Effect of Strain Rate on the Flame Structure of Syngas Flames in the Air-Fuel and Oxy-Fuel Condition

混合燃氣之拉伸極限影響火焰結構特性在空氣及純氧條件之研究

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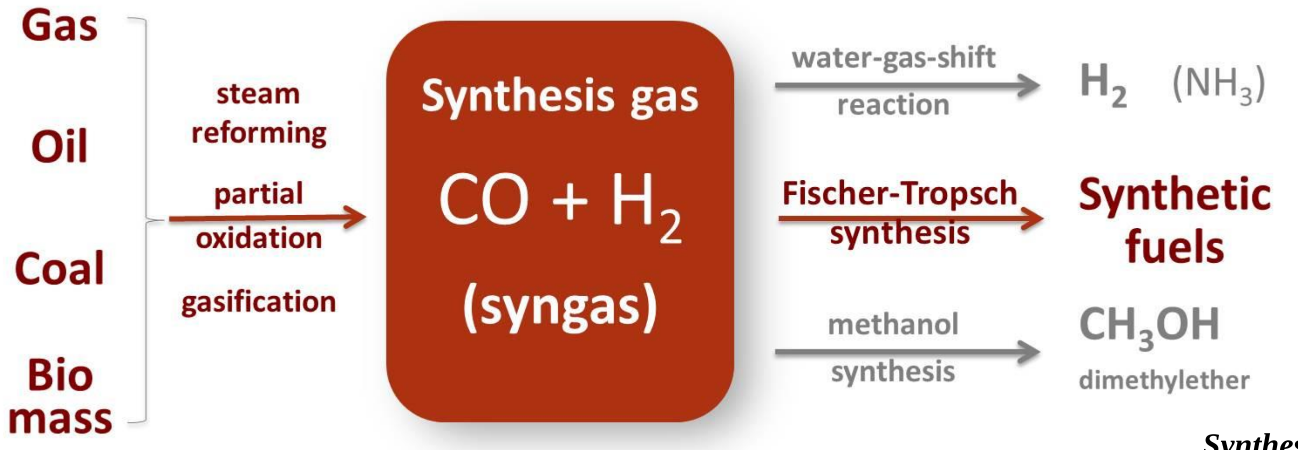
Introduction

The Energy issues

- Energy issues including fuel shortage and environmental pollutions have remained for several years. A number of strategies for reducing emission and utilizing renewable/clean energy have been investigated and developed.
- Syngas is being recognized as a viable energy source and an attractive fuel, particularly for stationary power generation with IGCC (Integrated Gasification Combined Cycle) Technology.



Synthesis Gas Chemistry and Synthetic Fuels.

Introduction—gas characteristics

- Species characteristics

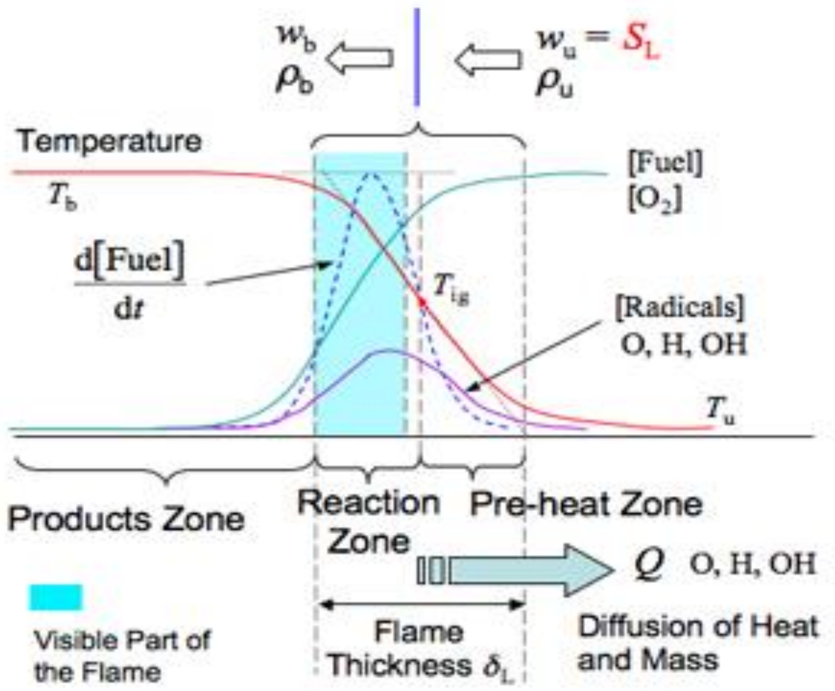
	Hydrogen (H_2)	Methane (CH_4)	Carbon monoxide (CO)
Molecular mass	2	16	28
Density (kg/m^3)	0.09	0.72	1.25
Heat Capacity (J/mole·K)	28.84	35.69	1.04
Heat value (kJ/kg)	119746	49915	10108
Ignition temperature (ºC)	571	632	608
Flammability(%)	4-75	5-15	12.5-74
Flame speed (cm/s)	170 @ ϕ=1	38.3 @ ϕ=1	28.5 @ ϕ=1

Paper survey

Laminar premixed flame structure

(Mallard & Le Chatelier, 1883)

- Laminar premixed flame divides into two distinct zones: **preheat & reaction zone**.



