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Response of heat release to equivalence ratio variations in high Karlovitz premixed H_2/air flames at 20 atm: a DNS study

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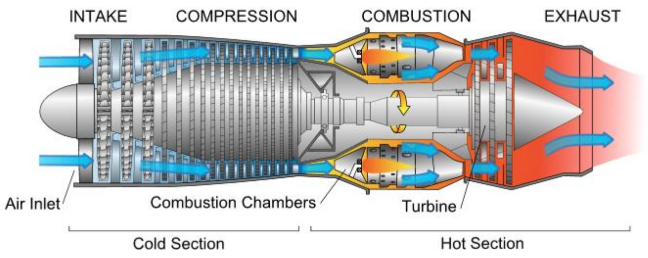
Outline

- ❑ Background
- ❑ Numerical method and computational cases
- ❑ Results and discussion
- ❑ Conclusions and future work

1 Background



- Lean premixed combustion has wide-ranging applications in industrial devices with the advantage of low NOx emission. In modern gas turbines, typical equivalence ratios at base load are in the range 0.45-0.6 [1].
- Turbulent flames in gas turbines are characterised by intense turbulence intensity and high pressure.
- Turbulent lean premixed flames are susceptible to equivalence ratio oscillation, which is one of the most significant mechanisms contributing to combustion instabilities.
- Objectives: To study the characteristics of lean H_2/air flames with various equivalence ratios under conditions relevant to gas turbines (High Ka, High P) by three-dimensional direct numerical simulations .

[1] Jansohn P. Modern gas turbine systems: High efficiency, low emission, fuel flexible power generation. Elsevier; 2013.

2 Direct numerical simulation

- ❑ DNS code: PENCIL CODE[1]
- ❑ Spatial discretization — six-order compact finite difference schemes
- ❑ Time advancement — low-storage third-order Runge-Kutta (RK3-2N)
- ❑ Chemistry calculation — Livermore Solver for ODE (LSODE)
- ❑ H_2/O_2 chemical mechanism developed by Li et al. (2004)

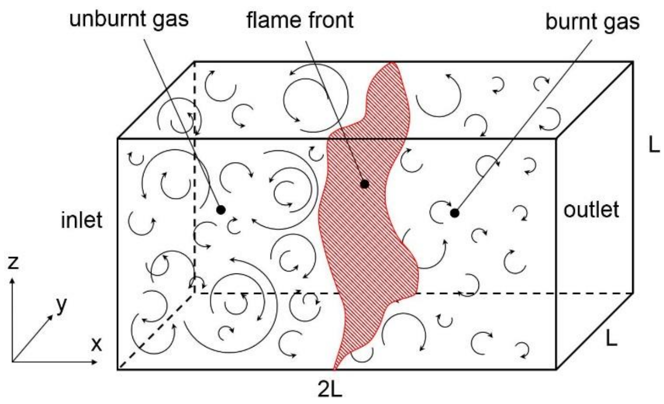


Fig. 1 Schematic of the computational domain .

Boundary conditions:

- ❑ Cross-flow direction: periodic boundary conditions
- ❑ Inlet/outlet: NSCBS

[1] Babkovskaia N, Haugen NEL, Brandenburg A. A high-order public domain code for direct numerical simulations of turbulent combustion. J Comput Phys 2011;230(1):1-12.

3 Computational Cases

Pressure=20atm

Table 1. Simulation parameters.

Case	A	B	C
ϕ	**0.4**	**0.5**	**0.6**
S_L (cm/s)	1.66	6.81	21.16
δ_L (cm)	2.54E-02	8.3E-03	3.3E-03
u′ (cm/s)	177	664	1941
v (cm²/s)	9.05E-03	9.34E-03	9.62E-03
l_t (cm)	2.54E-02	8.3E-03	3.3E-03
Δx (μm)	4.96	3.24	1.29
Re	497	590	666
Ka	**2376**	**2373**	**2368**

Turbulent Reynolds number $\mathrm{Re} = u' l_t / v$

Karlovitz number $\mathrm{Ka} = \left(u'^3 / v l_t\right)^{1/2} / \left(S_L / \delta_L\right)$

