Direct Numerical Simulation of Turbulent Lean Premixed H_2/Air Flames at Elevated Pressure

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1 Background

- There has been considerable interest in lean premixed H_2/air combustion which reduces peak temperature and consequently thermal NOx emission. No significant changes to current combustion facilities.

- It is hard to get detailed information of elevated pressure combustion in experiments. Most of DNS studies of flame structure and propagation are carried out at atmospheric pressure.

- 3D-DNS studies with detailed chemistry at elevated pressures are few and far inbetween. Understanding of combustion characteristics at elevated pressure is insufficient.

2 Objectives

- ❑ Study the instantaneous flame structure at different pressure levels
- ❑ Study the flame instability at different pressure levels

3 Numerical Approach DNS

- ❑ Navier-Stokes equations and chemical species transport equations are solved with six-order compact finite difference schemes for spatial discretization and low-storage third-order Runge-Kutta time advancing scheme is used for the time advancement.

- ❑ The Navier-Stokes Characteristics Boundary Conditions (NSCBS) are applied at the inlet / outlet and periodic boundary conditions are imposed in the spanwise and lateral directions.

3

Numerical Approach DNS

- Turbulence was generated in a periodic box, which was then fed into the inlet plane of the main simulation.
- A one-dimensional (1D) laminar flame was generated using detailed chemistry and detailed transport properties to initialize the three-dimensional turbulent flame simulation.
- Chemical mechanism is from Li et al.[1], involving 9 species and 21 reactions.

[1]Li, Juan, et al. "An updated comprehensive kinetic model of hydrogen combustion." *International journal of chemical kinetics* 36.10 (2004): 566-575.

4 Computational Cases

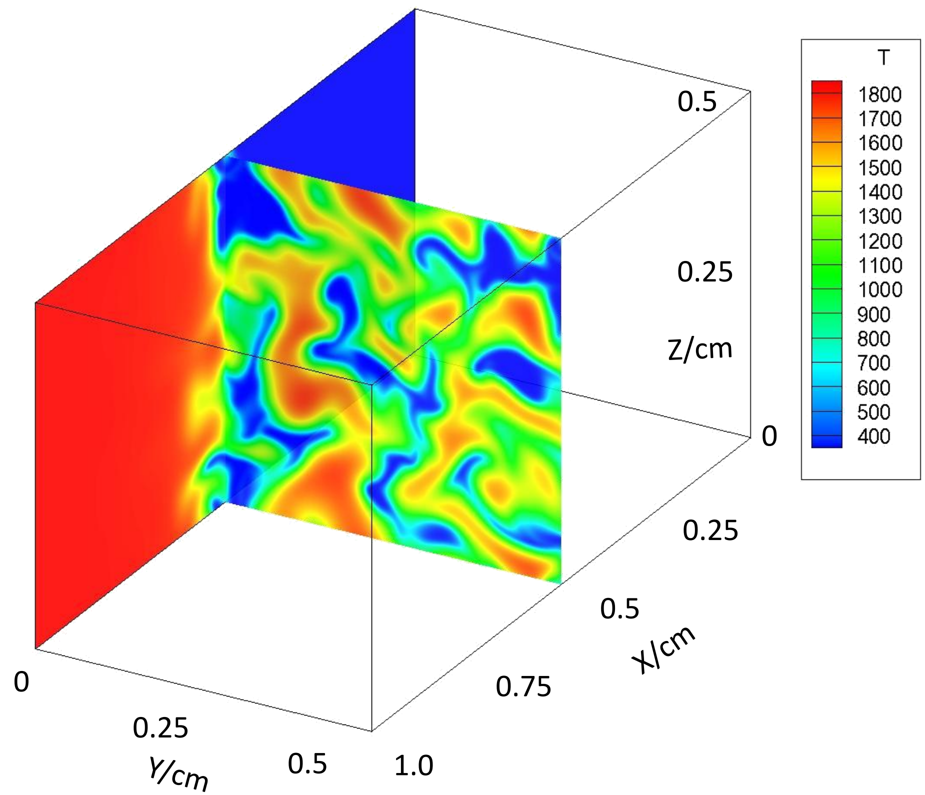


Fig.1 A schematic of computational domain .

