Low temperature combustion in ignition of turbulent dual fuel mixture

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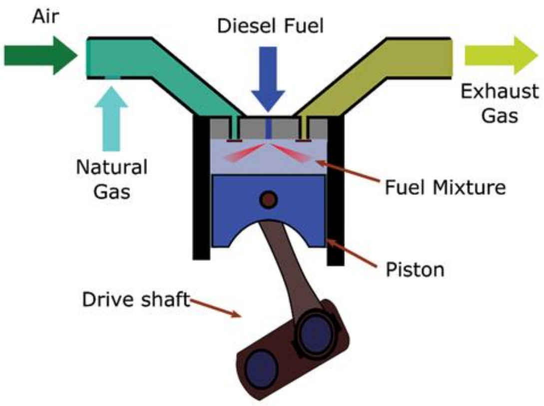
1.1 Motivation

- Lean premixed combustion of natural gas (NG) in IC engine is attracting to reduce particulate and NOx emission, with poor ignitability.
- Dual-fuelling, ignition of natural gas (NG) by a high-cetane fuel (e.g. DME), presents promise to ensure successful combustion initiation control.
- **Dual-fuel combustion** involves combined processes of **autoignition, diffusion flames, and flame propagation**, which is challenging for experimental measurement and numerical modelling.



Few fundamental numerical studies of dual-fuel ignition:

- Ignition in laminar heptane/CH4-air mixing layer (Wang et al. 2015).
- Heptane droplets ignition in CH4-air (Demosthenous et al. 2016).
- Pilot ignited DME/CH4-air (Soriano & Richardson)
- Dynamics of triple flames in igniting DME/CH4-air (Tai Jin, Kai Luo et al. PCI, 2018)

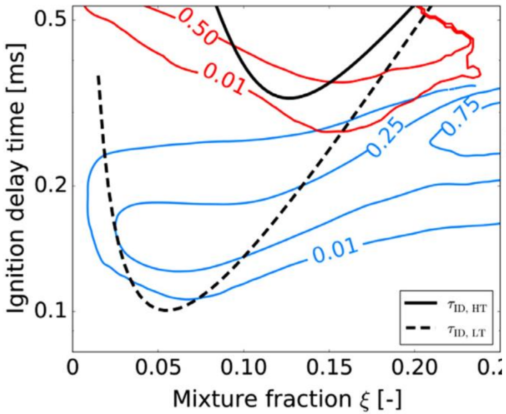
- **Understanding of the ignition dynamics in dual-fuel mixture is of great importance for design and control.**

1.2 Objectives

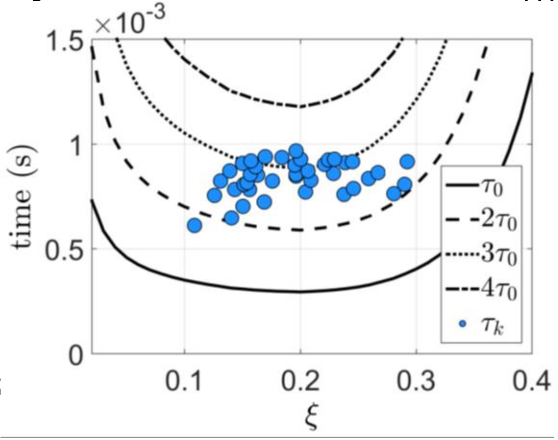
Autoignition in diesel engines occurs as a multi-stage process, involving **Low- and High-temperature combustion (LTC & HTC)**

Single-stage HTI in turbulent mixture no earlier than HID ($\tau_{HT,mr}$) (Mastorakos, 2009)
LT ignition (LTI) transits to propagating cool flame:

- Accelerate HTI, earlier and richer than τ_{HT} (Borghesi et al. (2015), Krisman et al. (2016, 2017), Borghesi et al. (2018))
- No accelerated HTI, vary between 2 and 3 times τ_{HT} in n-heptane jet (Krisman et al. (2017))



Borghesi et al. (2018)



Krisman et al. (2017)

LTI to cool flame?

Accelerate or not?

2.1 Ignition in dual-fuel mixture

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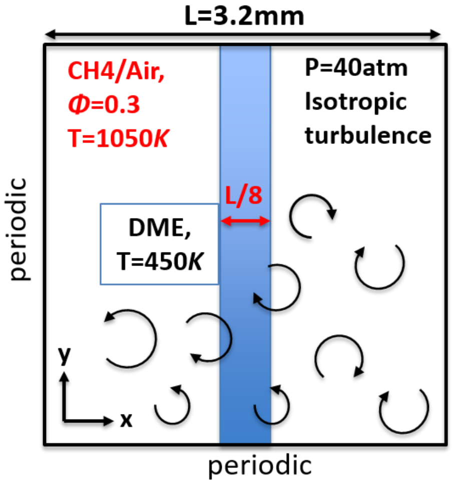
Configuration 1:
Pilot-ignited
DME/CH4-air

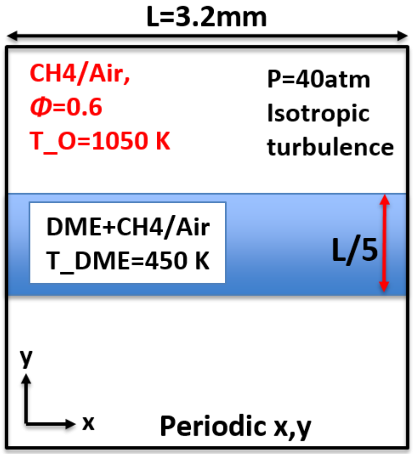


$\xi \in (0,1)$

Single ∇ ξ

Tai Jin et al., PCI (2018)

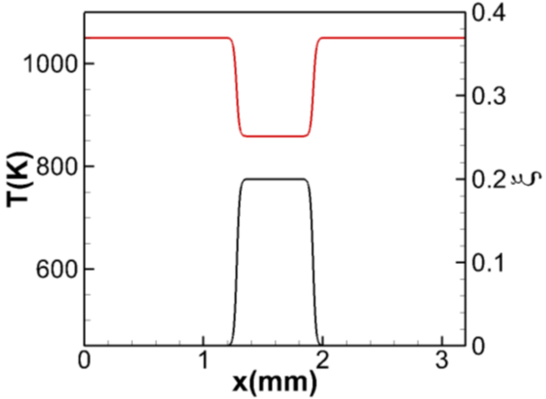
Configuration 2:
Partially mixing
Relevant to RCCI



$\xi \in (0,0.2)$, $\xi \in (0,0.4)$

Various ∇ ξ

Tai Jin et al., submitted



Initial scalar profile across mixing layer

Mixture fraction: $\xi = (Y_{N2} - Y_{N2,o})(Y_{N2,f} - Y_{N2,o})$

Initial scalar profiles: $\delta = 24\ \mu m$

$$f(x) = \left(\frac{f_1+f_2}{2}\right) + \left(\frac{f_1-f_2}{2}\right) \tanh\left(abs\left(\frac{x-x_c}{\delta}\right)\right)$$

