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Effect of hydrogen addition to methane-air jet flame based on Sandia flame D

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- Problem set up
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- Conclusions

Introduction

Motivation: hydrogen addition to methane combustion

Combustion of fossil fuels, like natural gas, is widely utilized in industrial production (power plant) and daily life (gas stove).

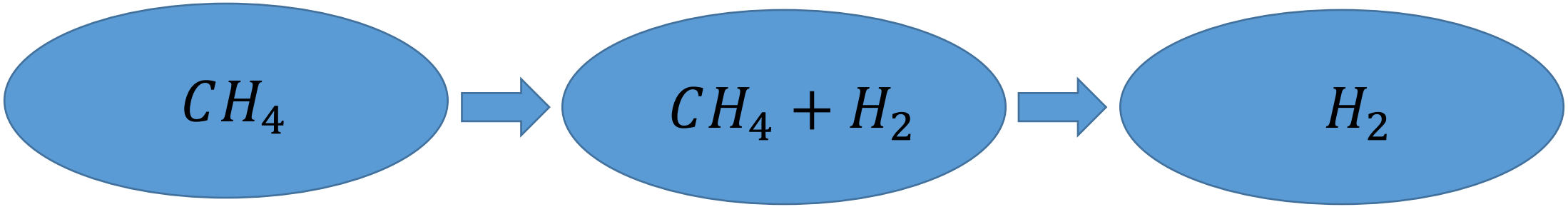
To limit the carbon dioxide emission for the low-carbon life style and environmental issues.

Hydrogen addition to natural gas is one of the effective methods, which can not only reduce the pollution from methane combustion, but also improve thermal efficiency and flame stability.

Fig.1 Hydrogen-methane jet flame example
(source: DLR flame from TNF workshop)

Introduction

Fuel types:



Problems:

- **A benchmark for validation**
- **An appropriate chemical mechanism for these three situations**
- **What way of hydrogen addition to affect the flame?**

Introduction

Four parts of flame simulations are conducted using Open FOAM. The $CH_4 - H_2$ blending jet flame is based on the **Sandia flame D** (CH_4-air jet flame benchmark, also tutorial in Open FOAM).

1. RANS simulations with reduced and detailed chemical mechanisms, including 1-step, 2-step, 4-step, DRM19, GRI-Mech 3.0 (the 4-step mechanism shows reasonable good results).

2. LES simulation with the 4-step mechanism and the WALE model (to further verify the 4-step mechanism on LES simulation).

3. LES simulation of $CH_4 - H_2$ blending jet flame ($5\%CH_4$+$20\%H_2$) (to verify RANS and LES simulations of $CH_4 - H_2$ blending jet flame can have similar and reasonable results).

4. RANS simulations of $CH_4 - H_2$ blending jet flame with different proportions, and also pure hydrogen jet flame.

Mathematical modelling

Governing equations: Multi-species compressible reacting flow Navier-Stoke equations

The mass conservation equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0$$

The momentum conservation equation

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i} = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i} + \rho \sum_{k=1}^{N} Y_k f_{k,j}$$

The energy conservation equation

$$\frac{\partial \rho h_s}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i h_s) = \frac{Dp}{Dt} - \frac{\partial q_i}{\partial x_i} + \frac{\partial}{\partial x_j}(\tau_{ij} u_i) + \dot{Q} + \dot{\omega}_T + \rho \sum_{k=1}^{N} Y_k f_{k,i} V_{k,i}$$

The species transport equation

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho(u_i + V_{k,i})Y_k\right) = \dot{\omega}_k$$

*Note: $\tau_{ij} = -\frac{2}{3}\mu \frac{\partial u_k}{\partial x_k}\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial u_i} + \frac{\partial u_j}{\partial x_i}\right)$, f_k is the volume force neglected, $\dot{\omega}_T$ is the heat release due to combustion neglected,

Mathematical modelling

Numerical settings for simulations

Tab.1 Numerical settings for RANS and LES simulations

	RANS	LES
Geometry	2D-wedge	3D-cylinder
Turbulence model	$k-\varepsilon$	WALE
Combustion model	EDC*	EDC
Chemistry solver	EulerImplicit/ODE	EulerImplicit
Chemical mechanisms	1-step, 2-step, 4-step, DRM19, GRI-Mech3.0	4-step
Numerical scheme	PISO	PISO
Flow-through time	10	10-15
Solver	reactingFoam, Open FOAM v-1906	

*EDC: Eddy Dissipation Concept model

Mathematical modelling

Chemistry kinetic mechanisms

Tab.2 Different chemical mechanisms for methane-air and hydrogen-air combustion

Chemical mechanisms	Species	Reaction steps	Author
1-step	5	1	Christ
2-step	6	2	Benedetta et al.
4-step	7	4	Jones & Lindstedt (JL)
DRM19	19	84	Kazakov & Frenklach
GRI-Mech 3.0	53	325	Gregory et al.
Keromnes ($H_2 - air$)	9	19	Keromnes et al.

