Direct Numerical Simulation analysis of localised forced ignition and flame propagation in turbulent droplet-laden mixtures

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Minimum ignition energy for turbulent droplet-laden mixtures

Introduction: Motivation

- Localised forced ignition (spark or laser) plays a dominant role in transportation and energy production
 - Applications in the Internal Combustion (IC) engines, and Gas turbines
 - Important from the point of view of accidental explosion and fire safety Hence, the importance of fully understanding the ignition phenomenon
- Ignition not only initiates combustion but also influences subsequent burning
- Droplet laden mixture combustion includes
 - The evaporation of the liquid droplets
 - Interaction of the droplets and fuel vapour with the flame and flow field is a complex phenomenon
 - A complex coupling between combustion, heat transfer, fluid dynamics.

Introduction: Objectives

- To demonstrate and explain the influences of initial droplet diameter, global equivalence ratio (total number of droplets present) and turbulence intensities on on the Minimum Ignition Energy (MIE) of droplet laden mixtures.
- To subsequently find and illustrate the sensitivity of the MIE on the above parameters

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: $\frac{dT_d}{dt} = \frac{\hat{T}(\vec{x}_d, t) - T_d - B_d L_v / C_p^d}{\tau_d^T}$

 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).

Gaseous Phase:

Eulerian Approach is used to solve for gas phase combustion.

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}_{ψ} is chemical reaction rate,

 \dot{S}_{q} is an appropriate source/sink term and

 \dot{S}_{ψ} 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.



Gaseous Phase:

Eulerian Approach is used to solve for gas phase combustion.

Addition of a source term to the energy equation to account for the energy deposition by the spark

$$\frac{\partial \rho E}{\partial t} + \frac{\partial \rho u_j E}{\partial x_j} = -\frac{\partial}{\partial x_k} u_k P + \frac{\partial}{\partial x_k} \tau_{ki} u_i + \frac{\partial}{\partial x_k} \left[\lambda \frac{\partial \hat{T}}{\partial x_k} \right] + \dot{w}_T + \dot{S}_{\psi} + q^{\prime\prime\prime}$$

• The source term (spark energy) follows a Gaussian profile

$$q^{\prime\prime\prime} = A_q \exp\left(-\frac{r^2}{2R_{sp}^2}\right) \qquad \dot{Q} = a_{sp}\rho_0 C_P \tau T_0 \left(\frac{4}{3}\pi l_f^3\right) \left[\frac{H(t) - H(t - t_{sp})}{t_{sp}}\right]$$
$$\dot{Q} = \int q^{\prime\prime\prime} dV \qquad t_{sp} = b_{sp}t_f \qquad a_{sp}\text{-Total ignitis}$$

$$\tau = (T_{ad(\phi=1.0)} - T_0)/T_0$$

 a_{sp} -Total ignition energy input parameter b_{sp} - Energy deposition duration parameter R_{sp} - Characteristic width parameter



- Compressible 3D DNS code SENGA¹
- Uniform Cartesian grid
- All boundaries are considered to be non-reflecting, pointwise inflow-outflow
- Initial turbulent field is generated by a pseudospectral method ² using Batchelor-Townsend Spectrum ³
- Spatial differentiation 10th order central difference scheme
- Time advancement Explicit low-storage 3rd order Runge-Kutta scheme



Geometrical description of the domain

¹ K.W. Jenkins, R.S. Cant, Proc. 2nd AFOSR Conference on DNS and LES (1999)

² R.S. Rogallo, NASA Ames Research Centre (1990)

³ G.K. Batchelor and A.A. Townsend, Proceedings Royal Society London (1948)

- Droplets are treated as sub-grid point sources.
- A modified single-step Arrhenius-type irreversible chemical reaction for the **n**-**heptane droplets** investigated in the present study:



Fuel + $s \cdot \text{Oxidiser} \rightarrow (1 + s)$ Products

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).