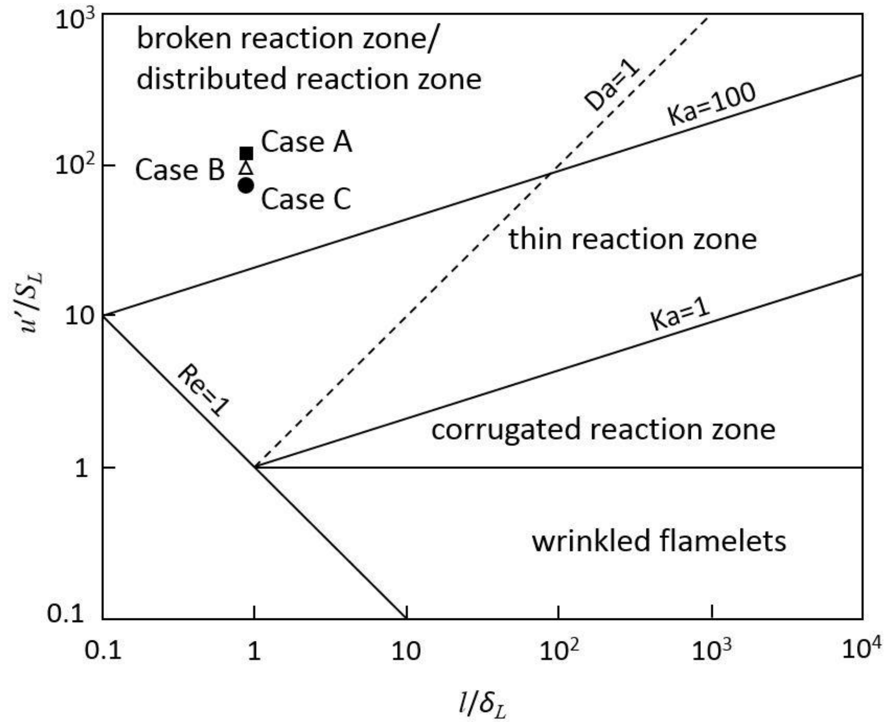


Fig. 2 Turbulent combustion regime diagram

Initial condition:

- Pre-generated 1D flame + turbulence
- 26 grids across the flame thickness
- Time step is determined by CFL condition: 1e-10~2.5e-9

Results: 1D laminar flame

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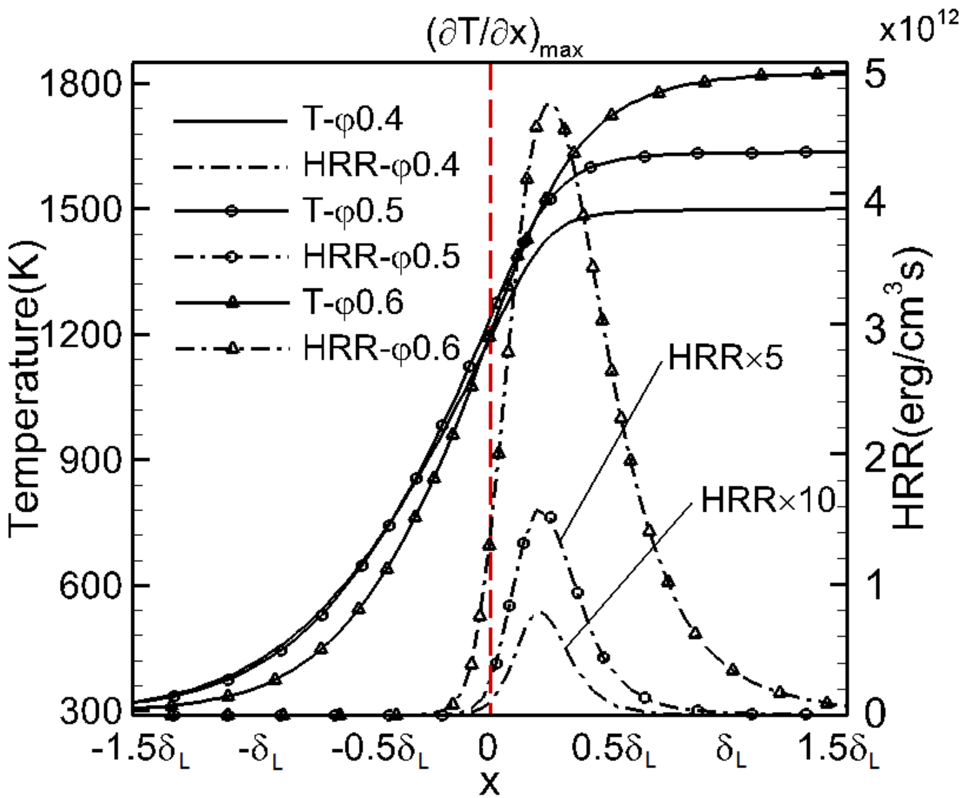