Mathematical modelling

The 4-step mechanism by JL

The 4-step mechanism: 4 reactions + 7 species (CH_4, O_2, CO, H_2, CO_2, H_2O, N_2)

$$CH_4 + 0.5O_2 \rightarrow CO + 2H_2 \quad (1)$$
$$CH_4 + H_2O \rightarrow CO + 3H_2 \quad (2)$$
$$CO + H_2O \leftrightarrow CO_2 + H_2 \quad (3)$$
$$H_2 + 0.5O_2 \leftrightarrow H_2O \quad (4)$$

Tab.3 Detailed reaction coefficients of the 4-step mechanism by JL

Reactions	a	b	r	$A[(m^3/kmol)^{r-1}s^{-1}]$	β	$T_a[K]$
(1)	0.5	1.25	1.75	$4.4 \cdot 10^{11}$	0	15095
(2)	1	1	2	$3.0 \cdot 10^{8}$	0	15095
(3)f	1	1	2	$2.75 \cdot 10^{9}$	0	10065
(3)b	1	1	2	$6.71 \cdot 10^{10}$	0	13688
(4)f	1	0.5	1.5	$7.91 \cdot 10^{10}$	0	17609
(4)b	1	-	1	$3.48 \cdot 10^{13}$	0	47907

Problem set up

Sandia flame D experiment: non-premixed methane-air jet flame

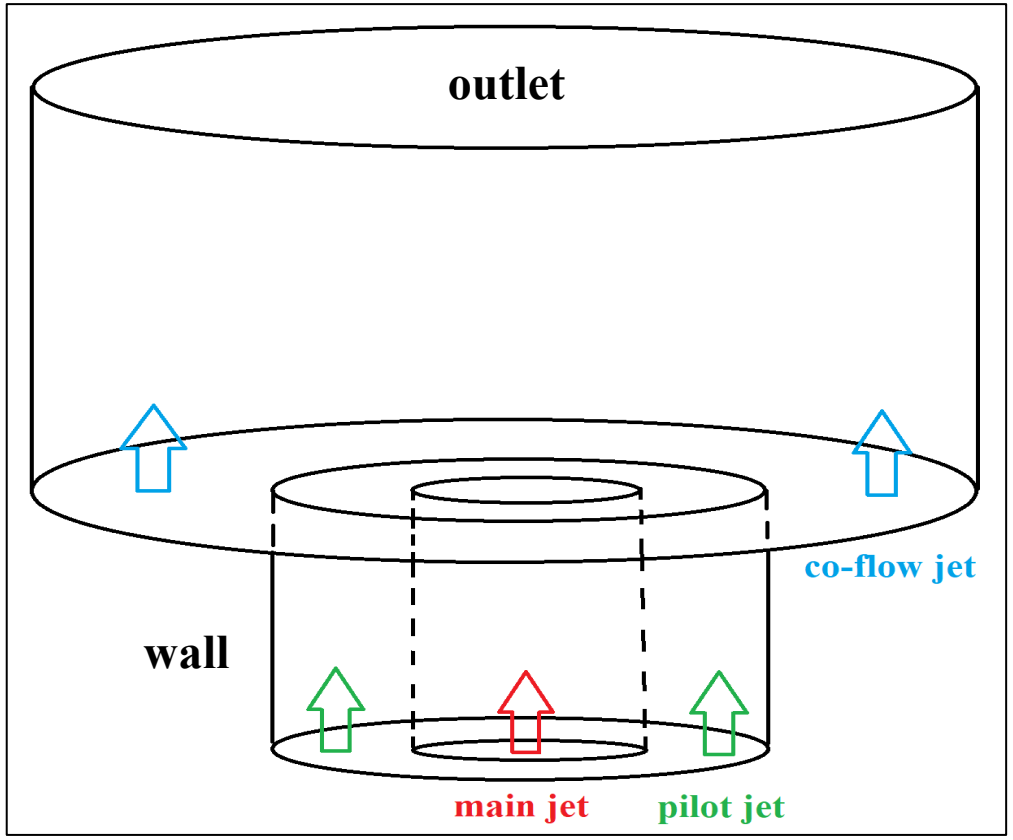


Fig.2 The sketch of Sandia flame D geometry