- Domain size of $9.6l_t \times 9.6l_t \times 9.6l_t$ equivalent to $51\delta_z \times 51\delta_z \times 51\delta_z$ (where $\delta_z = D_0/S_{L(\phi_g=1)}$ is the Zel'dovich flame thickness)
- Cartesian grid of 264 × 264 × 264, ensures:
 ▶10 grid points across the thermal flame thickness
 - $> \eta_k > \Delta x$ where η_k is the Kolmogorov length scale
- Spark location is at the centre of the domain
- Energy deposition duration (b_{sp}) and width (R_{sp}) kept constant, only spark power (a_{sp}) is varied to find the MIE



• Three turbulence intensities, overall equivalence ratios and initial droplet diameters

 $u'/S_{L(\phi_g=1.0)} = 0.0, 4.0.8.0$ (U00,U04,U08 resp.) $\phi_{ov} = 0.8, 1.0, 1.2$ (F08,F10,F12 resp.) $a_d/\delta_{th} = 0.03, 0.04, 0.05$ (D03,D04,D05 resp.) With all parameter combinations giving rise to a total of 27 cases

- N-heptane droplets initial temperature, $T_0 = 300$ K, yielding a heat release parameter of $\tau = 6.54$
- Atmospheric pressure conditions
- $a_d/\eta_k = 0.22, 0.29, 0.36$ for $a_d/\delta_{th} = 0.03, 0.04, 0.05$ respectively, thus sub-grid evaporation is not expected to significantly affect the ignition phenomena and subsequent flame-droplet interaction.



Direct Numerical Simulations

- Simulations carried out to evaluate the MIE for both **Ignition** and **Propagation**
 - Successful Ignition refers to a situation where T_{max} surpasses T_{ad} at any point in time. If T_{max} does not reach T_{ad} , it is referred to as a misfire. Simulations run a successful ignition is observed ($t = 3t_{sp}$).

Successful Propagation – obtained when the flame kernel burns without the aid of the ignitor after a successful ignition. It is determined by evaluating the temporal evolution of the burned gas volume, and if its temporal derivative is positive at $t = 10t_{sp}$, a successful self sustained propagation is obtained, otherwise it is considered to be quenched.

Results: Flame-turbulence interaction

Non-dimensional temperature:

$$T = \left(\frac{\hat{T} - T_0}{T_{ad(\phi_g=1)} - T_0}\right)$$

 \hat{T} is the instantaneous dimensional temperature,

 T_0 is the unburned gas temperature, $T_{ad(\phi_g=1)}$ is the adiabatic flame temperature for stoichiometric mixture

Normalised energy deposited by the spark:

 $\Gamma = IE / MIE_l^{\phi_g = 1.0}$

IE is the energy deposited by ignitor $MIE_l^{\phi_g=1.0}$ is the MIE for self sustained propagation of a laminar n-heptane premixed stoichiometric mixture



Isosurfaces of T at peak heat release coloured by reaction rate.

Results: Flame-turbulence interaction

- * **U00D05F12** at $t = 8.0t_{sp}$
 - The kernel retains its spherical structure
 - Droplets induce flame wrinkling, otherwise known as "dimpling"
- U08D03F08 at $t = 5.0t_{sp}$ and $8.0t_{sp}$
 - The extent of "dimpling" is dominated over by the effects of turbulence intensity
 - Kernel is warped and deformed



U00, U04, U08
$$u'/S_{L(\phi_g=1.0)}=0.0, 4.0, 8.0$$
D03, D04, D05 $a_d/\delta_{st}=0.03, 004, 005$ F08, F10, F12 $\phi_{ov}=0.8, 1.0, 1.2$

Results: MIE Variation

- As $u'/S_{L(\phi_g=1.0)}$ increases so does $\Gamma_{MIE}^{i/p}$, and the effects of turbulence dominate over the effects induced by changes in a_d and ϕ_{ov} , and this is most visible for Γ_{MIE}^p
- To observe the effects that a_d and ϕ_{ov} have on $\Gamma_{MIE}^{i/p}$ it is instructive to observe two sets off cases:



Results: MIE Variation

- The laminar cases for Γ_{MIE}^i :
 - > As ϕ_{ov} increases, Γ^i_{MIE} decreases
 - > As a_d increases, Γ_{MIE}^i increases
- The cases with $u'/S_{L(\phi_g=1.0)} = 8.0$ for Γ_{MIE}^p :
 - > As ϕ_{ov} increases, Γ_{MIE}^{p} decreases
 - > As a_d increases, Γ_{MIE}^p increases



The selected cases shown best illustrate these effects, however these observations hold across all cases investigated here.