張彥呈碩士論文, 2010

- $$S_L = \left[\left(\frac{\lambda}{\rho_u C_p}\right)\frac{(T_b - T_{ig})}{(T_{ig} - T_u)}\frac{W_b}{\rho_u}R_{av}\right]^{1/2} \propto \sqrt{\alpha R_{av}}$$

- $$R_{av} = \frac{dC}{dt} = k\prod_{i=1}^{N}(C_{M_i})$$

- $$k = AT^b exp\left(-\frac{E_a}{R_u T}\right)$$

Paper survey

Hydrogen addition to flame

- The hydrogen addition would lead to an increase of laminar burning velocity and a higher extinction strain rate. *(Scholte et al. 1959; Yu et al.1986)*

- *Vagelopoulos et al. (1994)* concluded that the increment in laminar burning velocity and extinction strain rate was led by the added H radicals, which would increase branching and accelerate the CO oxidation reaction by investigated the detailed kinetic mechanism using experiment and model prediction for H_2/CO/air and CH_4/CO/air systems.

Paper survey

Gas dilution of flame

- Results show that the flame propagation velocity S_L(Ar) > S_L (N_2) > S_L (CO_2) and each thermal diffusivity is αS_L (Ar) > αS_L (N_2) > αS_L (CO_2) and heat capacity C_p(CO_2) > C_p (N_2) > C_p (Ar). *(Suda et al. 2007; Masuko et al.2007)*

- *Suda et al. (2007)* revealed that heat capacity of gas seems to have a large effect on flame propagation velocity.

- *Chan et al. (2015)* the CO_2 was added, the methane combustion was diluted and the specific heat of the mixture increased, leading to a lower flame temperature and consequently the lower laminar burning velocity.

Paper survey

Comprehensive mechanisms

- Dominating species: (*Yetter et al. 1991)*

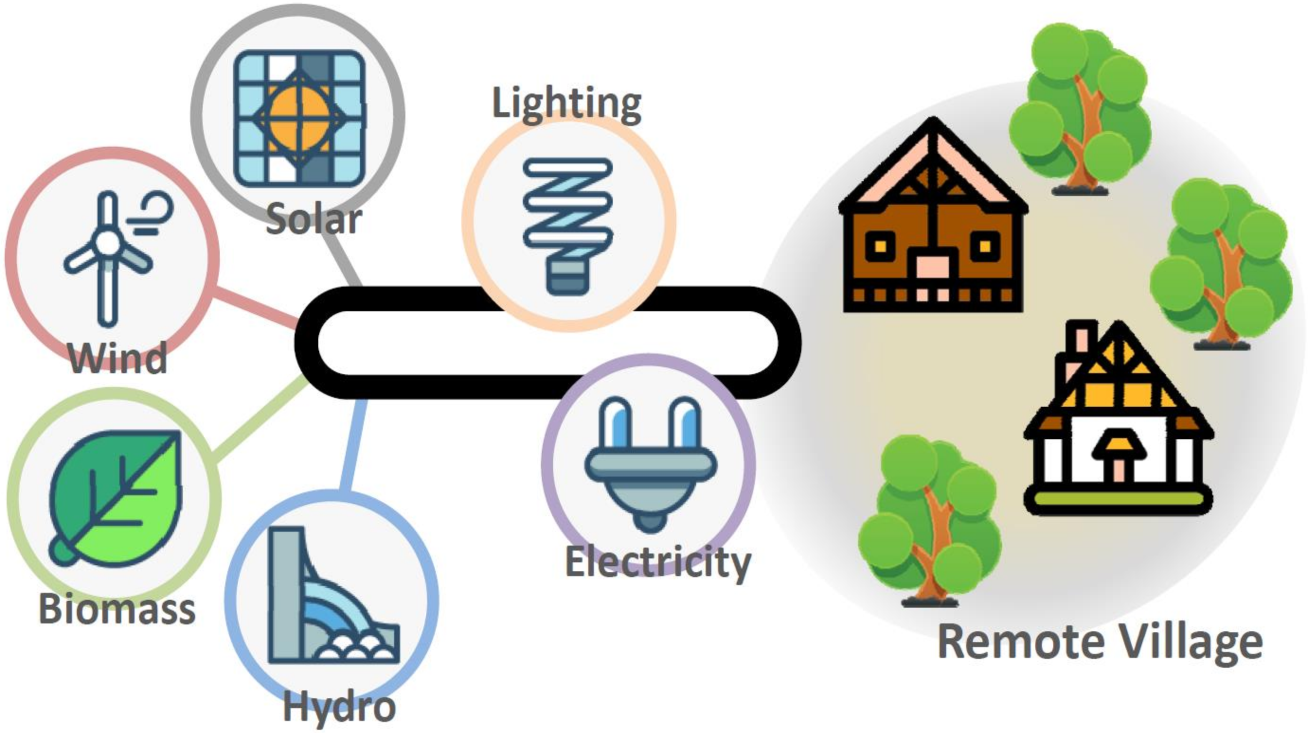
  High temperature (above 2000K) regime : H, O and OH radicals