Initial turbulence fluctuations:

$$E(k) = \frac{32}{3}\sqrt{\frac{2}{\pi}\frac{u'^2}{k_e}}\left(\frac{k}{k_e}\right)^4 exp\left[-2\left(\frac{k}{k_e}\right)^2\right]$$

2.2 Numerical Schemes

Governing equations: Continuity + Navier-Stokes + Species/Energy transport + EOS

A fully compressible in-house DNS code

1. Spatial discretization: Eighth-order central differencing scheme

$$f_i' = \frac{8/5\left(f_{i+1} - f_{i-1}\right)}{2h} - \frac{4/5\left(f_{i+2} - f_{i-2}\right)}{4h} + \frac{8/35\left(f_{i+3} - f_{i-3}\right)}{6h} - \frac{1/35\left(f_{i+4} - f_{i-4}\right)}{8h}$$

2. Temporal discretization: Fourth-order Runge-Kutta method (RK44)

3. Filtering: Explicit tenth-order filter method (suppress high wavenumber errors)

$$\widehat{f_n} = \frac{1}{2^{10}}\left[772 f_n + 210\left(f_{n-1} + f_{n+1}\right) - 120\left(f_{n-2} + f_{n+2}\right) + 45\left(f_{n-3} + f_{n+3}\right) - 10\left(f_{n-4} + f_{n+4}\right) + \left(f_{n-5} + f_{n+5}\right)\right]$$

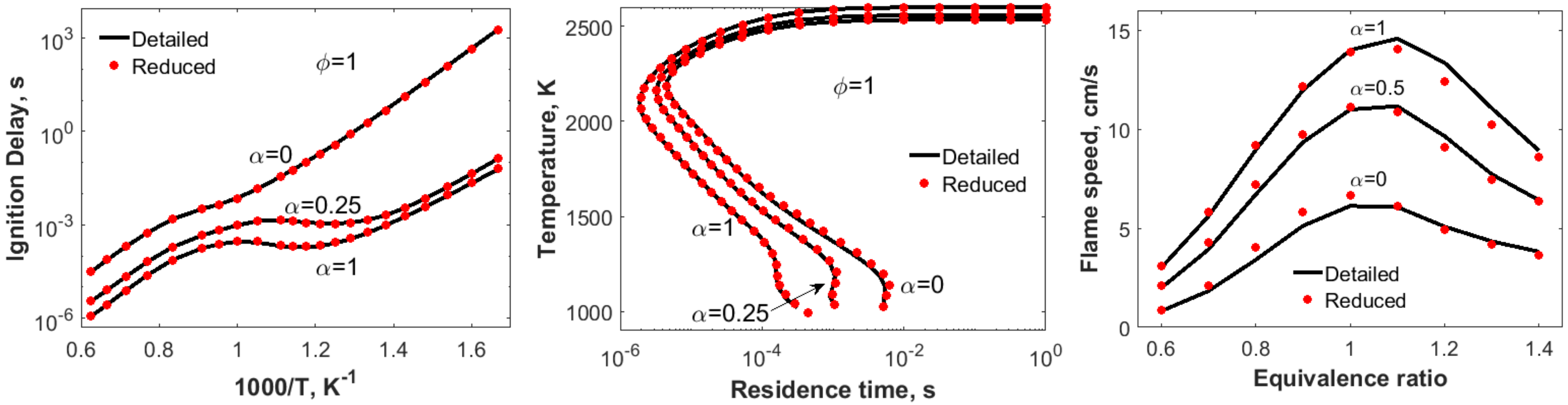
4. Boundary conditions

➢ Improved Navier-Stokes characteristic boundary conditions (NSCBC)

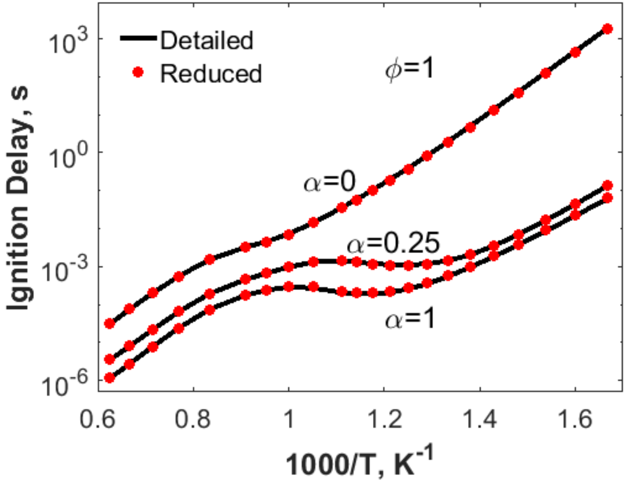
5. Parallel strategy: MPI communication + CPU decomposition

2.3 Chemical mechanism

- Reduced by Dr. Tianfeng Lu from a validated detailed DME/CH_4 mechanism (Mech_56.54) by Prof. Curran (2015)
- 25 species in 147 reaction steps
- Validated in ignition delay time, perfectly stirred reactor (PSR) extinction residence time, laminar premixed flame speed



2.4 Homogeneous Ignition Delay



Stoichiometric mixture

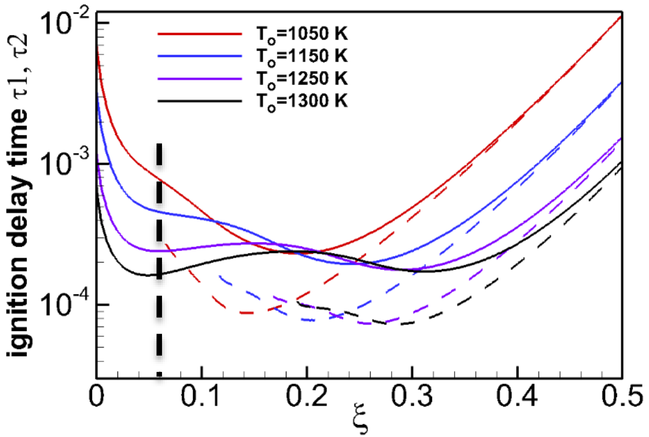
(Pure CH4, Pure DME, CH4+DME)+air

With DME added,

- Ignition delay (ID) decreases significantly,
- NTC effects.

