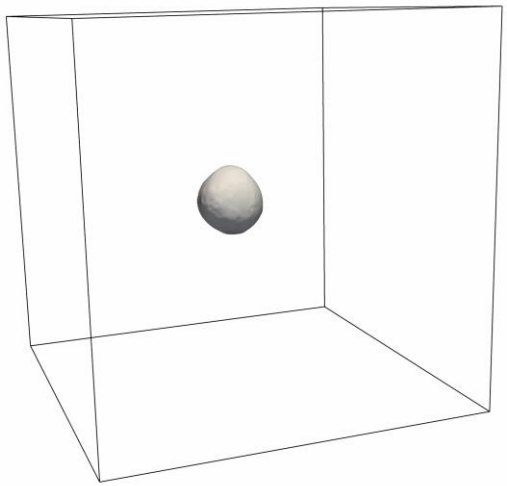
Mathematical Background

Simulation parameters:

- Initial rms: $u'/S_{b(\phi_g=1)} = 0.0\ and\ 4.0$
- Longitudinal integral length-scale: $L_{11}/\delta_{st} = 2.5$
- Droplet diameter: $a_d/\delta_{st} = 0.04, 0.05$ and 0.06
- Number density: $1.28 \leq (\rho_N)^{1/3}\delta_{st} \leq 2.18$
- Heat release parameter:

$$\tau = \frac{(T_{ad(\phi_g=1)} - T_0)}{T_0} = 6.54$$



Reaction progress variable, c:

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

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

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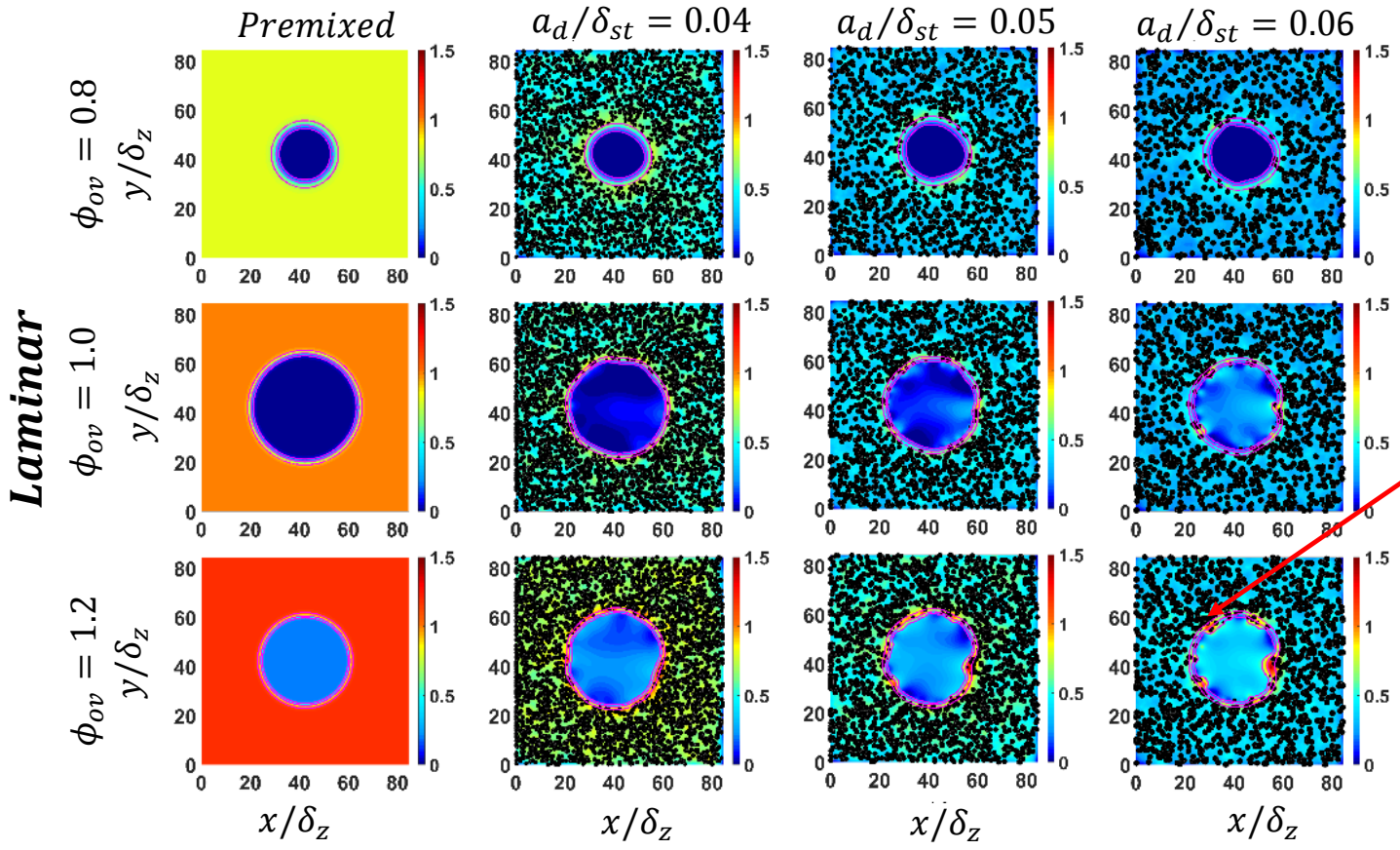
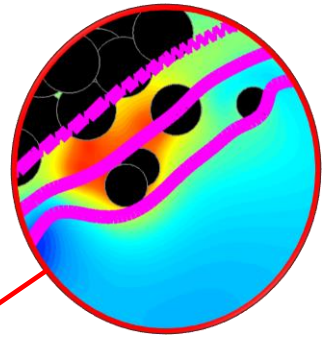
Results: Flame-droplet-turbulence interaction