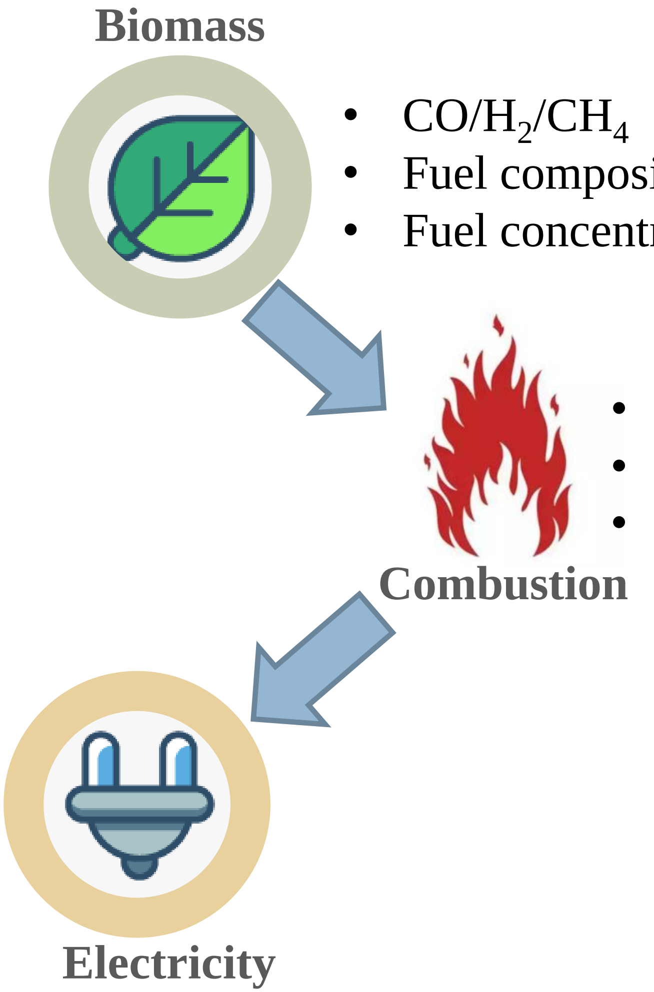
  Low temperature (below 1200K) regime : HO_2 and H_2O_2

  Intermediate temperature regime: the concentrations of H, O, OH, HO_2 and H_2O_2 intermediates are nearly the same order of magnitude.

- NO_x could catalyze the reaction of H_2/O_2 and $CO/H_2O/O_2$ systems at the temperatures below 1200K. (*Mueller et al. 1999)*