Fig.3 Laminar flame structures

- HRR is significantly increased when the equivalence ratio increases
- The burnt gas temperature increases from 1530 K to 1836 K
- The equivalence ratio increases, the reaction zone is obviously broadened.
- The scaled temperature gradient is larger under higher equivalence ratio

4 Results: flame structures

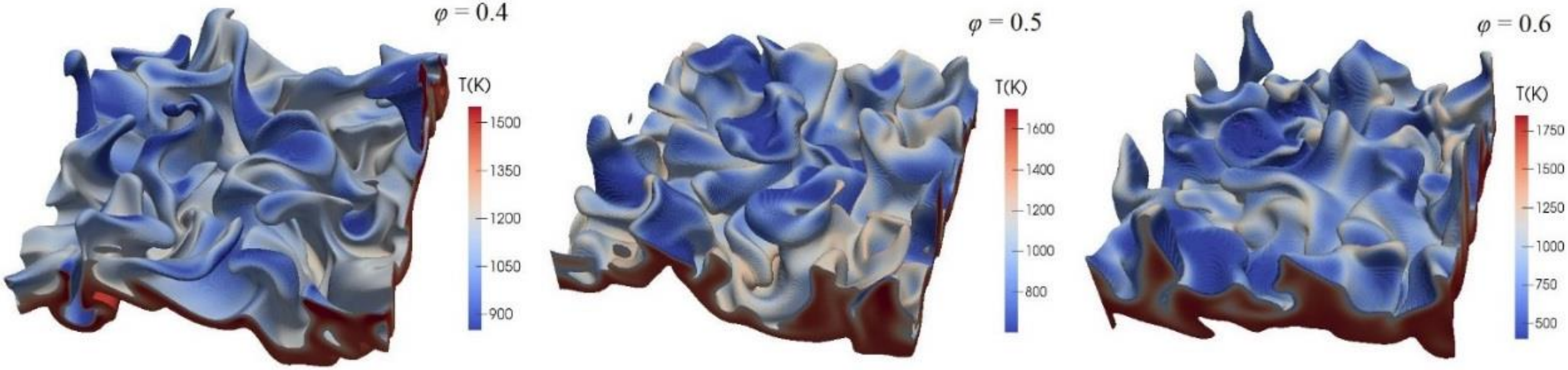


Fig. 4 Reaction zone structures at different equivalence ratios.

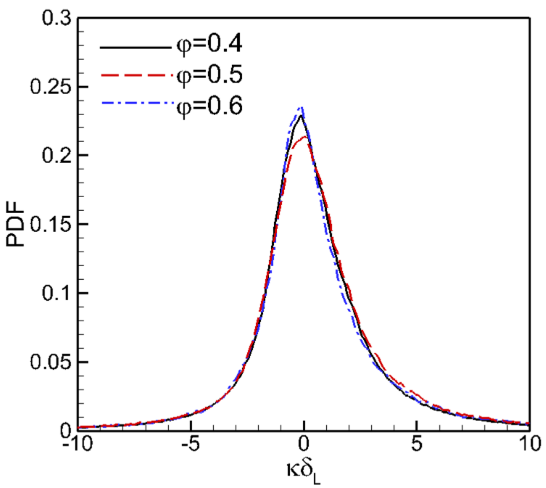


Fig.5 PDFs of mean curvatures of flame fronts

- ❑ the flame fronts are seriously wrinkled and stretched by turbulences
- ❑ Characterized by the same Ka, the flame front structures of the three flames are quite similar.
- ❑ The Pdf of mean curvatures of flame fronts are consistent.