$\phi_{ov} = 0.8, 1.0$ and 1.12 $a_d/\delta_{st} = 0.04, 0.05$ and 0.06





Distribution of Y_F/Y_{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 $t = 2.52\alpha_{T0}/S^2_{b(\phi_g=1)}$

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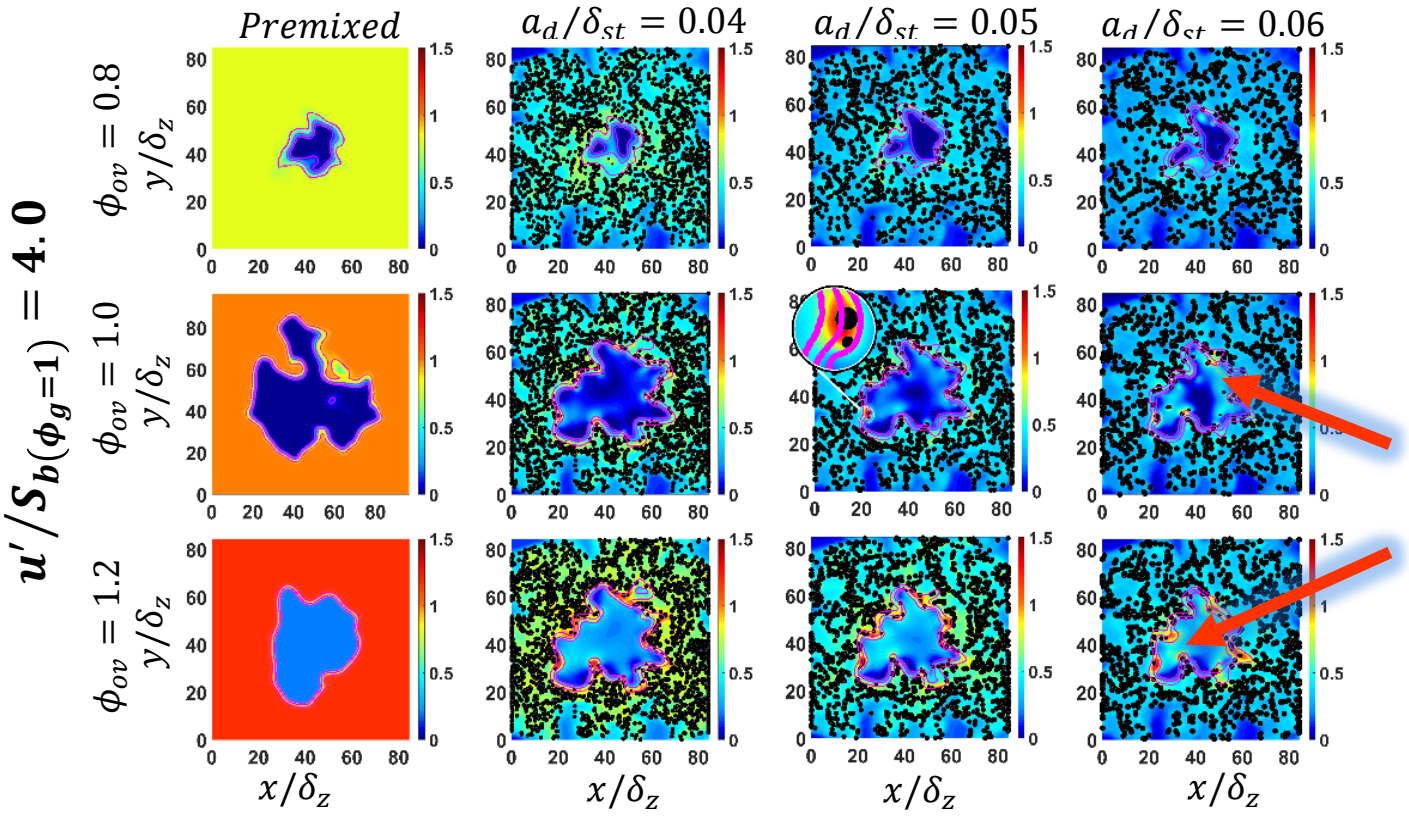
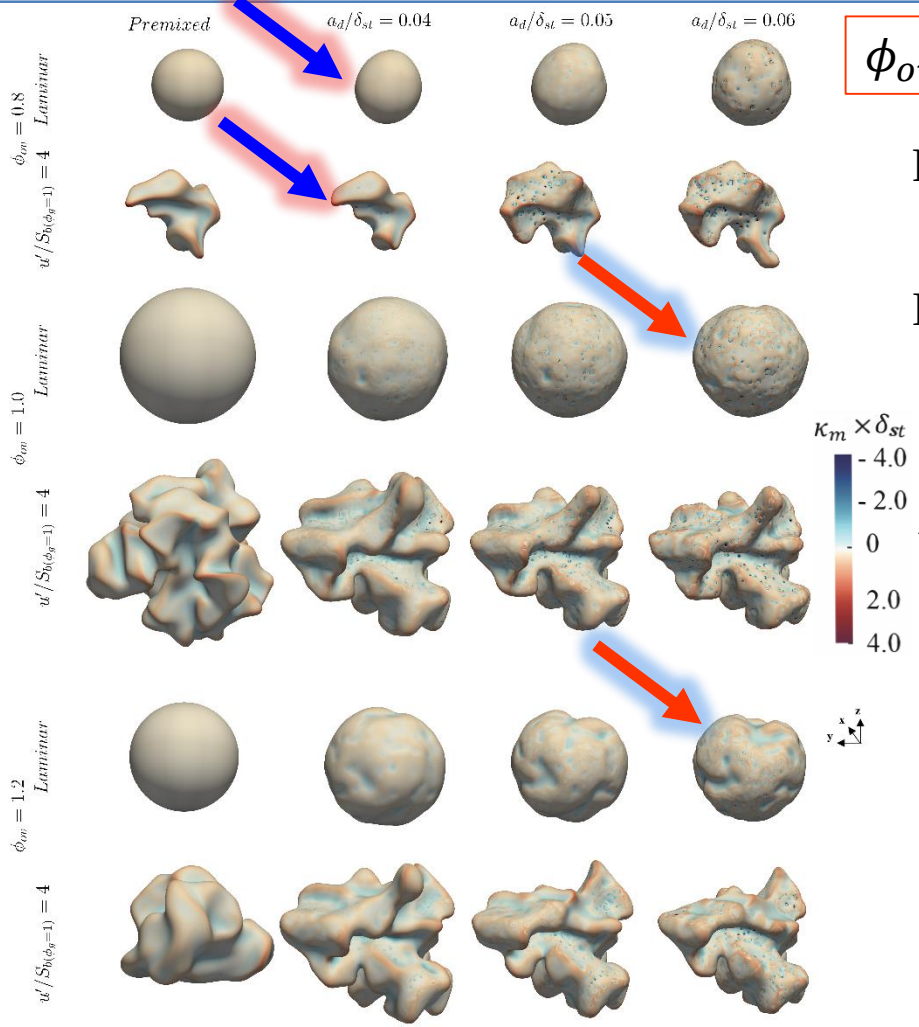
Results: Flame-droplet-turbulence interaction

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



Distribution of Y_F/Y_{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 turbulent flames with $\phi_{ov} = 0.8, 1.0$ and 1.2. All figures correspond to $t = 2.52\alpha_{T0}/S^2_{b(\phi_g=1)}$

Results: Droplet induced wrinkling



$\phi_{ov} = 0.8, 1.0, 1.2$ 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.