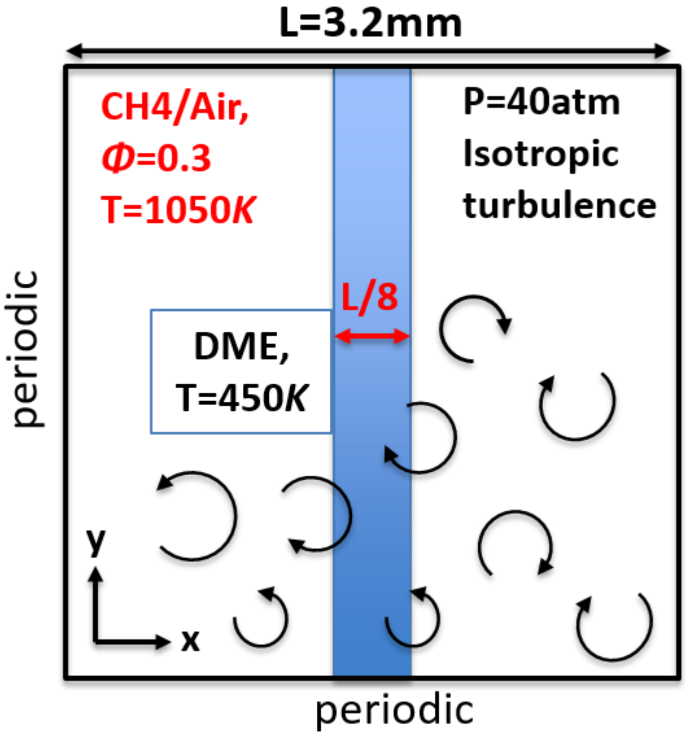
CH4-air (φ=0.6) → +DME

- One stage ignition → two stages
- T_o increase, ξ_{MR} for the two stage ignition increase
- τ_{st} decrease significantly



- $\xi = (Y_{N2} - Y_{N2,o}) / (0 - Y_{N2,o})$
- ξ increase: more DME added

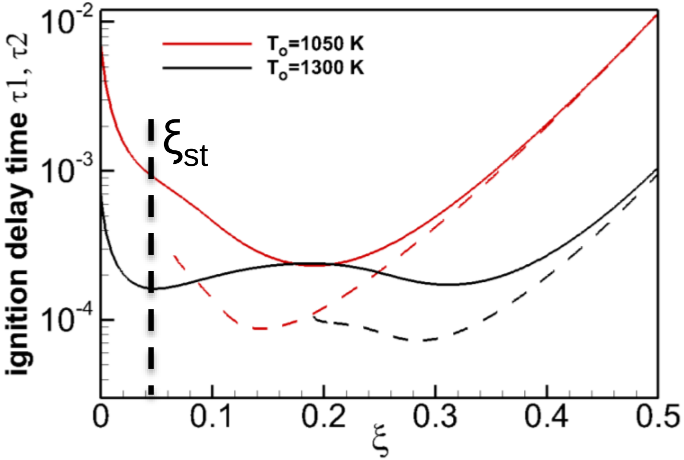
3. Pilot-ignited dual fuel combustion



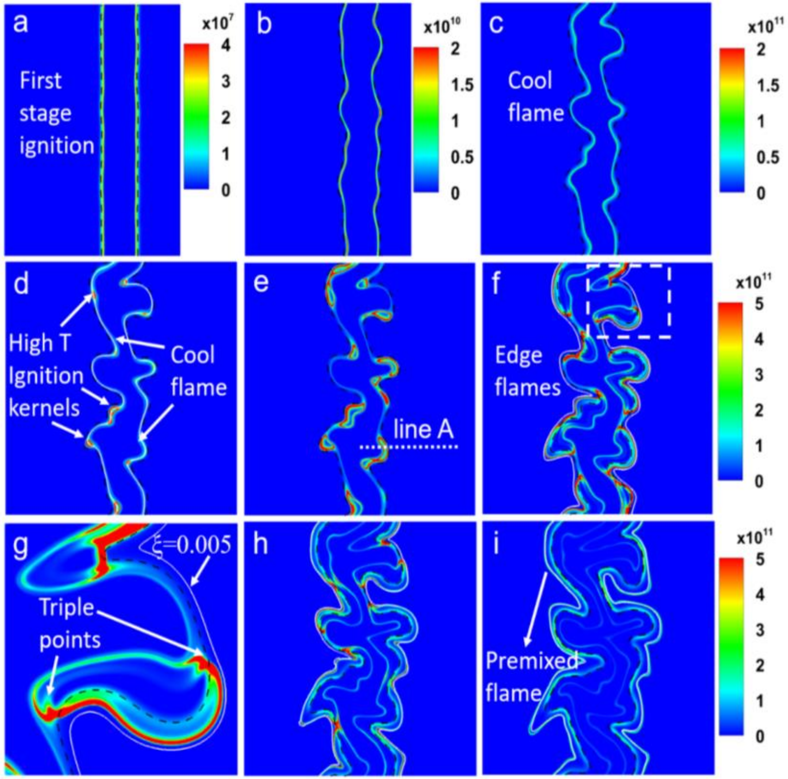
The computational domain with DME and methane-air mixture

Computational parameters

Case	φ	ξ_{max}	T_f (K)	T_o (K)	U' (m/s)	L11 (mm)
1	**0.3**	**1.0**	**450**	**1050**	**0.5**	**0.2**
2	0.6	1.0	450	1050	0.5	0.1
3	0.6	1.0	450	1050	1.0	0.1
4	0.6	1.0	450	1300	1.0	0.1



3.1 Ignition case 1



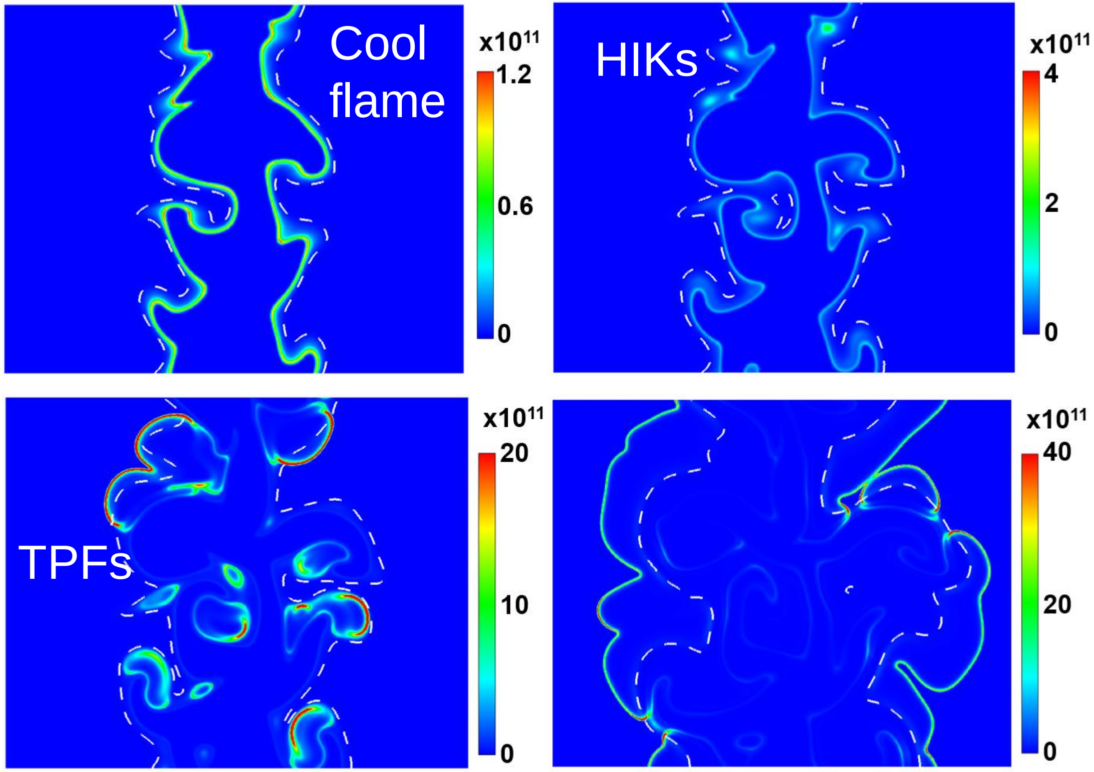
HRR (W/m^3), at 0.008, 0.06, 0.16, 0.23, 0.25, 0.29, 0.29, 0.33 and 0.41 ms