4 Results: flame structures

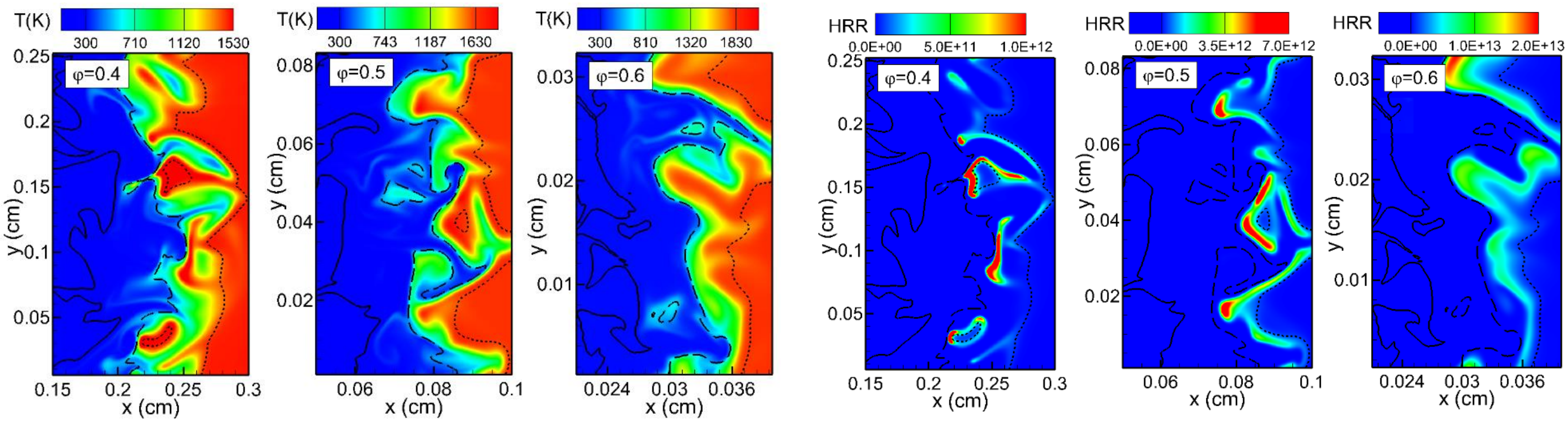


Fig. 6 2D snapshot of reaction zone structures at different equivalence ratios. The solid, dashed and dotted black lines correspond to c = 0.01, 0.5 and 0.99, respectively.

- The majority of heat release happens in region $0.5 < c < 0.99$
- the thickness of high-HRR regions is obviously increased, and the gradient is correspondingly decreased. In flame C, the high-HRR regions almost fill up the zone $0.5 < c < 0.99$, whereas there are only narrow strips in flame A.

4 Results: flame mean statistics

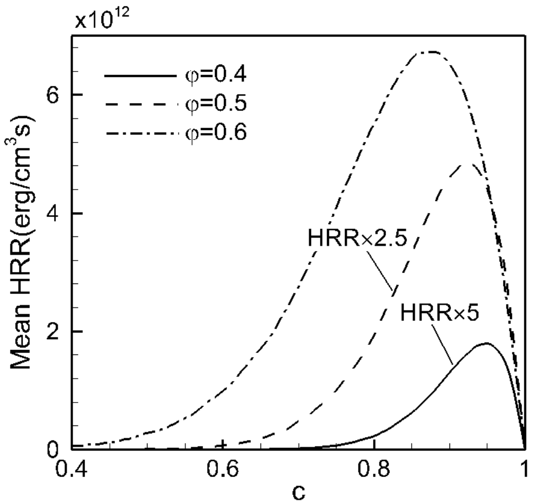


Fig.7 Mean heat release versus progress variable for turbulent flames

- the heat release of turbulent flames is enhanced, and the reaction layer is relatively broadened under high equivalence ratio.
- the extent of enhancement is reduced at high equivalence ratio.
- obvious heat release is observed from c = 0.4 for case φ = 0.6, while it happens after c = 0.7 for case φ = 0.4.