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 $t = 2.52\alpha_{T0}/S^2_{b(\phi_g=1)}$.

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Results: PDF of gaseous equivalence ratio

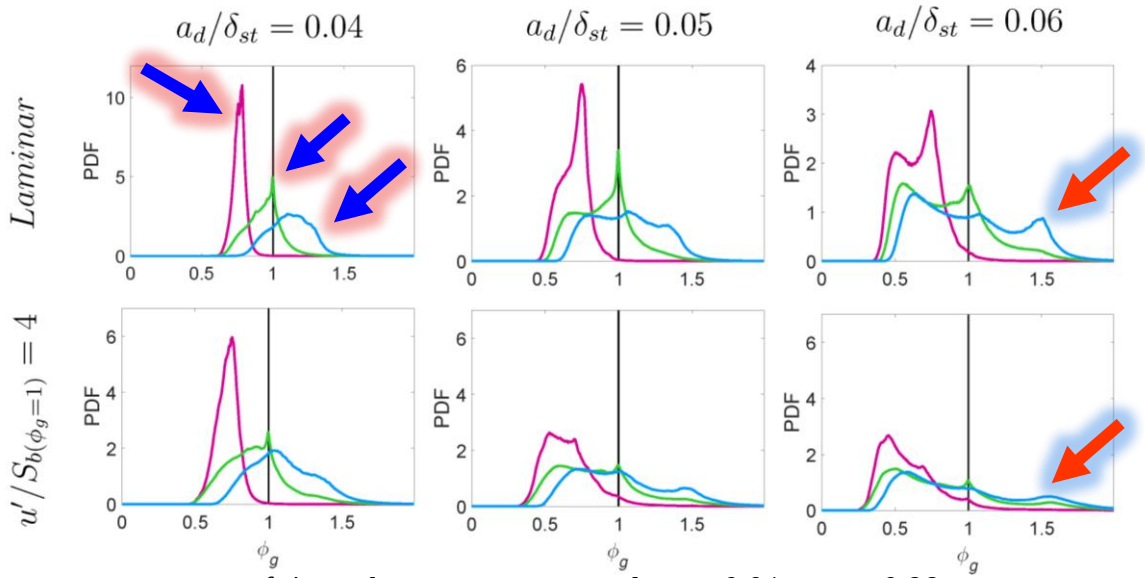
$\phi_{ov} = 0.8, 1.0$ and 1.2 $a_d/\delta_{st} = 0.04, 0.05$ and 0.06

Premixed Gas

$\phi_{ov} = 0.8$ $\phi_{ov} = 1.0$ $\phi_{ov} = 1.2$

Droplet Cases

$\phi_{ov} = 0.8$ $\phi_{ov} = 1.0$ $\phi_{ov} = 1.2$



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

- A peak of the ϕ_g-PDF at $\phi_g \approx \phi_{ov}$
- The probability of finding $\phi_g < \phi_{ov}$ supersedes the availability of $\phi_g > \phi_{ov}$

- Localised fuel-rich pockets are more frequent for large droplets and $\phi_{ov} = 1.2$

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Results: The evolution of flame surface area

A, flame surface area: $A = \int |\nabla c| dV$

r_A is the equivalent radius : $r_A = \sqrt{A/4\pi}$

S_A is a flame speed which can is defined based on based on the flame surface area.

$S_A = d\,r_A/d\,t$

	ϕ_{ov} = 0.8		ϕ_{ov} = 1.0		ϕ_{ov} = 1.2	
a_d/δ_{st}	Laminar	$u'/S_{b(\phi_g=1)} = 4$	Laminar	$u'/S_{b(\phi_g=1)} = 4$	Laminar	$u'/S_{b(\phi_g=1)} = 4$
0.04	3.30	3.48	5.46	7.96	6.17	10.12
0.05	3.90	5.30	4.87	6.93	5.60	8.48
0.06	4.57	5.97	4.69	6.78	5.17	7.59
Premixed	3.18	4.10	5.42	10.44	5.83	8.15

Normalised flame speed $S_A/S_{b(\phi_{ov})}$, which quantifies the growth rate of flame surface area *A*.