Tab.4 Initial conditions of species, temperature and velocity

		Streams		
		Main jet	**Pilot jet**	**Co-flow**
Radius(mm)		3.6	5.25	140.9
Temperature(K)		294	1880	291
Velocity(m/s)		49.6	11.4	0.9
Mass Compos-itions	CH_4	0.1561	0	0
	O_2	0.1996	0.0540	0.23
	CO_2	0.0000	0.1098	0.00
	H_2O	0.0000	0.0942	0.00
	N_2	0.6473	0.7342	0.77
Reynolds number		22400		

Results

1. RANS simulations of Sandia flame D with reduced and detailed chemical mechanisms

Consideration of the accuracy and the computational cost → the 4-step mechanism

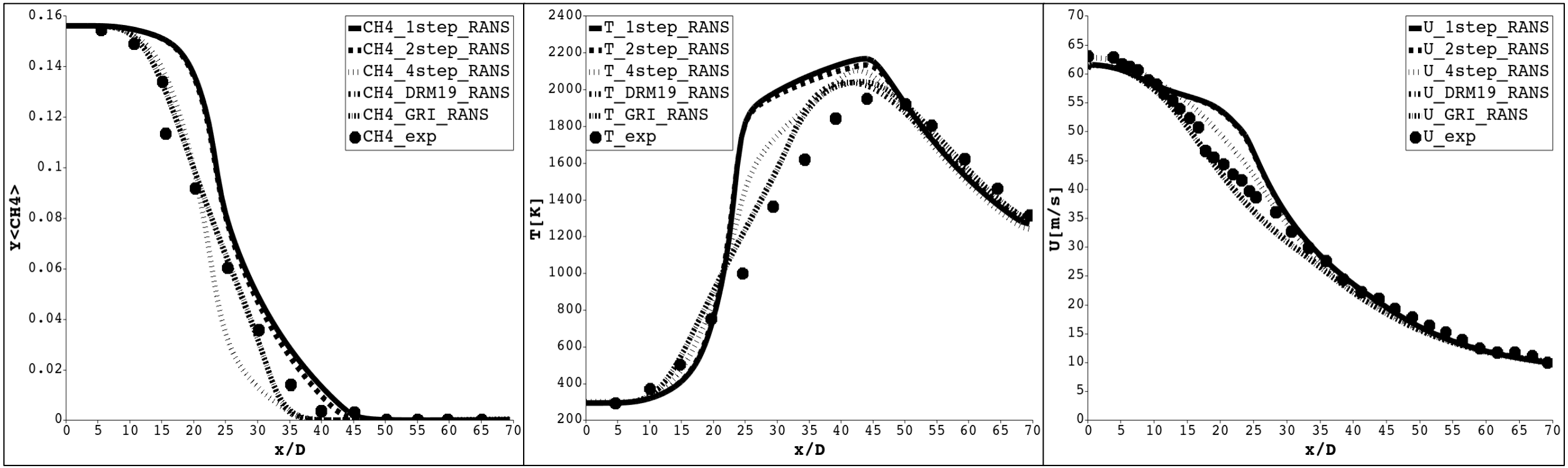


Fig.3 Mean CH_4*, temperature, and velocity along the centerline of Sandia flame D on RANS cases

*Y<CH_4> is the mass fraction of CH_4, D=7.2mm is the diameter of main jet

Results

2. LES simulation of Sandia flame D with the 4-step mechanism by JL

Further validation of the 4-step mechanism on LES simulation.