Results: Driving Physical Effects

- Igniting droplet-laden mixtures require more energy than igniting a homogenous mixture
 - The extra energy is initially required to evaporate the droplets, subsequently allowing for ignition
 - In turn as the kernel propagates, it has to overcome the losses due to turbulence, that would be present for a kernel propagating in a homogenous mixture, but also has to evaporate the droplets







Results: Driving Physical Effects



As $u'/S_{L(\phi_g=1.0)}$ increases (top to bottom), the peaks off the PDFs of ϕ_g slightly shift towards leaner conditions for the same droplet diameter and overall equivalence ratio



Probability density functions (PDF's) of the gaseous equivalence ratio (ϕ_g), extracted at $t = 5t_{sp}$, over the range 0.1 < c < 0.9

Results: Driving Physical Effects



As a_d increases (left to right), the gaseous mixture becomes increasingly leaner, and for $a_d/\delta_{th} = 0.05$ the PDFs peak outside the lean flammability limit (flammability limits indicated by the vertical dashed lines)

- *This is due to larger droplets requiring more energy to be evaporated
- As ϕ_{ov} increases, the probability of finding ϕ_g close to unity increases

This allows for easier ignition and propagation, in turn corresponding to smaller $\Gamma_{MIE}^{i/p}$ requirements

Conlusions-1

The MIE for uniformly dispersed n-heptane droplet-laden mixtures in homogenous isotropic turbulence has been numerically evaluated for three different turbulence intensities, overall equivalence ratios and initial droplet diameters, giving rise to the below observations:

- A smaller initial droplet diameter or a higher initial global equivalence ratio, reduces the MIE requirement and is beneficial towards successful ignition and subsequent self sustained propagation.
- The MIE has been found to increase with increasing u', and a significant increase of the MIE was observed for large turbulence intensities, in line with previous experimental and computational MIE studies.
- The MIE required for droplet laden mixtures, is higher than the relevant MIE required for a corresponding homogeneous mixture, due to the extra energy required to evaporate the droplets.
- * 1^{st} order effect u'
- * 2^{nd} order effects a_d and ϕ_{ov}

A DNS analysis of turbulent V-flames propagating into droplet-laden mixtures

- To demonstrate the evolution of the flame structure at different axial locations from the flame holder for rodstabilised V-flames in droplet-laden mixtures.
- To indicate and explain the influences of droplet diameter on the reaction zone structure and flame propagation characteristics at different axial locations from the flame holder.

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 $\bar{u}_{mean}/S_{b(\phi_g=1)} = 5$.
- Holder position (x,y): $(120\Delta x, 192\Delta y)$
- Heat release parameter: $\tau = 6.4$
- Droplet diameter: $a_d/\delta_{th} = 0.04, 0.05$ and 0.06
- Initial reacting flow field is generated by using a commercial software called as COSILAB



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 $t = 2t_{flow}$.

Results: Flame-turbulence interaction



Instantaneous fields of gaseous equivalence ratio, ϕ_g (blue lines show c = 0.1, 0.5 and 0.9 contours from outer to inner periphery) for initial $a_d/\delta_{st} = 0.04, 0.05, 0.06$ at $t = 2.0t_{flow}$. Grey dots show the droplets residing on the plane (not to the scale).

Results: Flame Brush Thickness (FBT)



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

Flame brush thickness (FBT) at locations A, B, C and flame angle θ for $\tilde{c} = 0.9$

a_d/δ_{st}	0.04	0.05	0.06
FBT at A	$3.53\delta_{st}$	$3.43\delta_{st}$	$3.21\delta_{st}$
FBT at B	$4.34\delta_{st}$	$4.06\delta_{st}$	$3.72\delta_{st}$
FBT at C	$4.74\delta_{st}$	$4.40\delta_{st}$	$4.04\delta_{st}$
θ	10.2°	11.0°	11.4°

Contours of $\tilde{c} = 0.1$ (solid line), 0.5 (dashed line) and 0.9 (dotted line) contours. The dashed purple lines show the sampling locations (A, B, C), and the dotted black line shows the flame center.