Case 1, φ=0.3, ξ_{max}=1.0, L_t=0.2 mm

- First stage ignition (LT) transits to propagating cool flame
- High T ignition kernel discretely located in fuel rich mixture
- Triple flames propagating along the ξ_{st} line
- Lean premixed branch initiates the premixed methane-air flame

Tai Jin, Kai H. Luo et al. Dynamics of triple-flames in ignition of turbulent dual fuel mixture: a direct numerical simulation study, PCI, 2018.

3.2 Ignition case 2

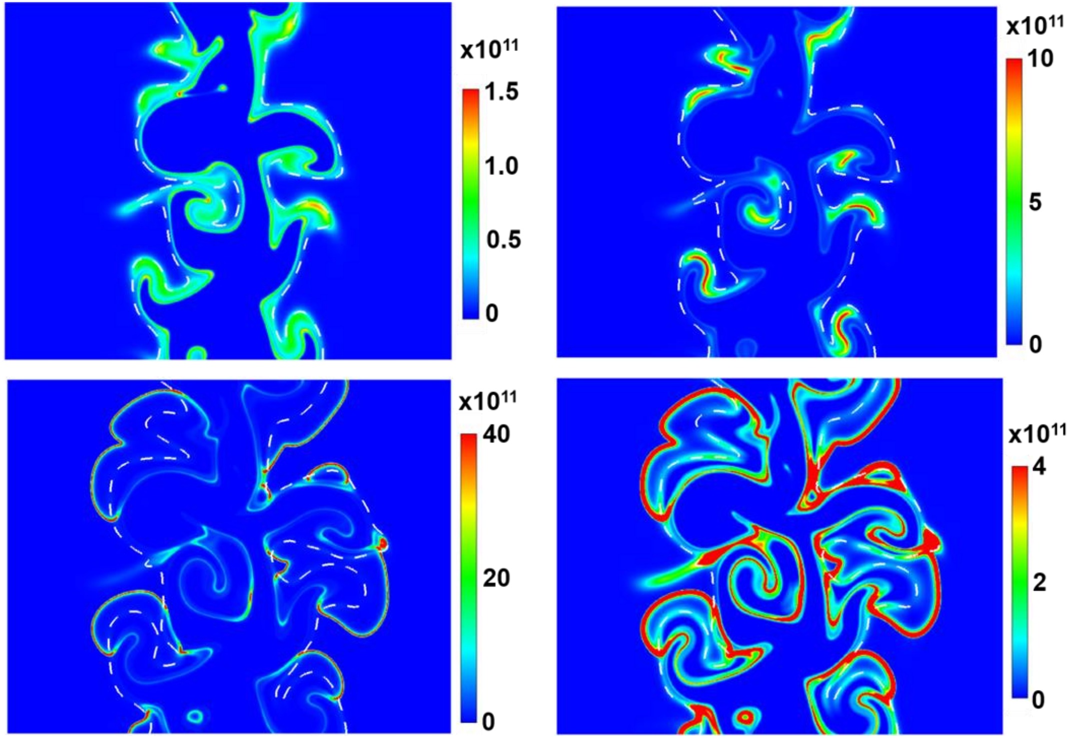


Temporal evolution of HRR (W/m³), t*=0.8, 1.2, 1.6, 2.0.

Case 2, φ=0.6, ξ_{max}=1.0, L_t=0.1 mm

The ignition and flame initiation process is qualitatively consistent with **φ=0.3**

3.3 Ignition case 3

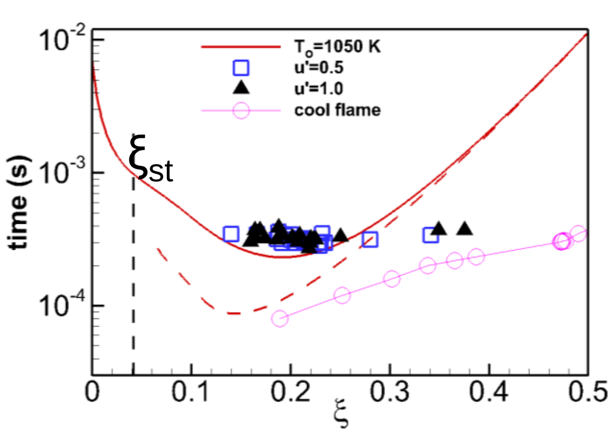


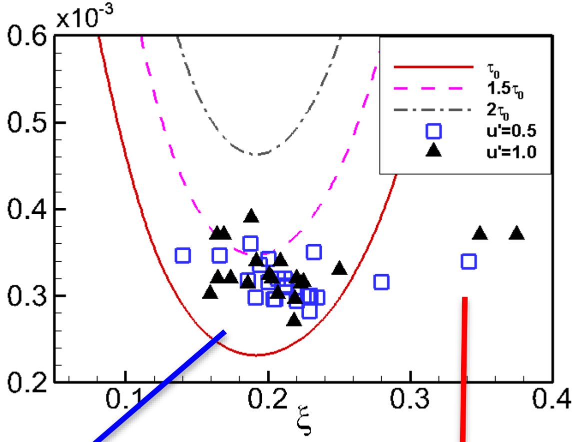
Time evolution of HRR (W/m^3), t*=0.864, 1.0, 1.2, 1.2.