Table 2 Characteristic parameters of reaction zones of laminar and turbulent flames

Case	HRR_{max_1D} (erg/cm^3s)	Mean HRR_{max_3D} (erg/cm^3s)	δ_{f_1D}	δ_{f_3D}
A	7.90E10	3.69E11	0.54 δ_L	1.25 δ_L
B	7.87E11	1.95E12	0.65 δ_L	1.63 δ_L
C	4.68E12	6.73E12	δ_L	1.86 δ_L

4 Results: local equivalence ratio $\varphi_L = \dfrac{Y_H/(2\cdot W_H)}{Y_O/W_O}$

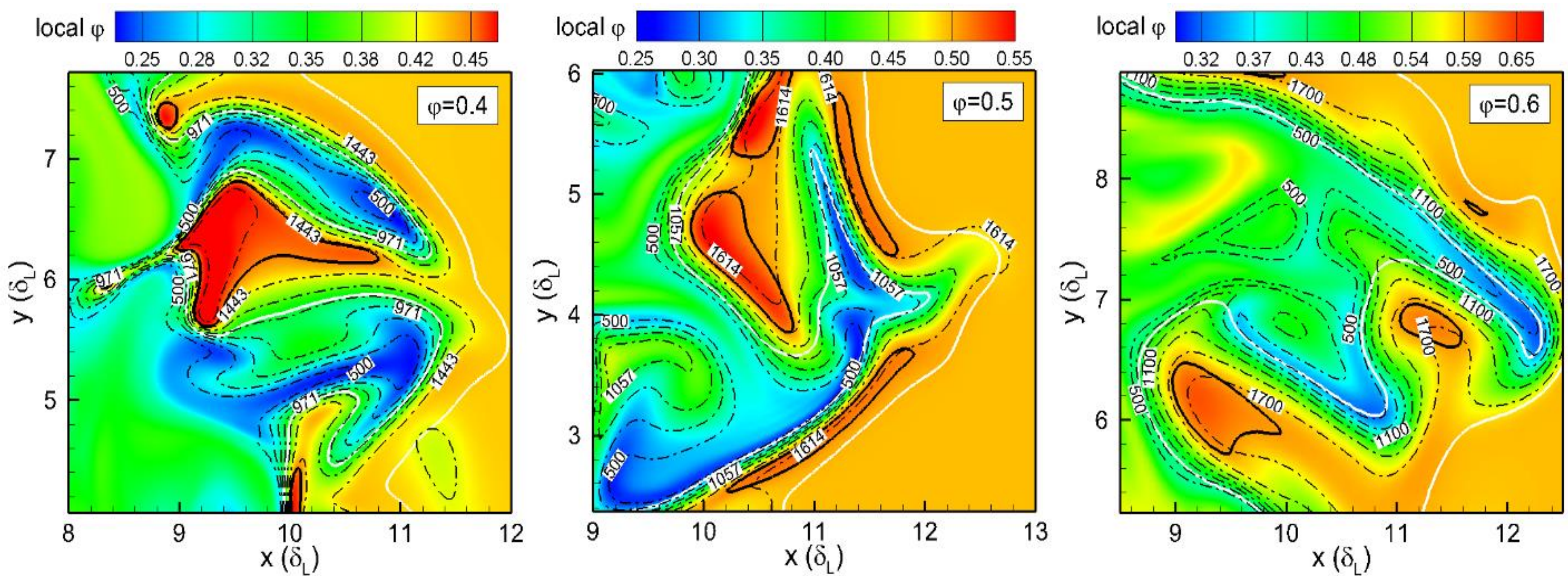
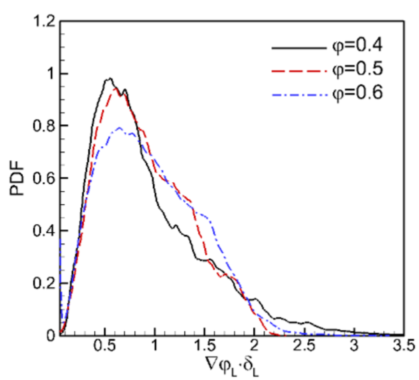