Table 1 Key parameters in computational cases

Case	P=1atm	P=2atm	P=5atm
Equivalence ratio	0.6	0.6	0.6
S_L (cm/s)	88.5	69.9	47.9
δ_L (cm)	3.85E-02	1.9E-0.2	8.24E-0.3
u' (cm/s)	1138	1138	1138
l (cm)	0.0628	0.0628	0.0628
Grid resolution (μm)	10.01	9.77	9.77
$\Delta x/\eta$	0.156	0.309	0.768
Re_T	21	54	181

*Note:

S_L - laminar flame speed

δ_L - laminar flame thickness

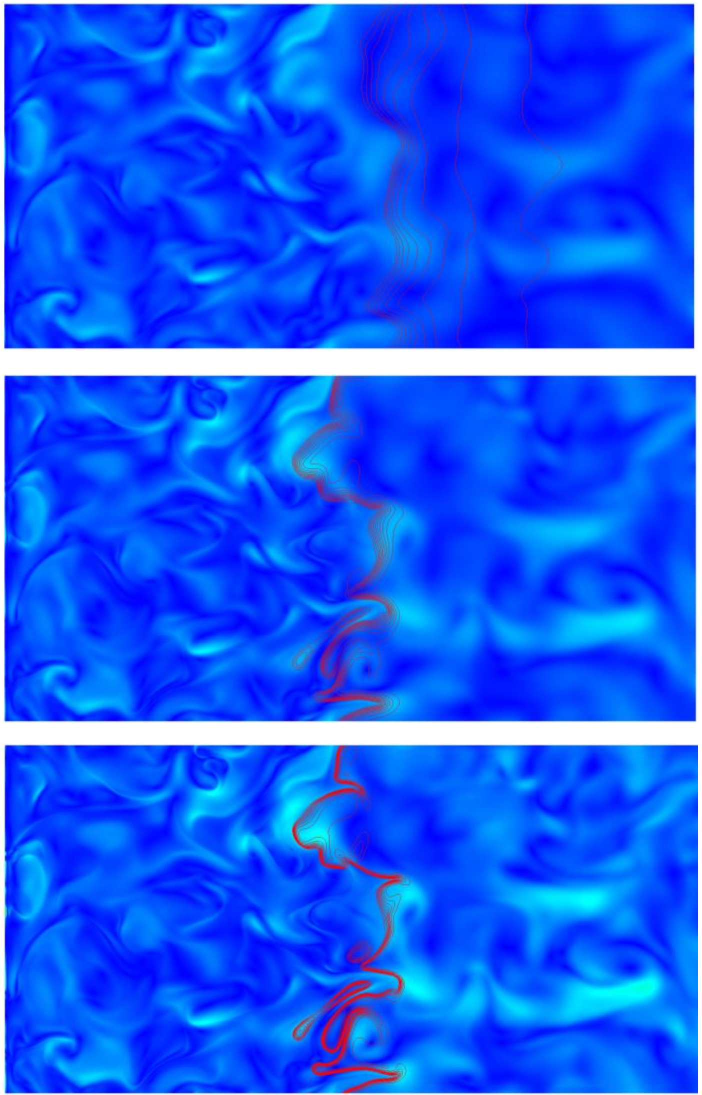
u' – Root-mean-square turbulent fluctuation velocity