- The presence of droplets enhances $S_A/S_{b(\phi_{ov})}$ for $\phi_{ov} = 0.8$ except for the initial $a_d/\delta_{st} = 0.04$.
- For $\phi_{ov} = 1.0$ and 1.2, only the small droplets with initial $a_d/\delta_{st} = 0.04$ under laminar conditions demonstrate higher $S_A/S_{b(\phi_{ov})}$ than the corresponding laminar premixed flame.
- $S_A/S_{b(\phi_{ov})}$ increases with increasing droplet diameter for $\phi_{ov} = 0.8$, whereas it shows just the opposite behaviour for $\phi_{ov} = 1.0$ and 1.2.

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Results: The evolution of burned gas volume

	ϕ_{ov} = 0.8		ϕ_{ov} = 1.0		ϕ_{ov} = 1.2	
a_d/δ_{st}	Laminar	$u'/S_{b(\phi_g=1)} = 4$	Laminar	$u'/S_{b(\phi_g=1)} = 4$	Laminar	$u'/S_{b(\phi_g=1)} = 4$
0.04	3.03	1.03	5.34 →	5.70	6.43 →	6.63
0.05	2.97	3.45	4.90	4.34	5.81	5
0.06	4.07	2.10	4.91	3.73	5.21	4.14
Premixed	3.55	2.32	5.5	6.63	6.25	7.28

Normalised flame speed $S_v/S_{b(\phi_{ov})}$, which quantifies the growth rate of burned gas volume V_b.

S_V is a flame speed which is defined based on based on the burned gas volume.

$$S_V = d\,r_V/d\,t$$

r_V is the equivalent radius which is calculated as : $r_V = (3V_b/4\pi)^{1/3}$

- The presence of droplets enhances $S_V/S_{b(\phi_{ov})}$ for $\phi_{ov} = 0.8$ with the initial $a_d/\delta_{st} = 0.06$ under laminar conditions .
- Turbulence significantly affects $S_V/S_{b(\phi_g)}$ and increases the growth rate of burned gas volume for large droplets with $\phi_{ov} = 0.8$ and for small droplets with $\phi_{ov} = 1.0$ and 1.2.

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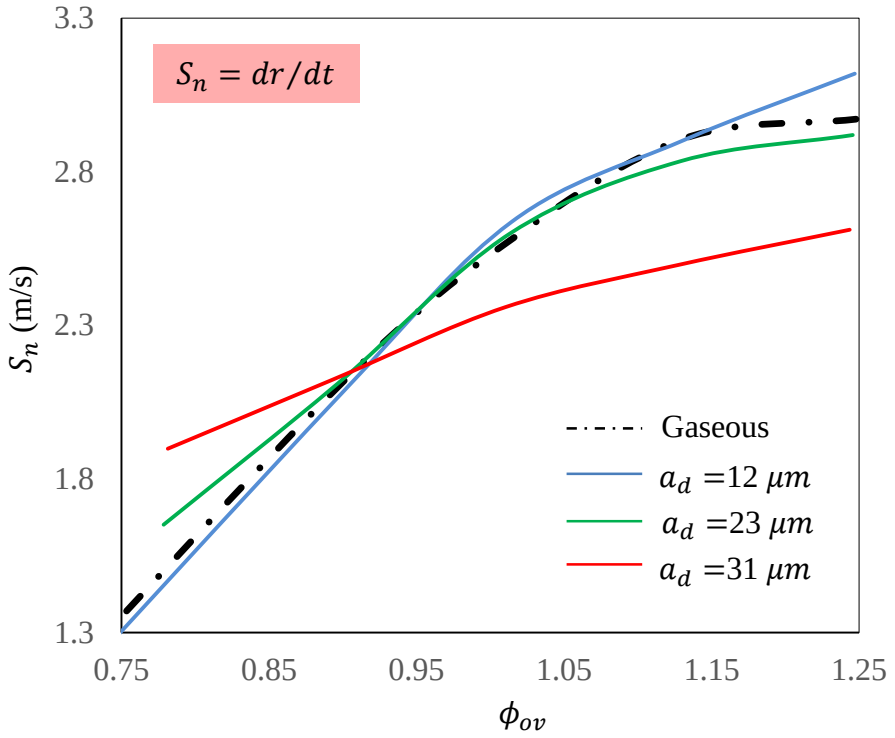
Results: The evolution of burned gas volume