Fig.8 Two-dimensional slices of the reaction zone coloured by local equivalence ratio



- ❑ φ_L is significantly lower than the fresh gas φ in the upstream near the reaction layer
- ❑ φ_L trenches and plateaus are situated on two sides of the left boundary of reaction zone
- ❑ With increasing equivalence ratio, the difference of gradients is reduced

4 Results: local equivalence ratio

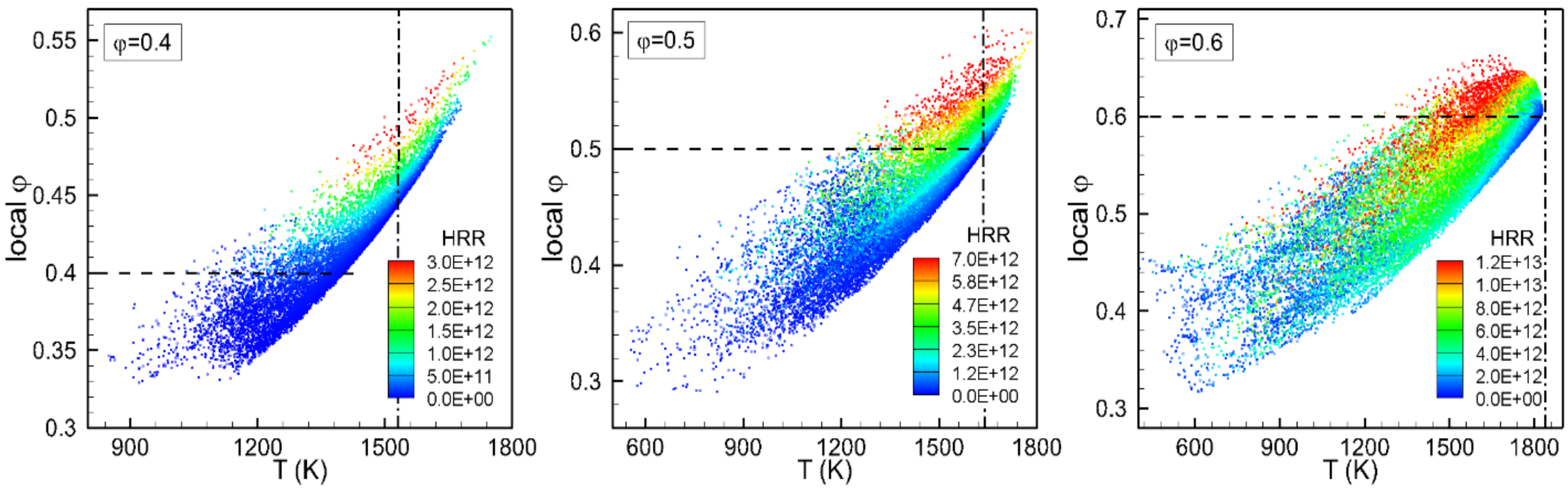


Fig.10 Scatter plots of local temperature and local equivalence ratio in the reaction zone.