l - Integral length scale

Turbulent Reynolds number $Re_T = \frac{u' l}{\delta_L S_L}$

Kolmogorov length scale $\eta = l \cdot Re_T^{-3/4}$

5 Instantaneous Flame Structure



P=1atm

P=2atm

P=5atm

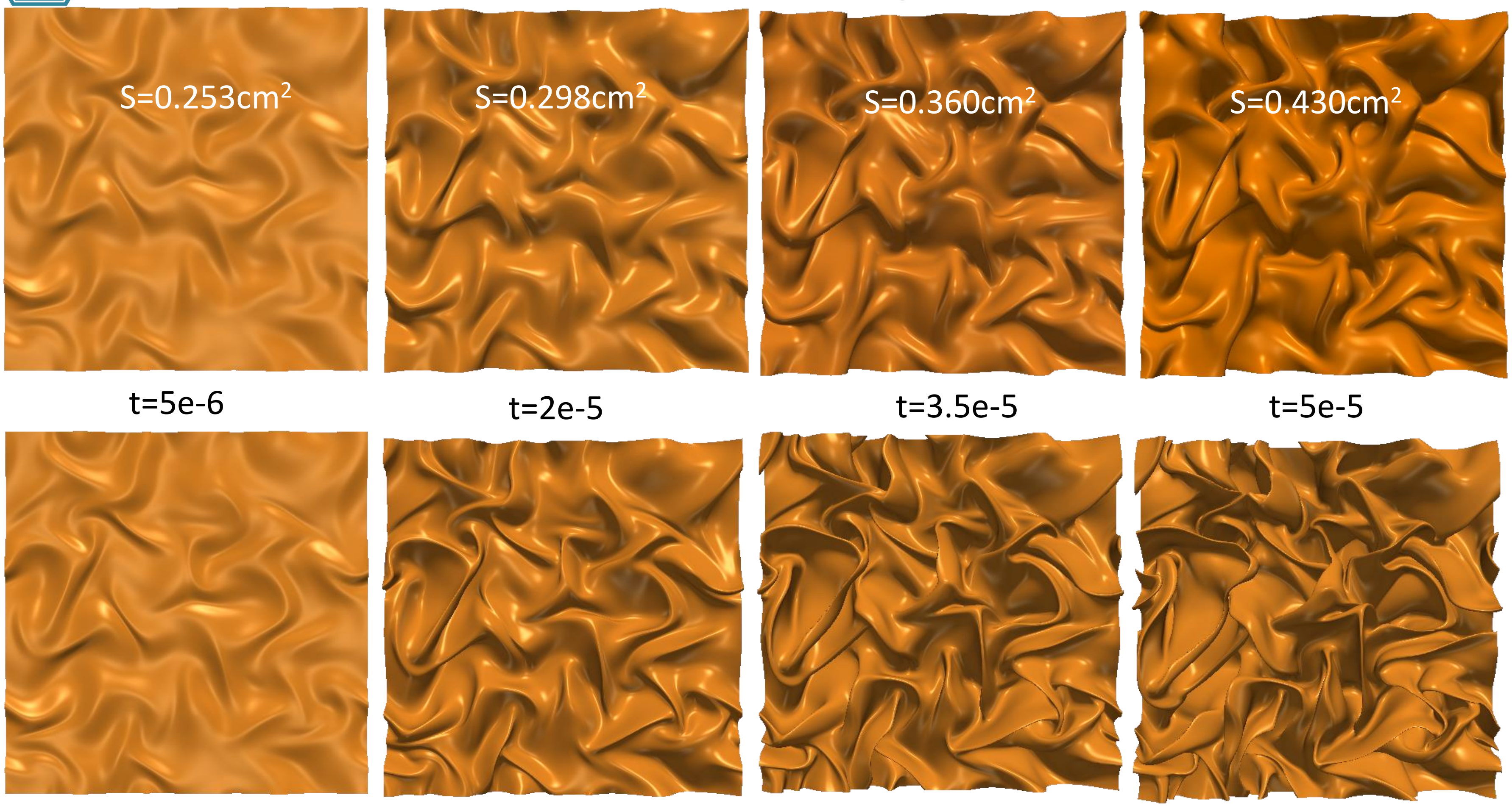
Fig.2 2D snapshots of vorticity field
(red lines for progress variable c=0.1-0.9)

Non-dimensional progress variable

$$c = \frac{T - T_u}{T_b - T_u}$$

- The three flames are considered within the Thin Reaction zone.
- The flame zone is considered to be bounded by c=0.1 and c=0.9. Small scale turbulent eddies could not enter the reaction zone.
- When P= 5atm, the reaction zone is much thinner than that under atmospheric pressure.