- * Favre averaging in time (i.e. over the time of t_{flow}) and space (i.e. spanwise z-direction)
- ✤ FBT increases in the downstream direction from the flame holder.
- ✤ FBT is greater for cases with smaller droplet diameters.

Results: Gaseous equivalence ratio





PDF of ϕ_q in the region corresponding to $0.01 \le c \le 0.99$ at different locations A, B and C

- The rate of burning, flame spread and both flamelet and flame brush thicknesses are dependent on the mixture composition within the flame.
- A high probability of having $\phi_g \approx 1.0$ for small droplet cases with initial $a_d/\delta_{st} = 0.04$ and 0.05.
- A mild peak at $\phi_g = 1.0$ at all locations but the probability of obtaining $\phi_g < 1.0$ remains greater than for the cases with small droplets.

Results: Flame-droplet interaction



- * 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.
- ♦ Case with initial $a_d/\delta_{st} = 0.06$ exhibits higher probability of finding high positive curvature values than the cases with initial $a_d/\delta_{st} = 0.04$ and 0.05

Results: Flame-turbulence interaction



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.

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

*
$$a_d/\delta_{st}$$
 / 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

Conlusions-2

The flame propagation behaviour for V-shaped turbulent flames in n-heptane droplet-laden mixtures has been numerically evaluated for three different initial droplet diameters and the axial distance from the flame holder giving rise to the below observations:

- The flame brush thickness is affected by both droplet diameter and the axial distance from the flame holder.
- The predominance of finding fuel-lean mixture within the flame decreases in the downstream direction due to evaporation of droplets and this effect is particularly strong for large droplets.
- The mean values of consumption speed are found to decrease with increasing droplet diameter because of greater likelihood of fuel-lean combustion in large droplet cases.

Ignition kernel development and subsequent flame propagation in a planar methane/air turbulent jet

Chemistry validation

- Preferred over the classical modified one-step chemistry¹ :
 - Captures the flame speed accurately over the whole flammability range
 Good prediction of the flame expansion in rich mixtures
 Better characteristics for the prediction of auto-ignition and quenching



Simulation parameters:

- Slot (jet) width : $h = 7.8\delta_{th}$
- Computational Domain: $37h \times 37h \times$ $37h (1920 \times 990 \times 225 \text{ cells}) \text{ and}$ $h/\Delta x = 52$
- Boundary conditions : Periodic in transverse (y/z), NSCBC partiallyreacting outflow, fully-reacting inflow (imposed **u**, Y_k , T, ρ using a scanning plane in $Re_{\tau} = 395$ channel flow)
- Simulation time (reacting): $t_{sim} \approx 80t_{sp} \approx 60t_j$ (main) and $t_{sim} \approx 20t_{sp} \approx 15t_j$ (stochasticity)

Inflow and thermo-chemistry:

- Inlet velocity: $V_b = 23.5s_l^0$ $U_c = 0.1U_b = 2.35s_l^0$ $Re = (\rho_0 U_b h)/\mu_0 = 650$
- Inlet Composition: > $X_f = 0.275, X_o = 0.725$ > $Y_{CH_4} = 0.174, Y_{O_2} = 0.233$
- Thermo : $\tau = 4.5$, $T_0 = 415K$, $\gamma = 1.4$
- *Transport:* Pr = Sc = 0.7 (*Le* = 1)
- Spark: $a_{sp} = 10$, $b_{sp} = 0.34$, $R_{sp}/\delta_{th} = 1$



osition	.s :					
Pos	x^+	y^+	z^+	$\widetilde{\xi}$	$ ilde{\xi}/\xi_{ m st}$	${\cal F}$
0	0	15	0	0.53	1.68	0.37
1	-1	10	0	0.43	1.35	0.28
2	0	7.5	0	0.82	2.60	0.08
3	0	22.5	0	0.44	1.40	0.68