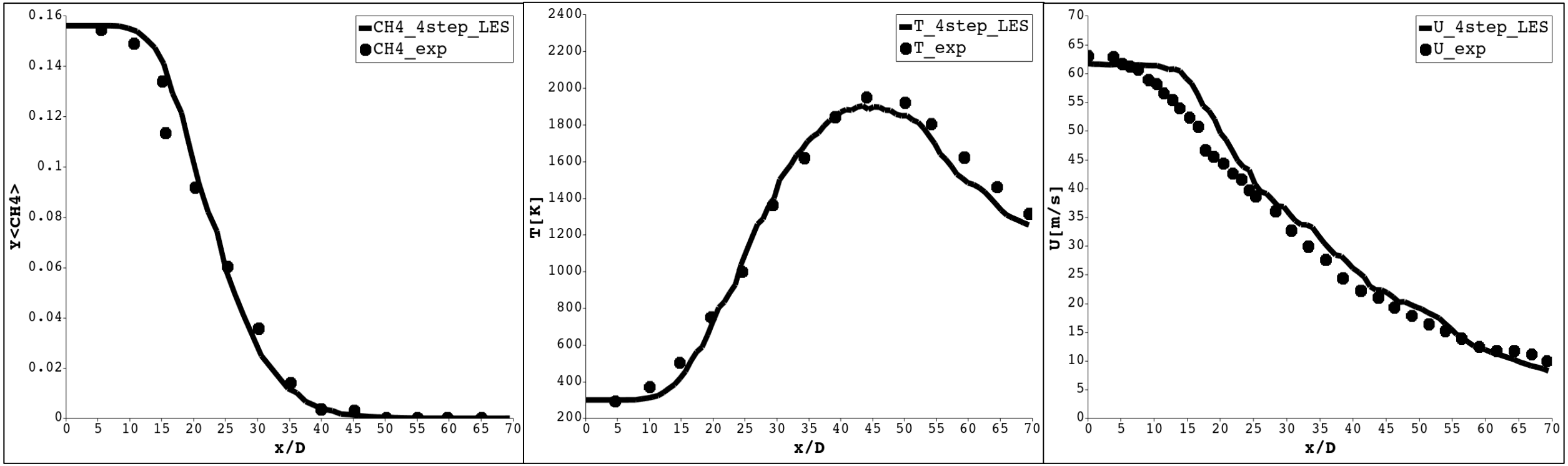
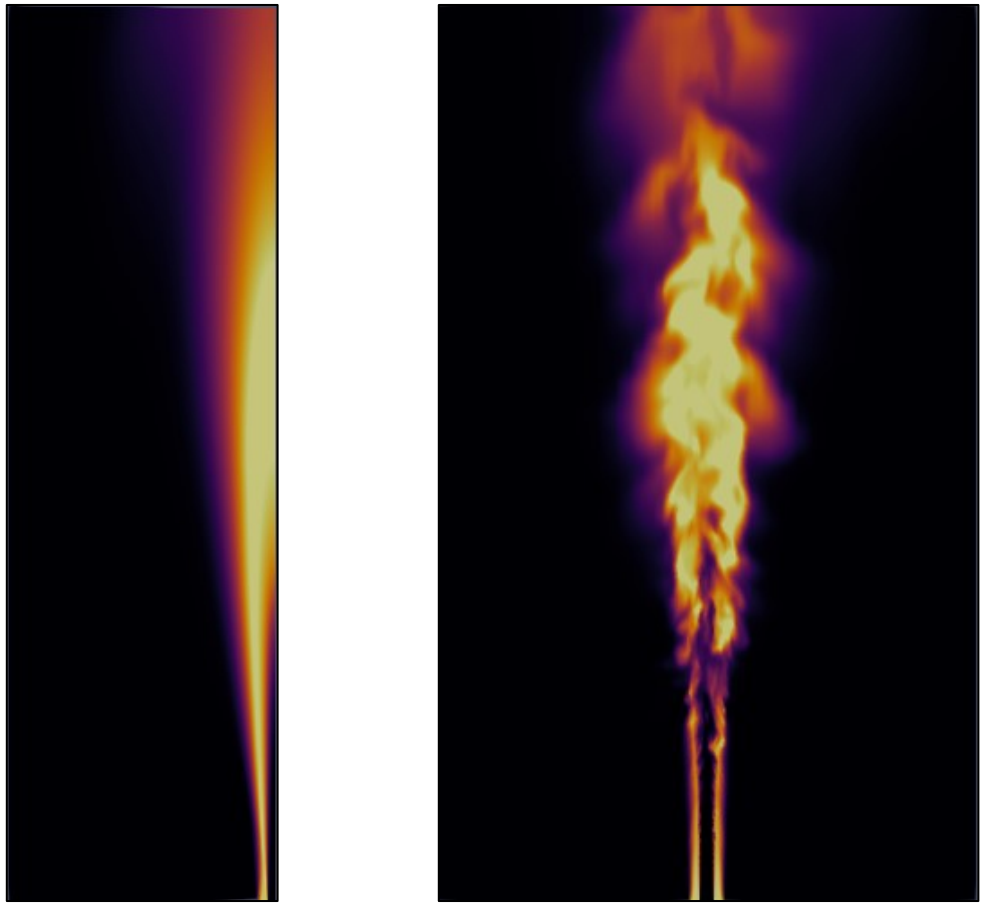