5 Instantaneous Flame Structure



P= 1atm

t=5e-6 t=2e-5 t=3.5e-5 t=5e-5

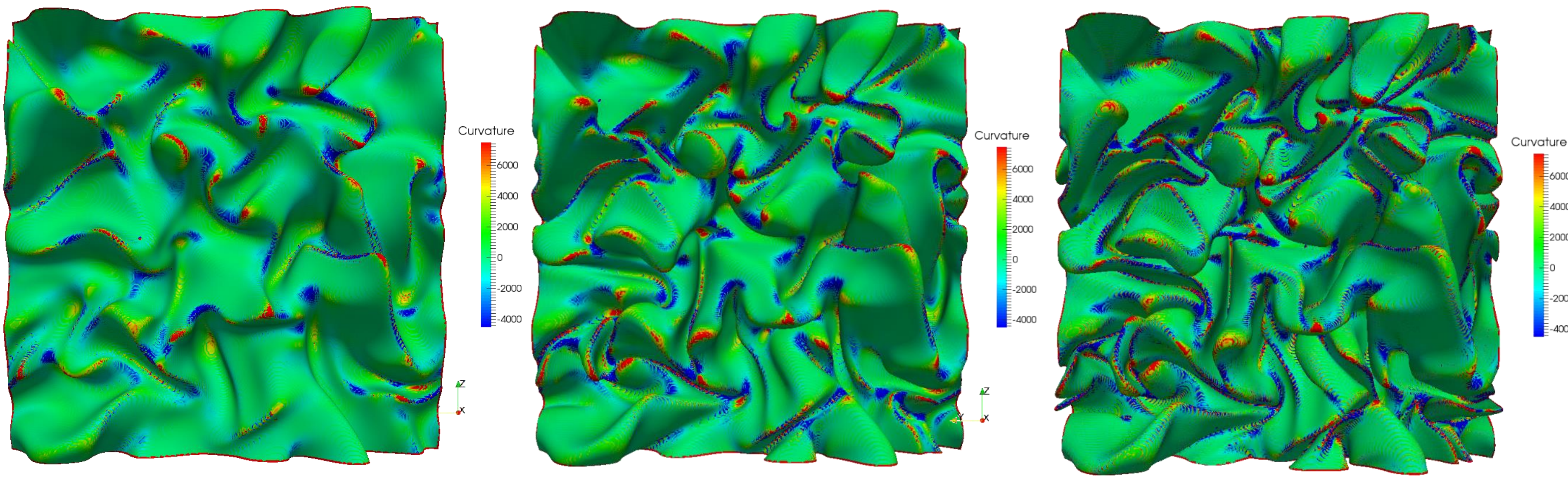
P= 5atm

t=5e-6 t=2e-5 t=3.5e-5 t=5e-5

Fig.3 sequences of flame propagation(iso-surface c=0.5)

5 Instantaneous Flame Structure

S=0.430cm^2 S=0.635cm^2 S=0.908cm^2



P=1atm P=2atm P=5atm

Fig.4 Iso-surfaces of flame front, coloured by curvature (t=5e-5, c=0.5)

5 Instantaneous Flame Structure

P=1atm P=5atm

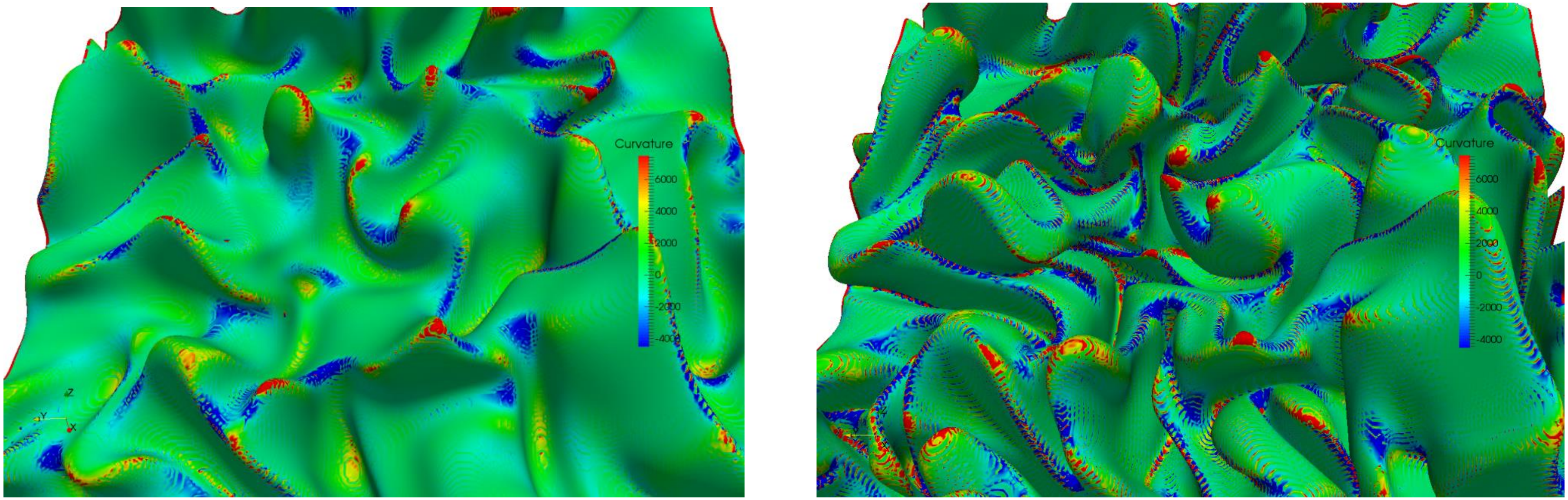
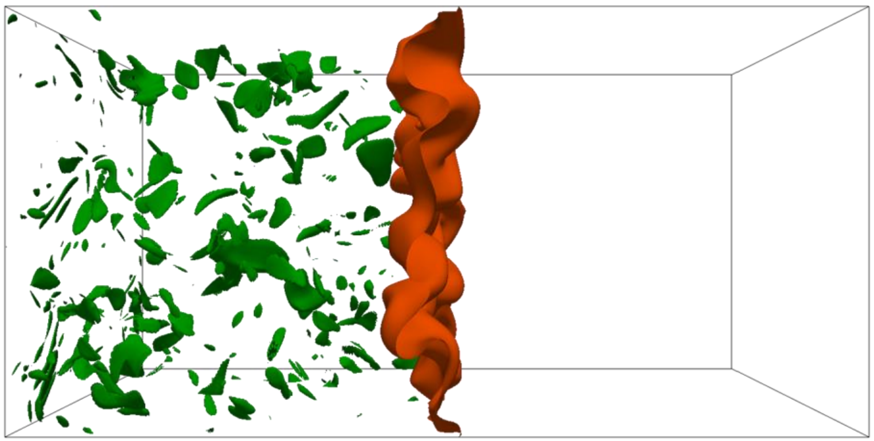