Case 4, φ=0.6, T_o=1300K

- The ignition process is qualitatively consistent with **Cases 1&2**
- **High T ignition kernels much bigger**

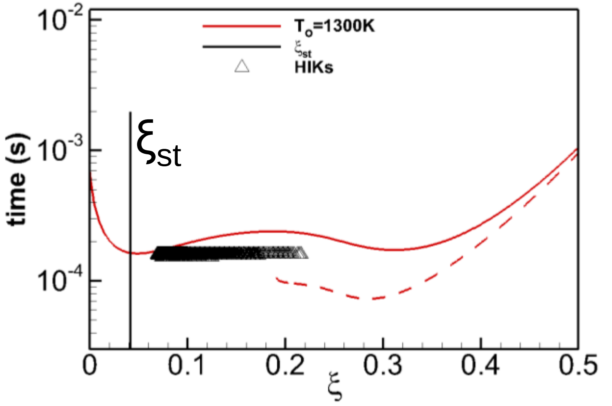
3.4 HT ignition kernels





No obviously accelerated

accelerated



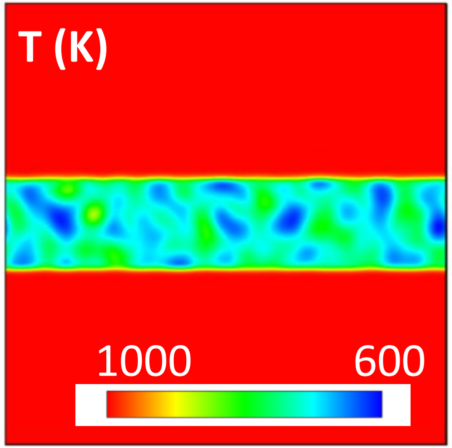
- Most of HIKs located around ξ_{mr}
- HIKs in fuel rich mixtures are accelerated
- Velocity fluctuation, no significant change time of HIKs

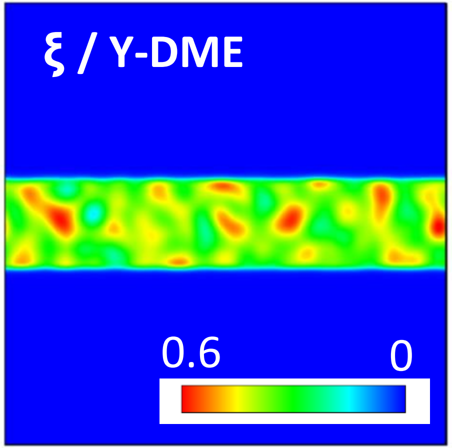
- HIKs located in a wide range of ξ (fuel rich)
- HIKs are accelerated

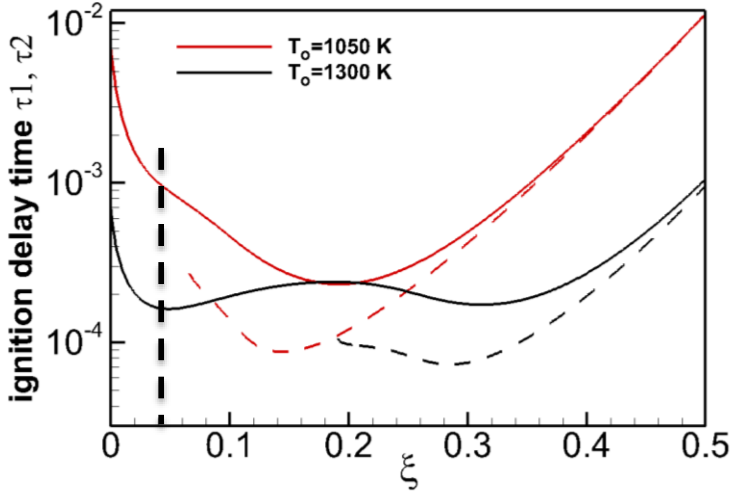
4. Ignition in turbulent dual-fuel mixture

case	T_o (K)	$\bar{\xi}$	ξ'	ξ_{MR}	ξ_{st}	ID @ ξ_{MR}	1st ξ_{MR}	1st ID
1	1050	0.4	0.025	0.19	0.0413	2.3e-4	0.14	8.71e-5
2	1050	0.2	0.015	0.19	0.0413	2.3e-4	0.14	8.71e-5
3	1300	0.4	0.025	0.046	0.0413	1.62e-4	0.289	7.29e-5