Fig.4 Mean CH_4, temperature, and velocity along the centerline of Sandia flame D on LES case

Results

RANS + LES simulations of Sandia flame D with the 4-step mechanism by JL



Tab.5 Mesh, core, and calculation time

MPI	Cell	Core	Time step	CPU Time
RANS-4step	9.0×10^3	4	0.1 sec	≈ 10min
LES-4step	3.5×10^6	160	0.15 sec	≈ 180h

Note: Co=0.4

Fig.5 Snapshots of mean temperature and transient temperature of Sandia flame D on RANS and LES cases

Results

$CH_4 - H_2$ blending jet flame: same geometry of Sandia flame D and constant Re number

To guarantee constant Reynolds number (Re=22400) with different proportions of $CH_4 - H_2$ blending fuel, the inlet velocity of main jet will be revised according to the corresponding blending proportions.

The dynamic viscosity of blending mixture is calculated as

$$\mu_{mix} = \sum_{\alpha=1}^{N} \frac{x_\alpha \mu_\alpha}{\sum_\beta x_\beta \phi_{\alpha\beta}}, \phi_{\alpha\beta} = \frac{1}{\sqrt{8}}\left(1+\frac{M_\alpha}{M_\beta}\right)^{-\frac{1}{2}}\left[1+\left(\frac{\mu_\alpha}{\mu_\beta}\right)^{\frac{1}{2}}\left(\frac{M_\beta}{M_\alpha}\right)^{\frac{1}{4}}\right]^2$$

Tab.6 Different inlet velocity of main jet to guarantee constant Re with d=7.2mm (original: $25\%CH_4 + 75\%air$)

Cases	$U[m/s]$	$\rho_{mix}[kg/m^3]$	$\mu_{mix}[kg/(m \cdot s)]$
$20\%CH_4 + 5\%H_2$	50.8527	1.03108	1.68535
$15\%CH_4 + 10\%H_2$	53.155	1.00226	1.71242
$10\%CH_4 + 15\%H_2$	55.651	0.973451	1.74129
$5\%CH_4 + 20\%H_2$	58.3647	0.944639	1.77215

Results

3. LES results of $CH_4 - H_2$ blending ($5\%CH_4$+$20\%H_2$) jet flame with the 4-step mechanism by JL

Despite the gap, the results between RANS and LES are still similar and reasonable → RANS