Fig.5 Details of iso-surfaces

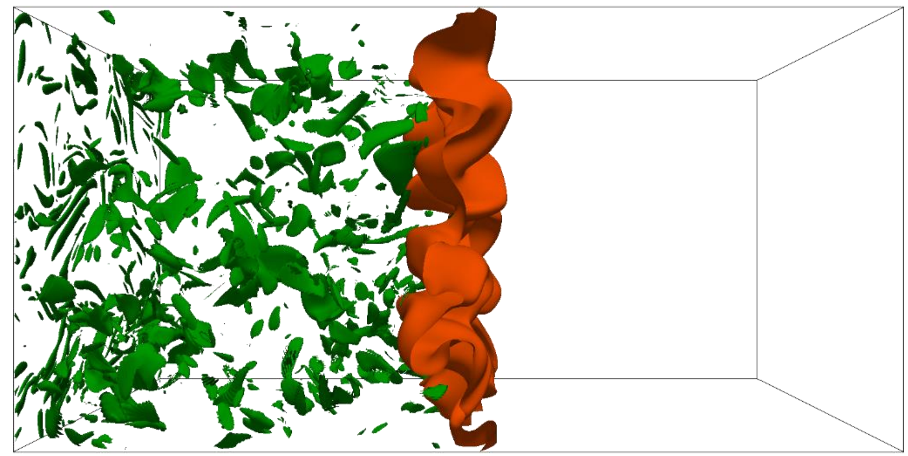
- The three cases are initialized with same turbulence field. The flame surface is wrinkled immediately after initiation of propagation.

- The flames under higher pressure exhibit more small scales structures and as a result flame wrinkling is getting stronger. It is associated with flame instabilities and turbulent levels at elevated pressure.

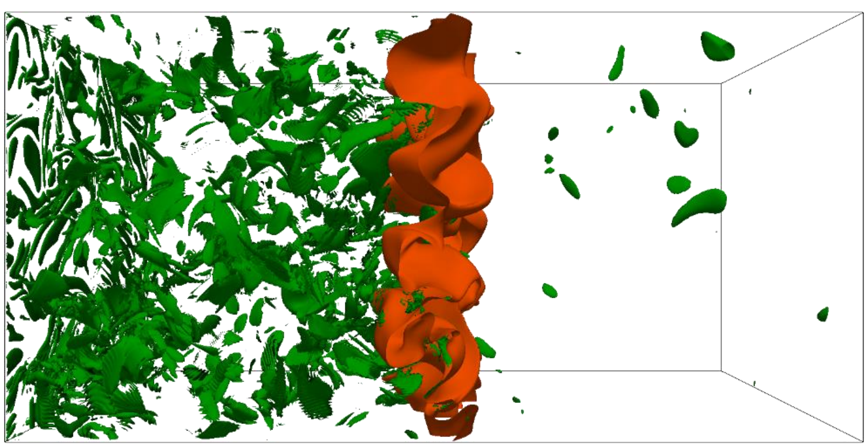
7 Influence of turbulence



P=1atm



P=2atm



P=5atm

Fig.6 Instaneous vortex structures at different pressures (red surface c=0.5)