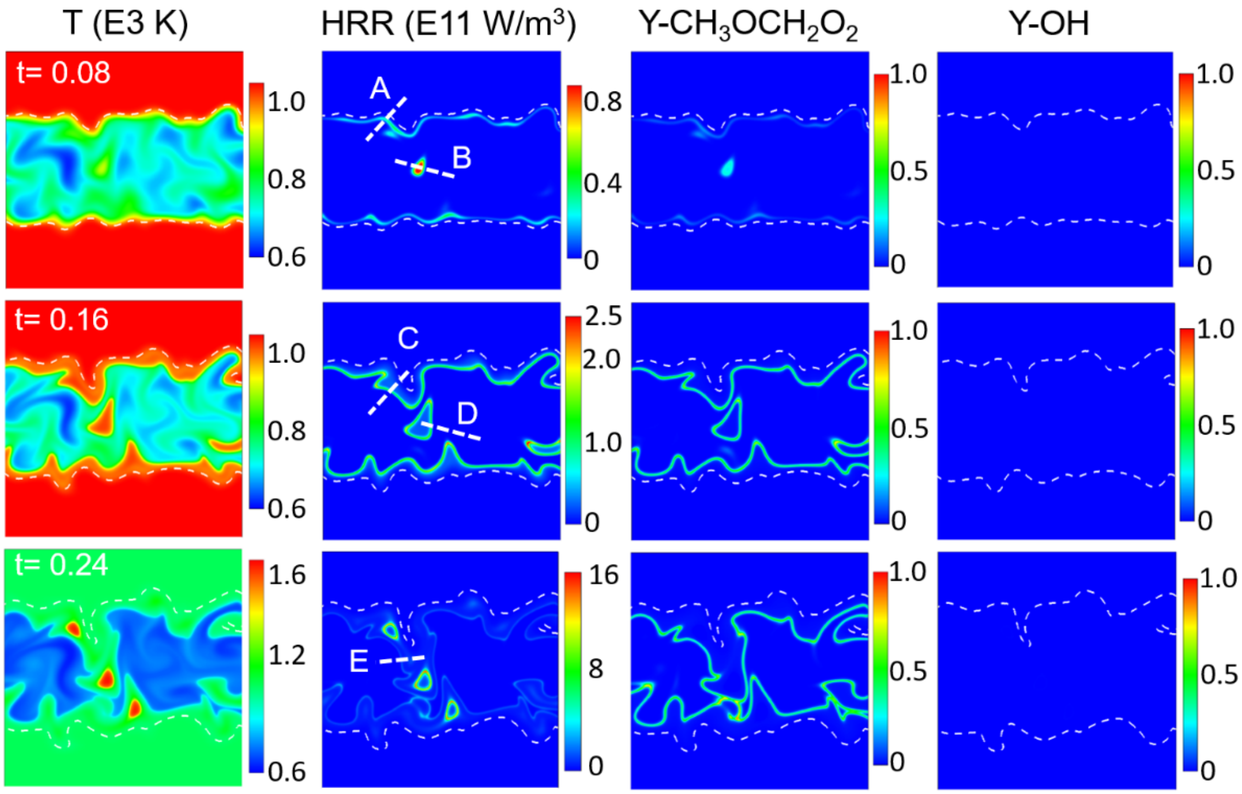
Computational parameters







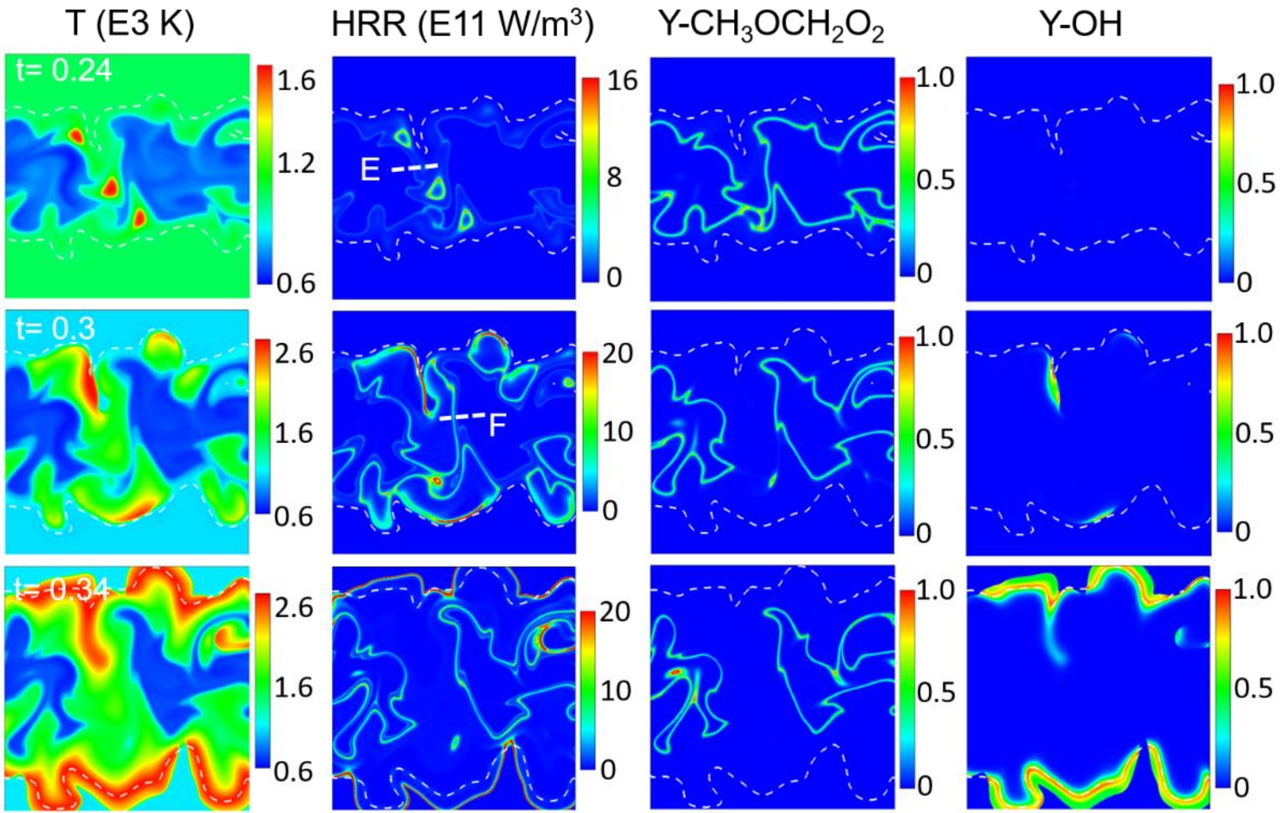
4.1 Ignition-case 1



Case 1, $\bar{\xi}$=0.4

- First stage ignition (LT) transits to propagating cool flame
- High T ignition kernel discretely located in fuel rich mixture

4.1 Ignition-case 1



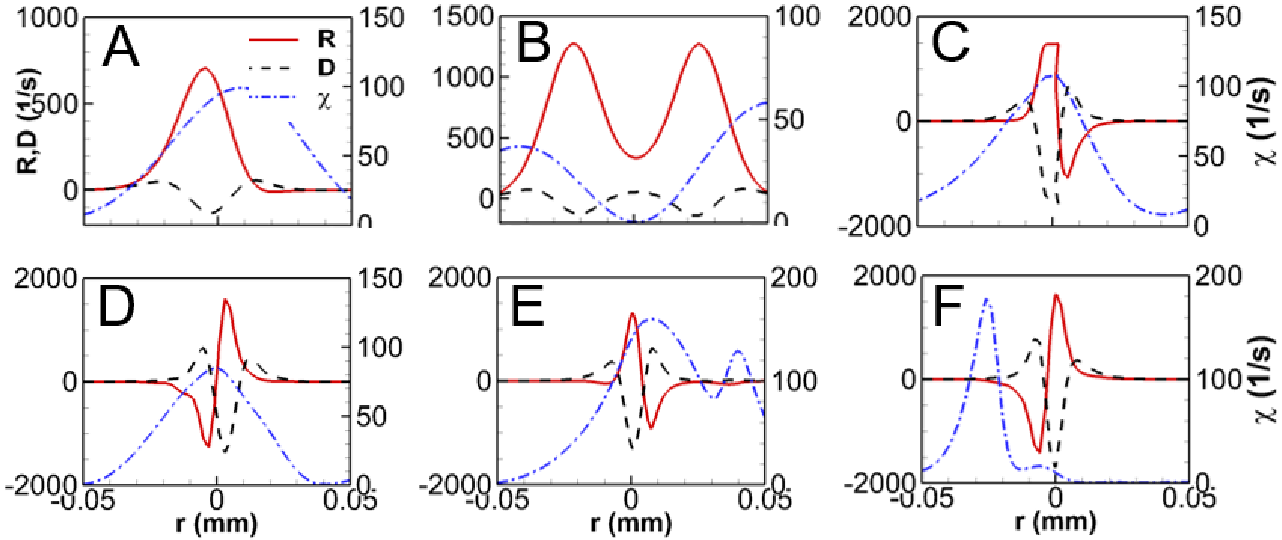
Case 1, $\bar{\xi}$=0.4

- High T flames connected
- No obvious propagating triple flames
- Lean premixed branch initiates the premixed methane-air flame

4.1 Ignition-case 1

The role of diffusion in supporting the cool flame, transport budget analysis for the **LTC marker $Y_{CH3OCH2O2}$**