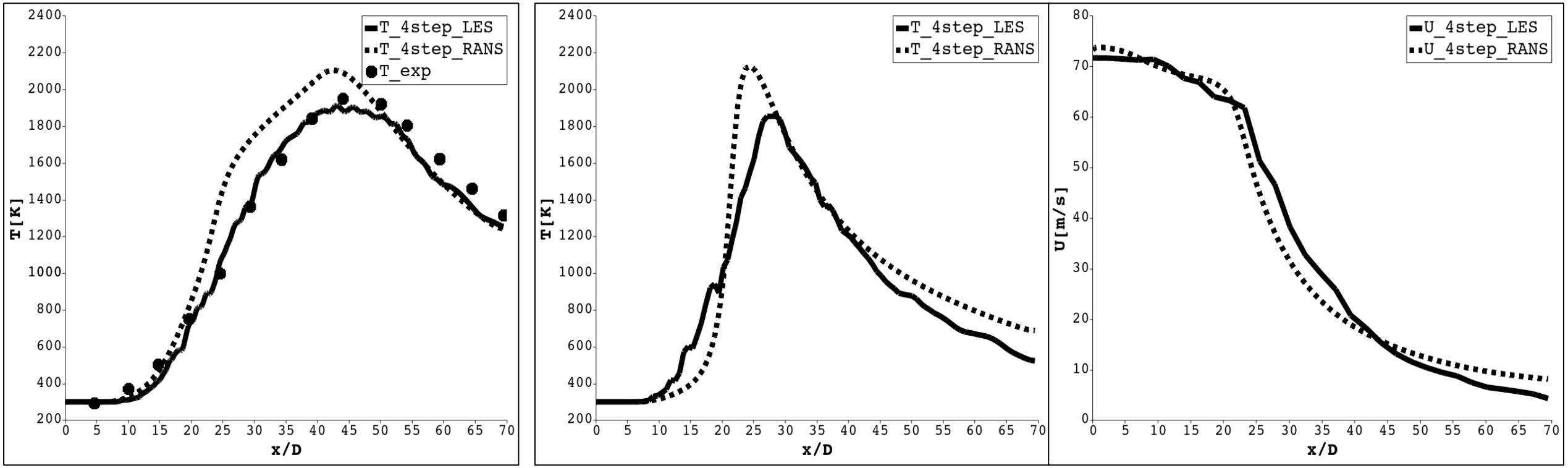


Fig.6 Mean temperature along the centerline of Sandia flame D (pure CH_4) (left),
mean temperature and velocity along the centerline of $CH_4 - H_2$ blending jet flame (mid, right)

Results

4.1 RANS simulations of $CH_4 - H_2$ blending jet flame with the 4-step mechanism by JL

The emission of CO_2 is decreased as the decrease of CH_4 proportion in the main jet.

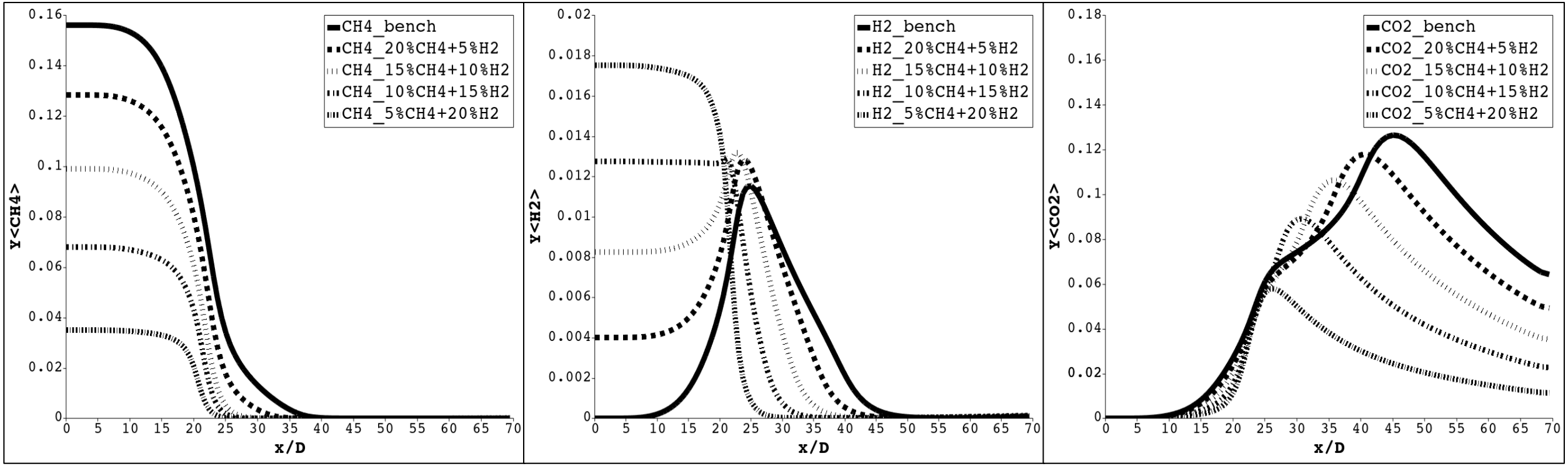


Fig.7 Mean CH_4, H_2, and CO_2 along the centerline of $CH_4 - H_2$ blending jet flame on RANS cases

*bench: benchmark is the RANS simulation of Sandia flame D (25%CH_4) with the 4-step mechanism

Results

4.1 RANS simulations of $CH_4 - H_2$ blending jet flame with the 4-step mechanism by JL

The consumption of O_2 is also decreased, and the peak temperature keeps consistent.