Q_criterion $$Q\_ = \frac{1}{2}\frac{\partial u_i}{\partial x_j}\frac{\partial u_j}{\partial x_i}$$

- ❑ Under high pressure, the vortex structures tend to be complex and unsteady, which contributes to more small flame cells

7 Dissusion

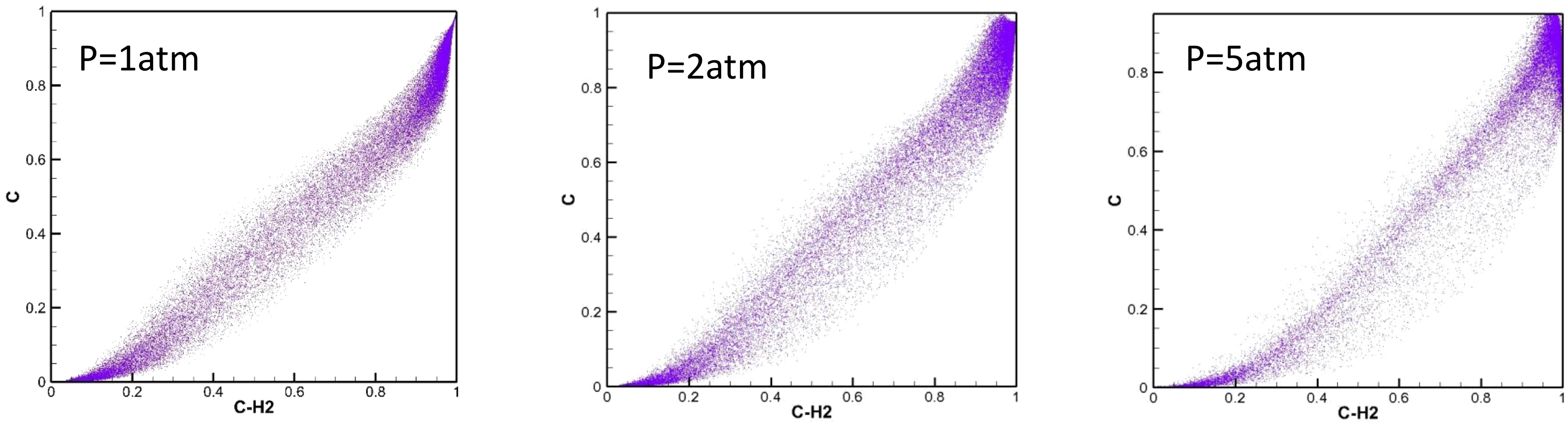
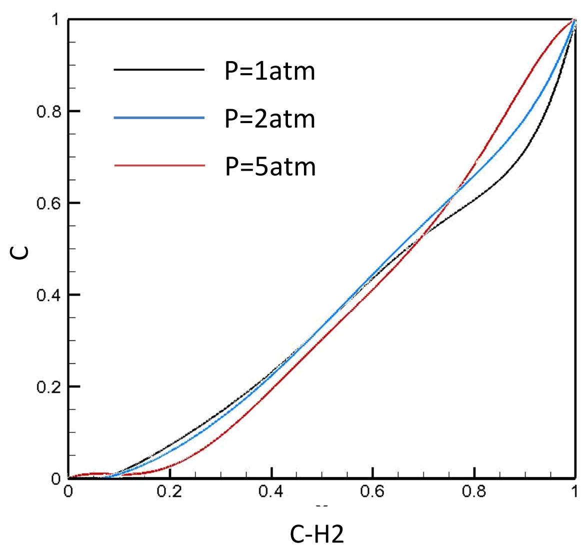


Fig.7 Scatter plot for progress variable(T) and progress variable(H2)



Progress variable defined by H_2 concentration

$$c\!-\!H_2 = \frac{Y_{H_2,u} - Y_{H_2}}{Y_{H_2,u} - Y_{H_2,b}}$$

- ❑ In preheat zone, the H_2 concentration is lower for the high pressure case. More H_2 diffuses from preheat zone to reaction zone. Differential diffusion is enhanced in this case.

7 Conclusions and plans

- The reaction zone is seriously narrowed at elevated pressure for turbulent lean premixed H_2/Air combustion.
- Under high pressure, there are more small flame structures than low pressure. Flame wrinkling tends to be stronger.
- Under high pressure, differential diffusion is enhanced and vortex structures tend to be complex and unsteady.
- In the future, we will focus on: the influence of differential diffusion and turbulent levels on flame properties at elevated pressure.

Acknowledgement

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Thank you!