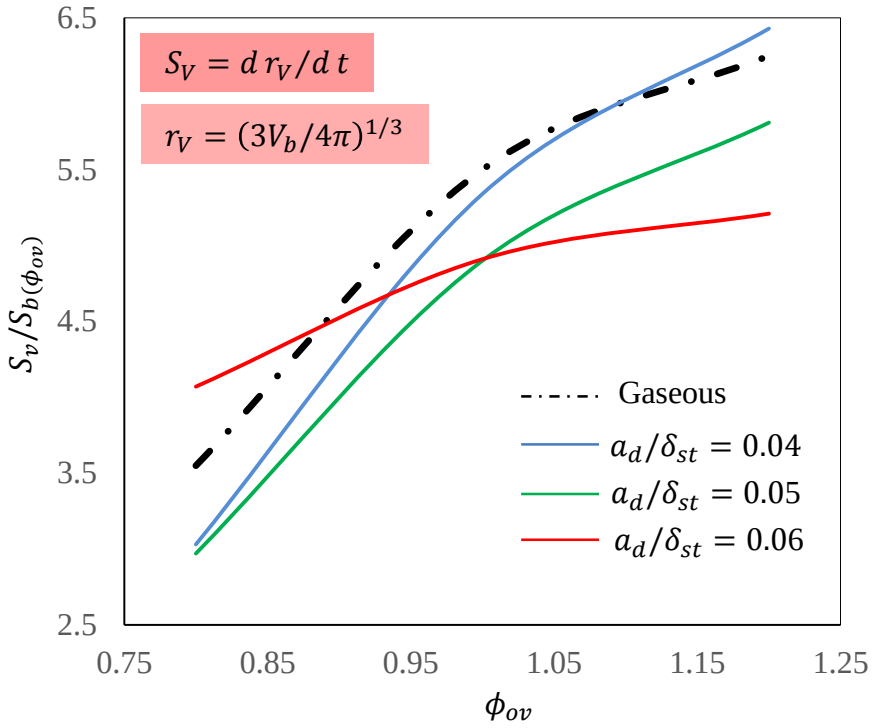
Laminar

Experiment



[1]Comparison S_n of for gaseous and aerosol ethanol-air at various ϕ_{ov}.

DNS



Normalised flame speed $S_v/S_{b(\phi_{ov})}$, which quantifies the growth rate of burned gas volume V_b.

[1]Saat, A.: Fundamental Studies of Combustion of Droplet and Vapour Mixtures. PhD Thesis, The University of Leeds, (2010).

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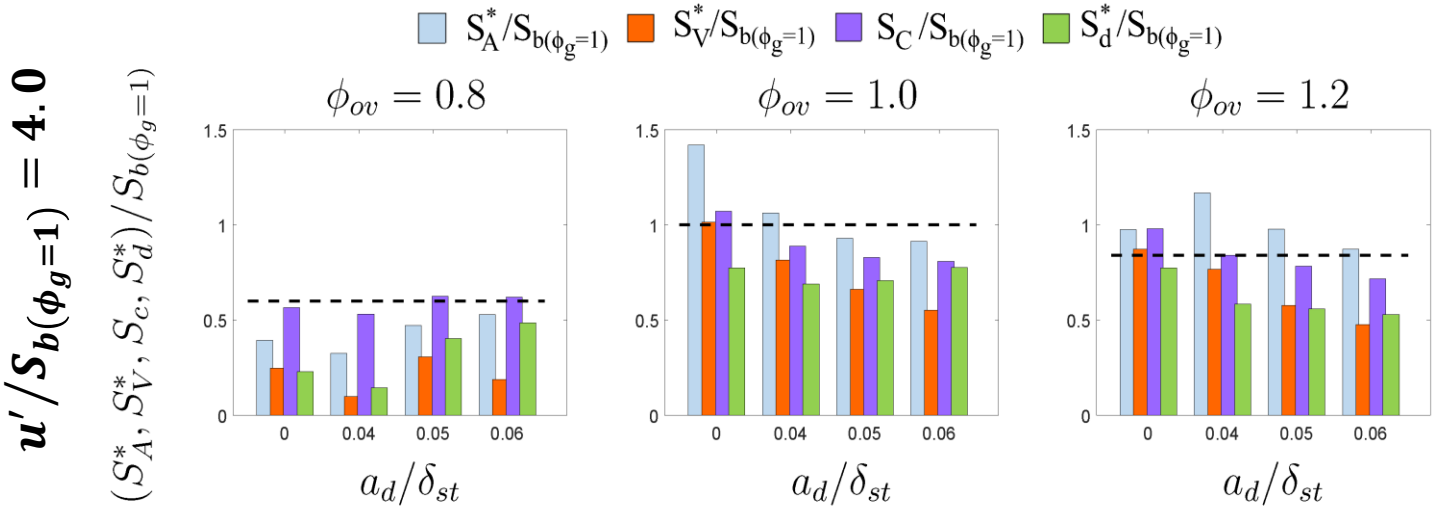
Results: Mean flame speed statistics