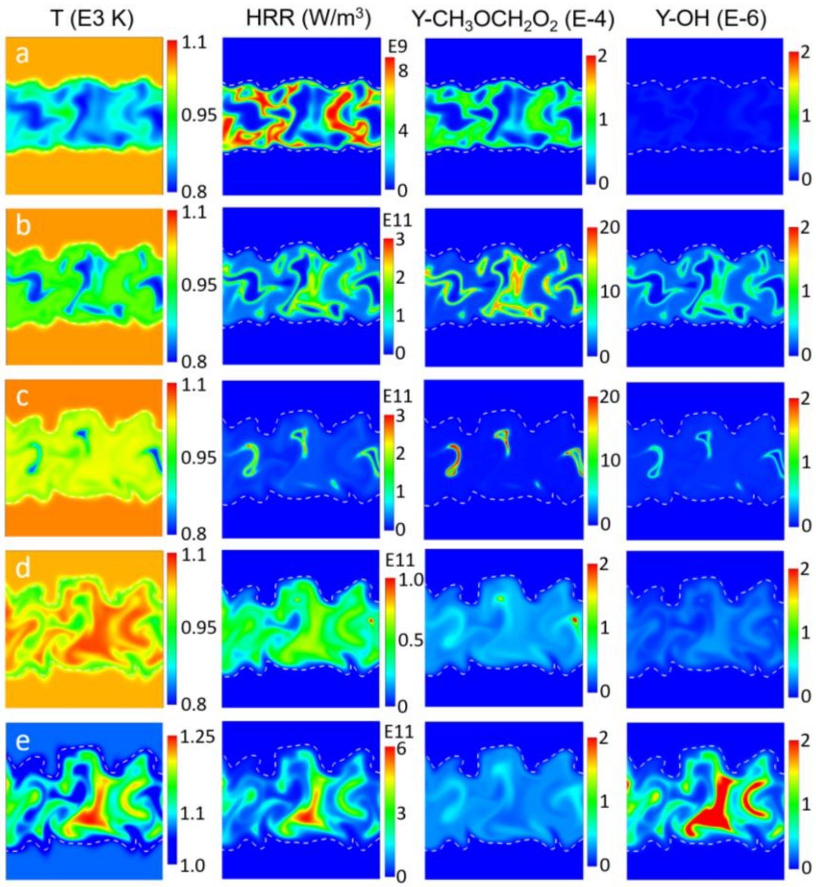
Ignition front: R>>D, Propagating flame front: R≃D (R-reactive, D-diffusion terms)



- A.B:
R>>D, ignition front,
χ relatively low

- C-F:
R&D increase, R≃D,
cool flame front

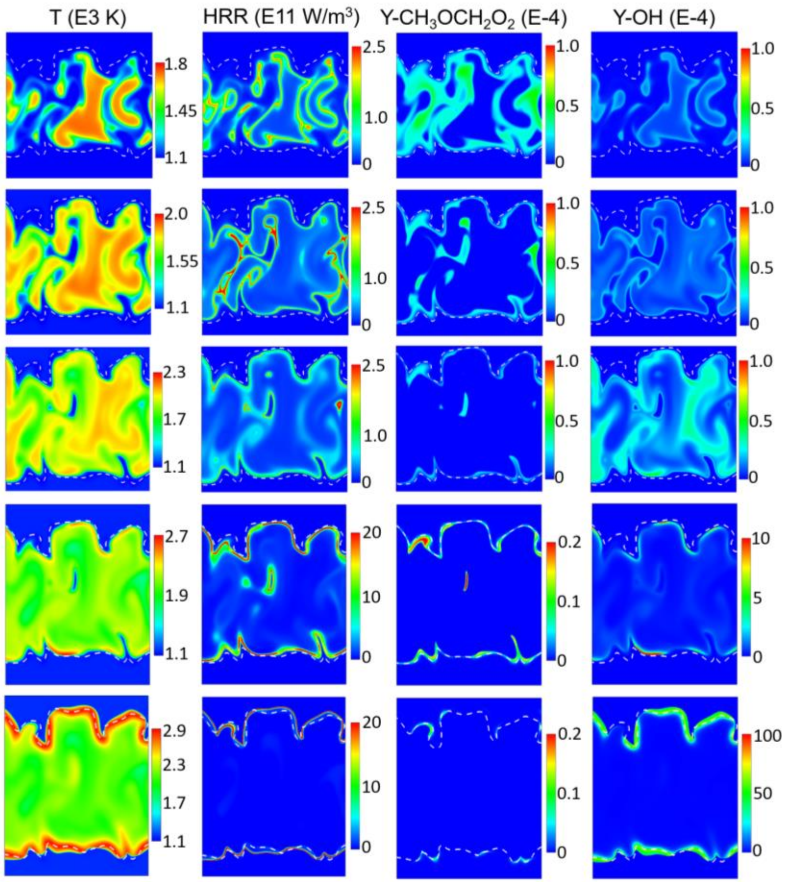
4.2 Ignition-case 2



Case 2, $\bar{\xi}$=0.2

- Cool flame exists around low T mixture (high ξ, larger 1st stage ignition delay)
- HRR, Y-$CH_3OCH_2O_2$, relatively high around cool flame
- High T ignition occur in a large area, not in discrete kernels