- The scatter distribution shows a positive correlation between φ_L and temperature
- Hot spots with temperature higher than the adiabatic temperature are observed under ultra-lean conditions

4 Results: HRR marker

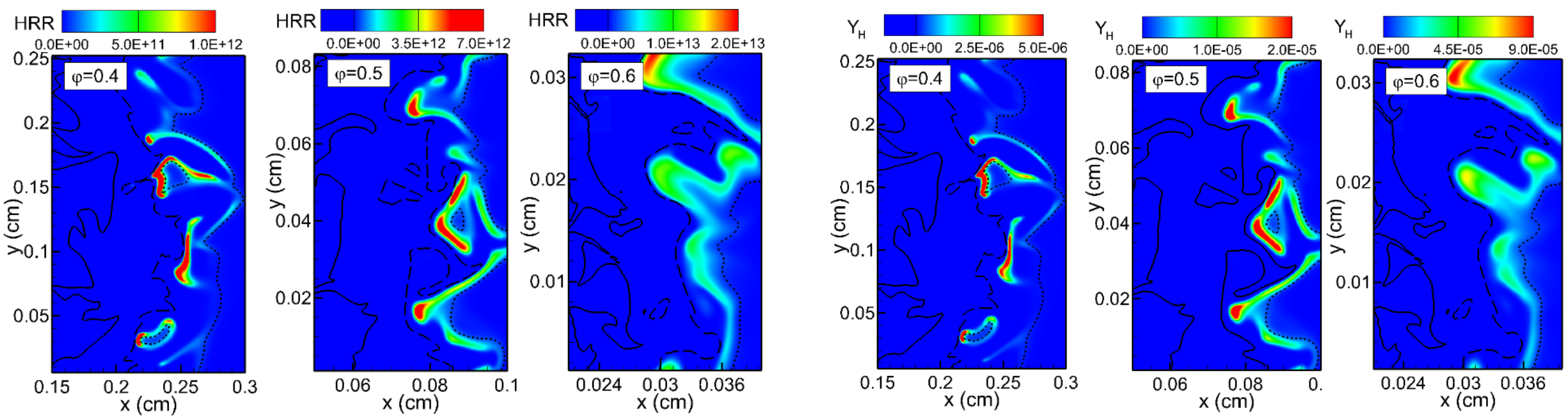


Fig.11 Two-dimensional snapshots of regions around reaction zones showing heat release rates, and H mass fraction for the cases with equivalence ratios 0.4, 0.5 and 0.6. The solid, dashed and dotted black lines correspond to c = 0.01, 0.5 and 0.99, respectively.

- In experimental studies, the heat release regions cannot be directly measured
- the contour of H mass fraction agrees well with the contour of HRR
- H could be used as a reliable HRR marker in high-pressure lean flames with varying equivalence ratios?