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 $S_V^*/S_{b(\phi_g=1)}$. The value of $S_{b(\phi_g=\phi_{ov})}/S_{b(\phi_g=1)}$ is shown by the horizontal black dashed line.

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

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

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

$S_V^* = \rho_b\, S_V/\rho_0$

$S_A^* = \rho_b\, S_A/\rho_0$

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Conlusions and ongoing work

- O**verall equivalence ratio**, **droplet size** and **turbulence** have an important influence on the flame structure.
- The presence of droplets leads to **dimples on the flame surface** for large droplet diameters and large droplet number densities.
- **The gaseous phase mixture** within the flame is predominantly fuel-lean in comparison to the overall equivalence ratio for $\phi_{ov} = 1.0$ and 1.2 droplet cases.
- **The growth rate of flame surface area** increases with increasing droplet diameter under fuel-lean mixture conditions, whereas an opposite behaviour has been observed for $\phi_{ov} = 1.0$ and 1.2.
- **Displacement** and **consumption speeds** can be related with the **rates of flame area generation** and **the burned gas volume** in spherically expanding spray flames.

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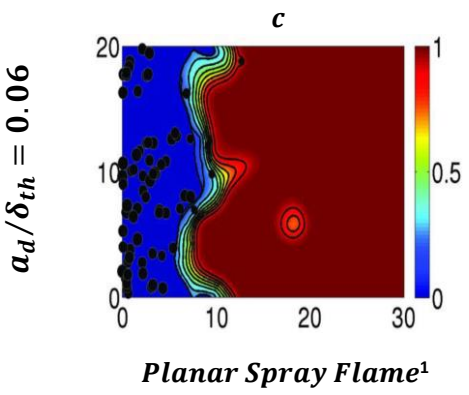
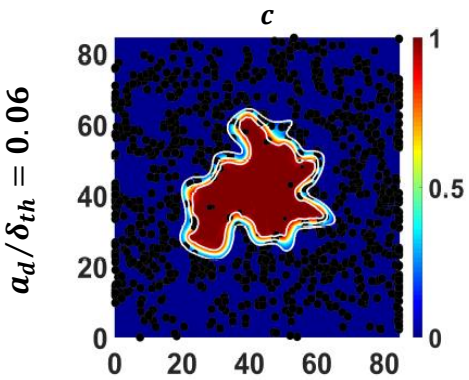
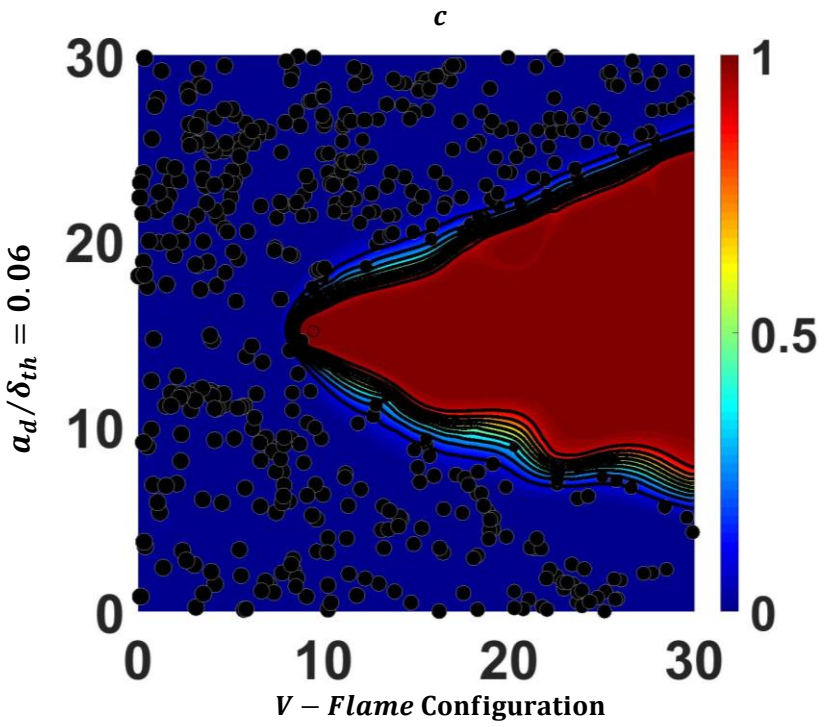
Conclusions and ongoing work