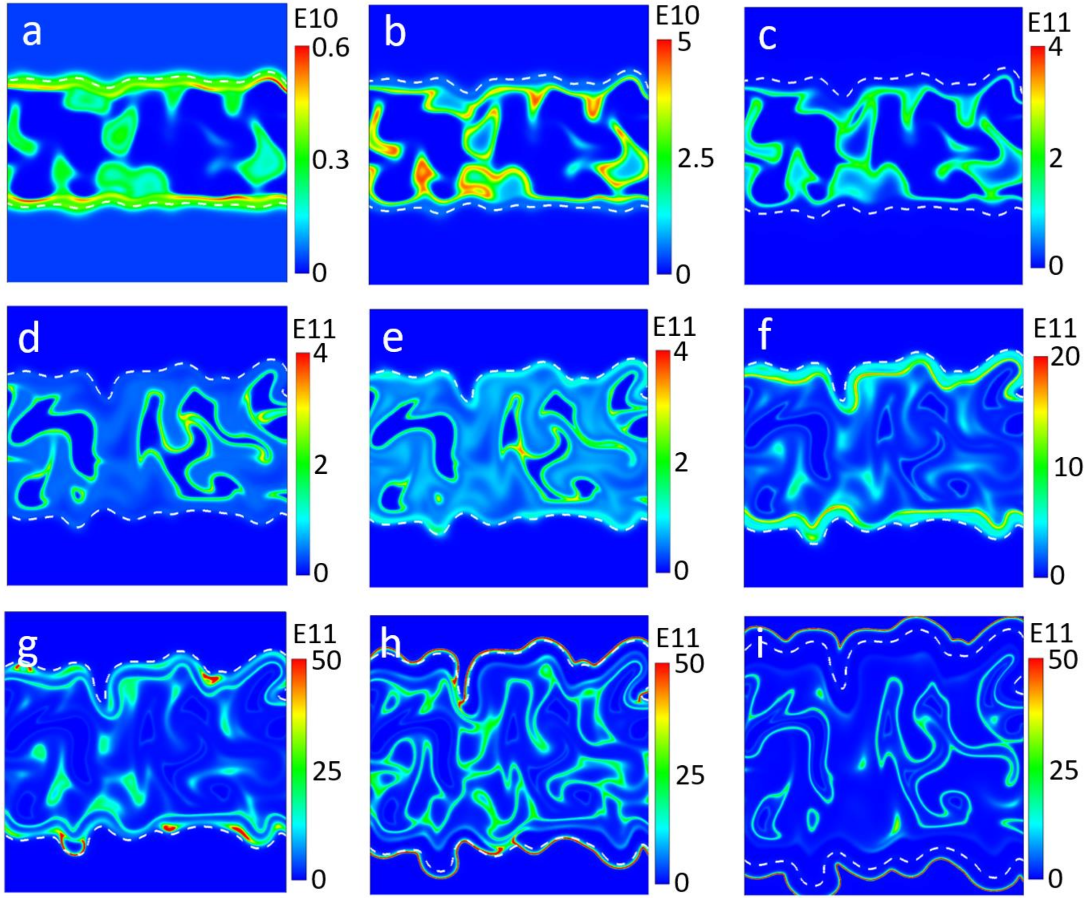
4.2 Ignition-case 2



Case 2, $\bar{\xi}$=0.2

- High T flames emerge with each other
- High T flames connected, propagate across ξ_{st}, and initiate the premixed methane-air flame

4.3 Ignition-case 3



Case 3, $\bar{\xi}$=0.4, T_o=1300K

- Cool flame develops both in the central region and in the mixing layer
- HTI first initiate along ξ_{st}, around single-stage ξ_{mr}
- third-stage ignition kernels

4.4 HT ignition kernels

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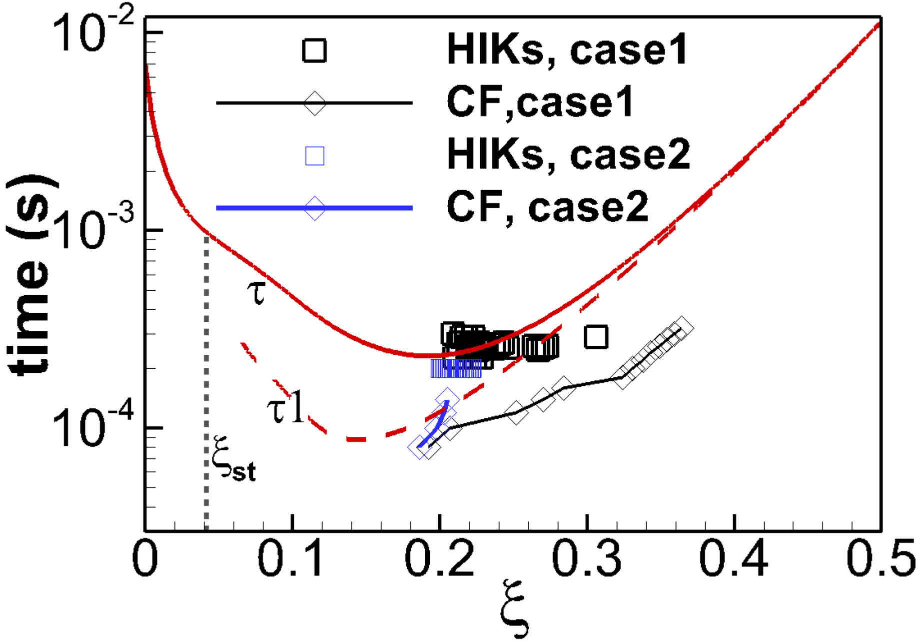


Time of HIKs compared with homogeneous ignition delay times

Case 1, $\bar{\xi}$=0.4

HIKs in fuel rich mixture, accelerated

Comparable with $\tau_{HT,mr}$

Case 2, $\bar{\xi}$=0.2

HIKs in fuel rich mixture

HT ID shorter than the shortest $\tau_{HT,mr}$

ID of CH_4/air: 6.98ms

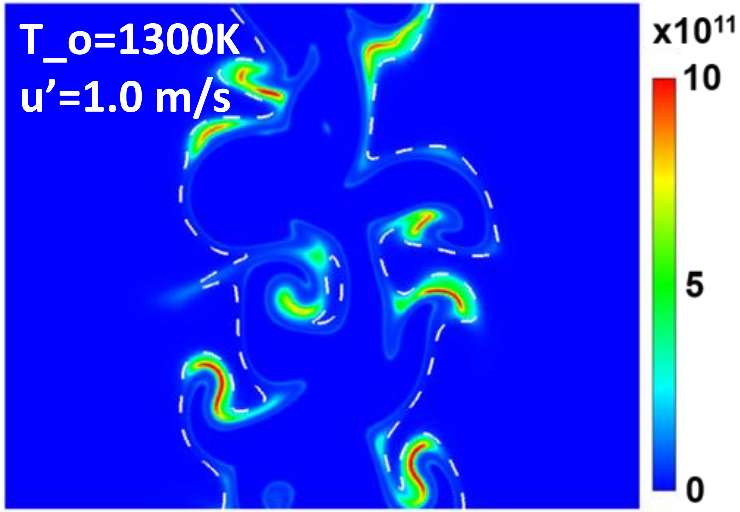
Premixed CH_4/air flame initiation time:

Case 1: 0.34ms

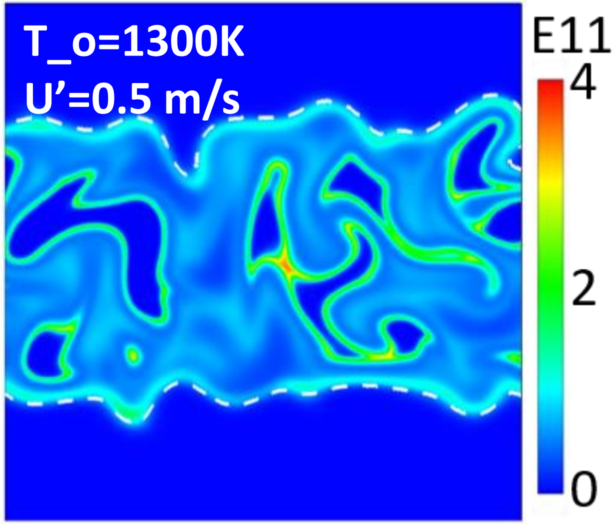
Case 2: 0.26ms

4.4 HT ignition kernels

ξ∈(0,1)
Single ∇ ξ



ξ∈(0,0.4)
Various ∇ ξ



5. Conclusions

Ignition dynamics in turbulent DME/methane-air mixture via DNS

- The ignition process involves both LTC and HTC, varies with the thermo-chemical conditions, as well as turbulence
- Low temperature combustion plays a vital role

LTI to cool flame?

- Depends on the mixture fraction gradient (ignition delay gradient)

Accelerate or not?

- High-T ignition in fuel quite rich mixture is accelerated by passage of cool flame
- High-T ignition can be shorter than the shortest $\tau_{HT,mr}$

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Questions or comments?

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