Time :
$$t_{inj}/t_j \approx 0(a), \ 20(b), \ 40(c), \ 60(d)$$

•
$$N_y = \frac{\nabla Y_f}{|\nabla Y_f|}, N_z = \frac{\nabla \xi}{|\nabla \xi|}$$

•
$$T_1 = \frac{N_y \times N_z}{|N_y \times N_z|}, T_2 = N_z \times T_1$$

•
$$s_d = -\frac{\dot{w}_c + \nabla \cdot (\rho D \nabla Y_f)}{\rho |\nabla Y_f|}$$
, $s_z = -\frac{\nabla \cdot (\rho D \nabla \xi)}{\rho |\nabla \xi|}$

•
$$s_e = V_e \cdot T_2 = \frac{s_d - ks_z}{\sqrt{1 - k^2}}$$
 with $k = N_y \cdot N_z$

• Laminar value¹:
$$s_e^{theo} \approx s_l^0 \sqrt{1-\tau} \approx 2.35 s_l^0$$

•
$$W_e = \frac{u \cdot T_2}{|T_2|} + s_e$$
 and $W_{e,x} = W_e \times T_{2,x}$



¹Ruetsch, G.R. et al., Phys. Fluids 7:1447-1454 (1995)

Results: Kernel evolution - 3 mains phases - Case 0a



- Ignition :
 - > Early growth sustained by the large temperature values
 - > Near spherical shape at the end of ignition
- Radial growth and advection :
 - Advection of the kernel downstream
 - Increased growth rate due to the propagation of the downstream edge
 - Growth in the transverse direction (low SDR values)
 - > Triple flame structure appears in a shear layer
- Edge flame propagation and onset of stabilisation :
 - Multiple triple flame structures
 - Flame sheet almost spans the whole jet width
 - Edge flames start to propagate upstream onset of stabilisation

Results: Edge flame evolution- Case 0a



- Kernel initially near spherical and formed of a single flame sheet
- Local extinctions occurs in regions that are beyond the lean/rich flammability limits
- Edge flame structure appears in regions of low SDR
- Longer premixed rich branch than the lean one and almost negligible non-premixed branch
- Survives in region of very high SDR values

Results: Temporal evolution of some statistics



- Flame height (measured with T or \dot{w}_T)
 - Increases after energy deposition
 - Starts to propagate when the edge flame structure is fully established
 - ➤ Converges towards a single value (x⁺ ≈ 18 - 20) for all initial locations
- Mean edge flame speed
- Mean edge flame absolute displacement speed

Results: Temporal evolution of some statistics



- Flame height (measured with T or \dot{w}_T)
- Mean edge flame speed
 - Converges towards a single value $(\langle s_e |_{ef} \rangle / (s_e^{theo}) \approx 2 3)$
 - Positive influence of SDR, Y_f and ξ curvatures and u' on s_e
- Mean edge flame absolute displacement speed

Results: Temporal evolution of some statistics



- Flame height (measured with *T* or \dot{w}_T)
- Mean edge flame speed
- Mean edge flame absolute displacement speed
 - $\langle W_{,xe}|_{ef} \rangle / s_l^0 ≤ 0 \implies$ edge flame
 propagates upstream

$$> -5 \le \langle W_{,xe} |_{ef} \rangle / s_l^0 \le 8$$

Large positive values initially for cases 0a and 1a rapid convection downstream

Conlusions-3

Kernel growth and early stages of flame propagation in a planar methane/ air turbulent jet has been numerically evaluated for different energy depositing position and timing, giving rise to the below observations:

- Ignition and propagation qualitatively similar for all cases
- Edge flame behaviour:
 - ➤Large influence on the success of ignition/propagation
 - ≻If the growing kernel transition to a set of tribrachial flame → successful propagation
 - Mean edge flame speed relatively fast $(\langle s_e |_{ef} \rangle / (s_e^{theo}) \approx 2 3) \implies$ locally the edge flame propagates faster than the flow and the flame base stabilises.
- For low values of x^+ , local conditions are very important.
- Different modes of failure captured (quenching due to local mixture composition, SDR value, no transition to edge flame, etc.)

Thank you for your time and attention

Questions ?

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