4 Results: HRR marker

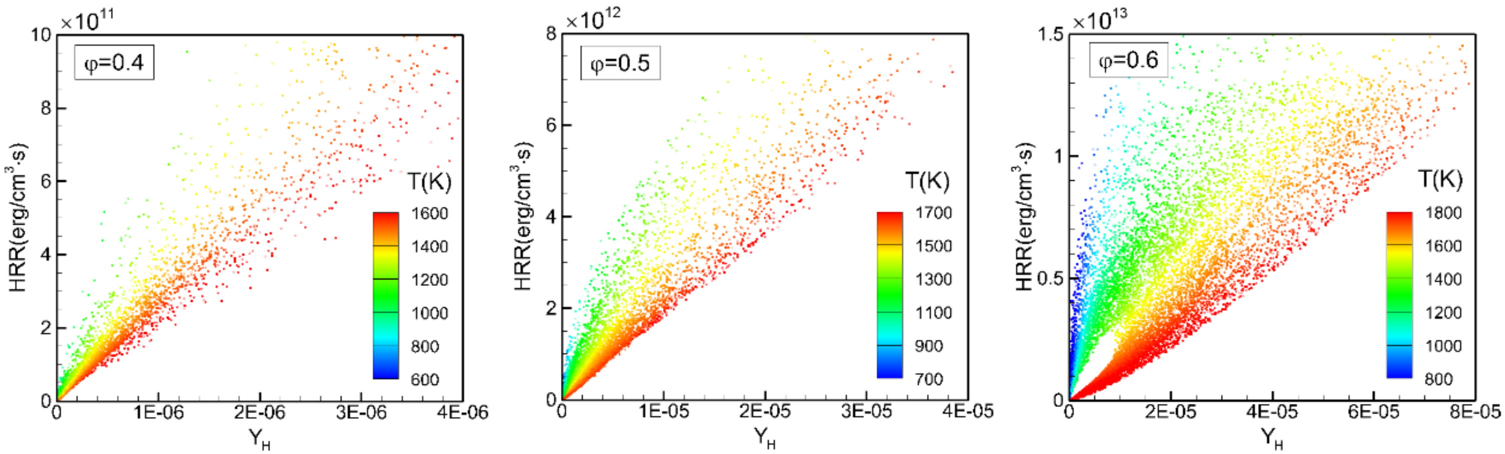
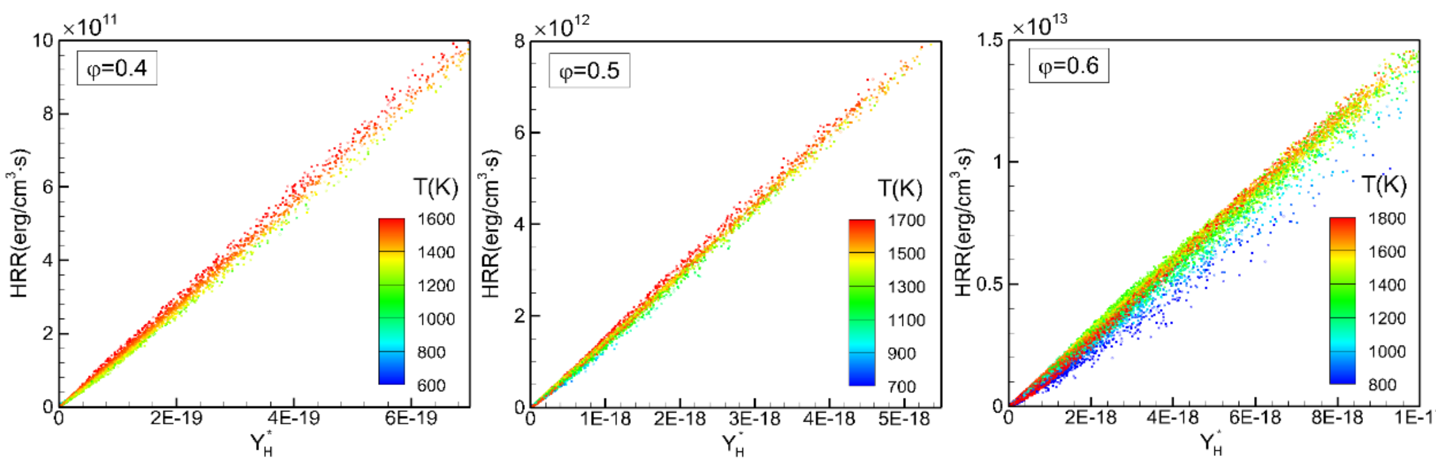


Fig.12 Scatter plots of H mass fraction and heat release



$$Y_H^* = Y_H / T^n$$

$$n = 4$$

$$\mathrm{HRR} = \alpha Y_H / T^4$$

$$\alpha = 1.43e30 - 1.5e30$$

Fig.13 Scatter plots of scaled H mass fraction and heat release

6 Conclusions

- The characteristics of heat release under various equivalence ratios are investigated by three-dimensional direct numerical simulations of lean H_2/air flames under conditions relevant to gas turbines.
- Under different lean conditions (φ = 0.4, 0.5, 0.6), the turbulent flame fronts show similar topological structures for the three cases under the same Karlovitz number.
- Trenches of local equivalence ratio φ_L are located at concave structures outside the reaction zone, while φ_L plateaus are situated at convex structures inside the reaction zone.
- With increasing equivalence ratio, the difference of gradients in convex and concave regions is reducing.
- φ_L is found to be significantly higher than mixture φ under ultra-lean conditions, resulting in hot spots in the reaction zone.
- Radical H could be used as a perfect HRR marker when it is scaled by temperature.

Thank you!

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