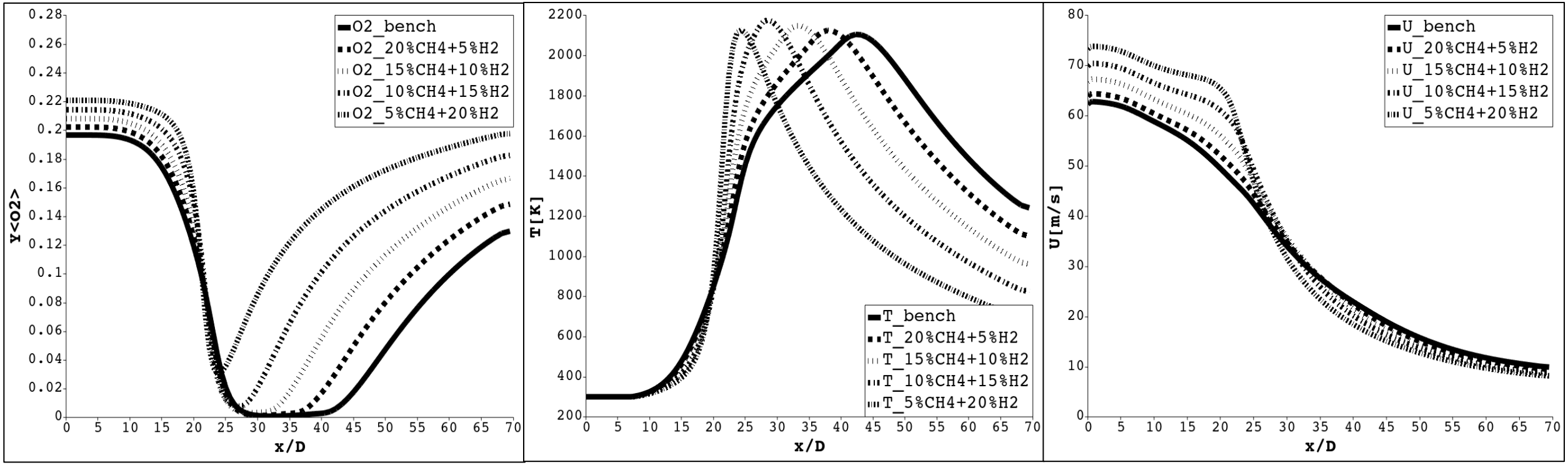


Fig.8 Mean O_2, temperature, and velocity along the centerline of of $CH_4 - H_2$ blending jet flame on RANS cases

Results

4.2 RANS simulations of pure 25% H_2 jet flame with different chemical mechanisms.

This 25% H_2 jet flame is based on Sandia flame D geometry.

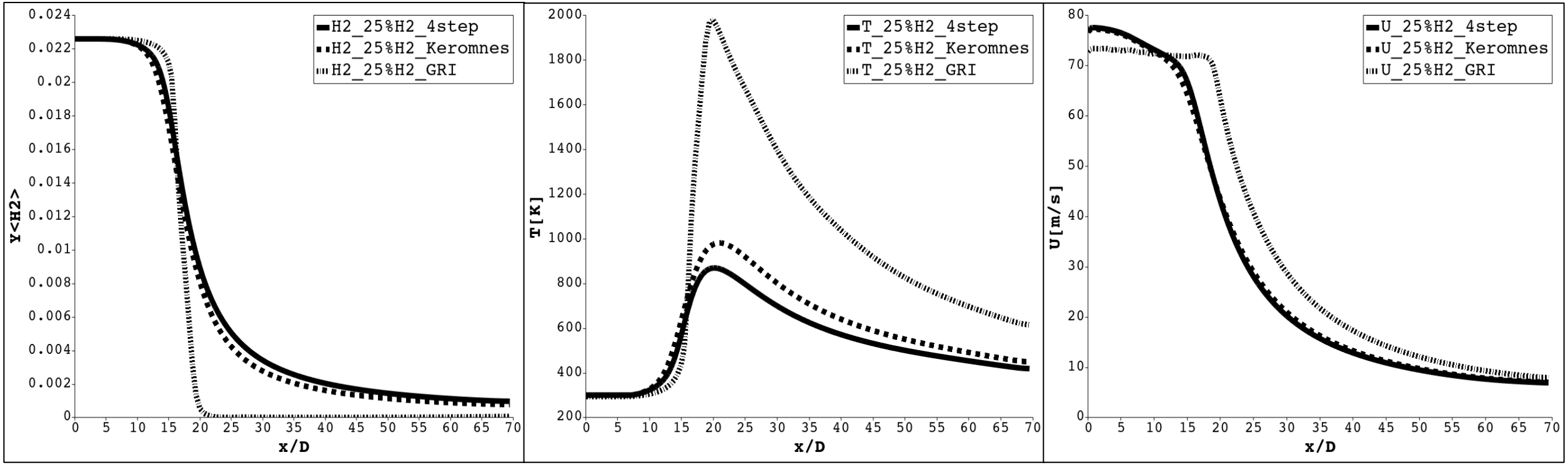


Fig.9 Mean H_2, temperature, and velocity along the centerline of pure 25% H_2 jet flame on RANS cases