Planar Spray Flame[1]



Spherical Expanding Spray Flame[2]



$V - Flame$ Configuration

[1]D.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).

[2]G. 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)

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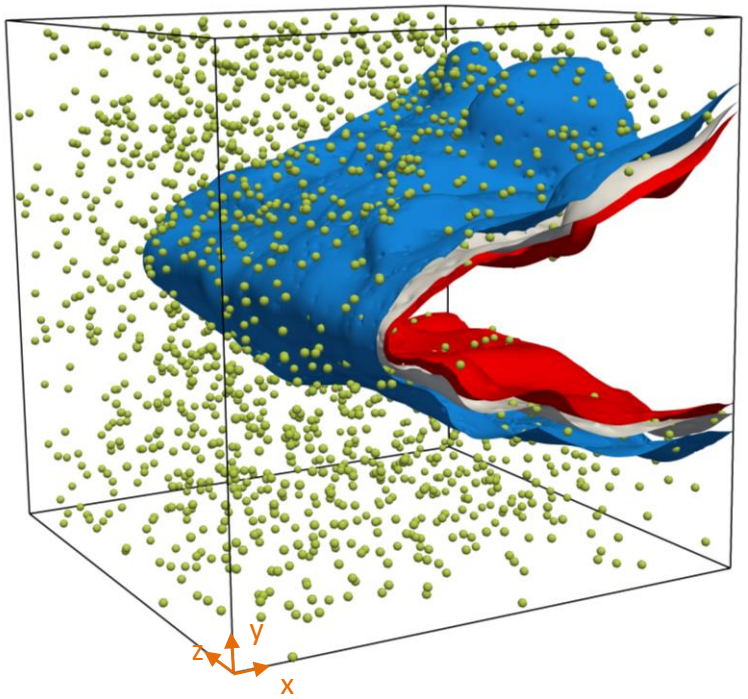
Conclusions and ongoing work

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 =0.1, 0.5 and 0.9 for a_d/δ_{th} = 0.06 initial droplet diameter, at $t = 1.5t_{flow}$.

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Publications:

Journal Papers:

1. Ozel Erol, G., Hasslberger, J., Klein, M., Chakraborty, N., A direct numerical simulation analysis of spherically expanding turbulent flames in fuel droplet-mists for an overall equivalence ratio of unity. **Phys. Fluids.** 086104, (2018)
2. Ozel Erol, G., Hasslberger, J., Klein, M., Chakraborty, N., A Direct Numerical Simulation investigation of spherically expanding flames propagating in fuel droplet-mists for different droplet diameters and overall equivalence ratios. **Combust. Sci. Technol.** (printed online), (2019)

Conferences:

1. Ozel Erol, G., Hasslberger, J., Klein, M., Chakraborty, N., Spherically expanding turbulent flames in fuel-droplet mists: A Direct Numerical Simulation analysis, **Turbulence, Heat and Mass Transfer 9**, Rio de Janeiro, Brazil (10.07.2018 - 13.07.2018)
2. Ozel Erol, G., Hasslberger, J., Klein, M., Chakraborty, N., Evolution of Spherically Expanding Turbulent Flames in Droplet-Laden Mixtures: A Direct Numerical Simulation Analysis, **37th International Symposium on Combustion**, Dublin, Ireland (29.07.2018 - 02.08.2018)

THANK YOU

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