Results

4.3 RANS simulations of pure H_2-air jet flame experiment from Barlow and Flury*

Results of the 4-step mechanisms are close to Keromnes mechanism.

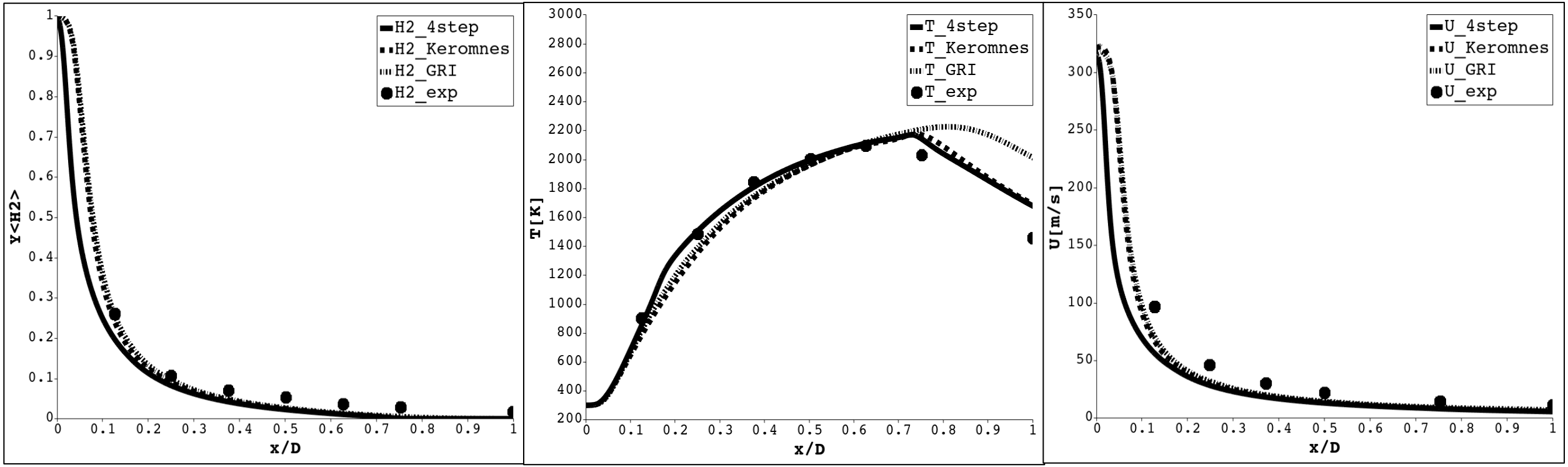


Fig.10 Mean H_2, temperature, and velocity along the centerline of H_2 jet flame on RANS cases

*: Unlike Sandia flame D, this pure H_2-air jet flame has high inlet velocity (296m/s) and more slender burner, D=67.5mm is the visible flame length

Conclusions

A series of CH_4, $CH_4 - H_2$ blending, and H_2 fuel jet flames are simulated using reactingFoam.

- Results with the 4-step mechanism by JL agree with experimental data on both RANS and LES simulations of Sandia flame D. Other reduced and detailed mechanisms are not attractive because the accuracy or computational cost is insufficient.

- The addition of hydrogen to methane fuel would lead to a trend of earlier occurring temperature peak, and then temperature also drops faster. The flame velocity differs in the region near to the exit of nozzle, but it finally drops to the same level.

- It means the addition of hydrogen accelerates the propagation and attenuation of jet flame under conditions of same geometry and constant Re number. But it allows the flame to maintain the same peak temperature while reducing carbon dioxide emission and oxygen consumption.

- The 4-step mechanism by JL can be regarded as a global mechanism when it is applied in pure hydrogen-air jet flame simulation.

Thank you