Motivation





- $CO/H_2/CH_4$
- Fuel composition
- Fuel concentration

- Flame characteristics
- Combustion stability
- Gas emission

Purpose

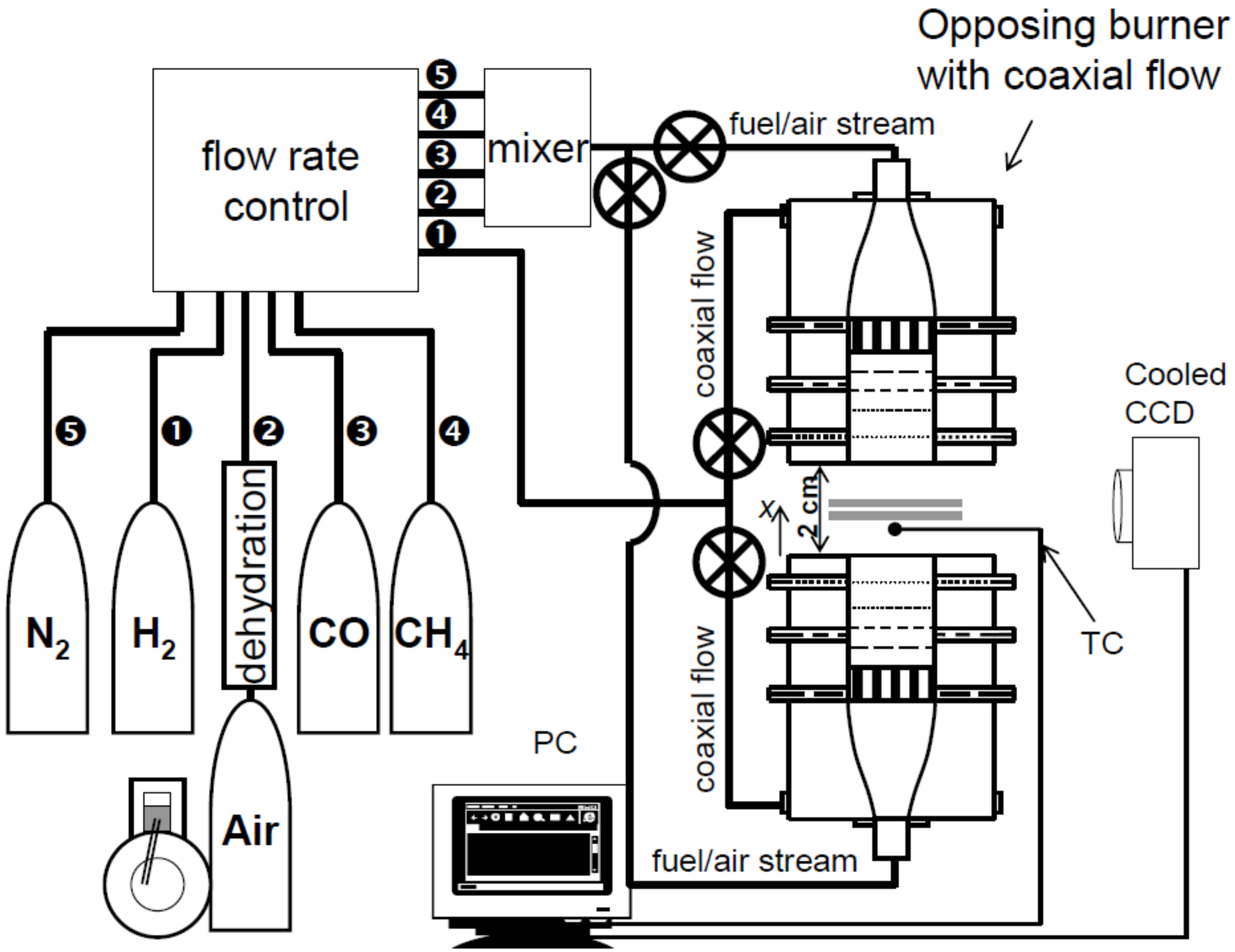
- Thermal effect
- Chemical effect
- Dilution effect
- Aerodynamic effect
- Concentration effect

Syngas combustion

➢ Simulation ：

- Adiabatic flame temperature
- Laminar flame velocity
- Extinction strain rate
- Concentration distribution
- Net reaction rate

Experimental methodology



Wu et al.,2009

- The opposed-jet burner consists of two water cold, well-contoured circular nozzles (ID=2cm) with slow coaxial shielding flows.
- Observed the flame phenomenon by varying the strain rate , equivalence ratio and fuel ratio.
- Equivalence ratio(ϕ) = 0.4, 0.6, 0.8
- Global strain rate(a) = 200, 300, 400

$$a=\frac{2V_o}{L}\left(1+\frac{|V_f|\sqrt{\rho_f}}{|V_o|\sqrt{\rho_o}}\right) \quad \text{unit : } s^{-1}$$

Experimental condition

- The initial condition：300 K and 1 atm.

Flame NO.	$H_2/CO/CH_4$ Fuel ratio (%)			$H_2/CO/CH_4$ Mole fraction(vol%)			ϕ Air(vol%)			
	H_2	CO	CH_4	H_2	CO	CH_4	0.4	0.6	0.8	1.0
1	0	20	5	0	64	16	90.2	86.4	82.6	79.2
2	1	20	5	3.04	61.52	15.36	90.1	86.2	82.4	78.7
3	2	20	5	5.92	59.28	14.80	90.0	86.1	82.2	75.3
4	3	20	5	8.56	57.12	14.32	86.1	85.9	82.0	77.9
5	4	20	5	11.04	55.20	13.76	89.7	85.8	81.9	77.6
6	5	20	5	13.36	53.36	13.36	89.6	85.6	81.7	77.3
7	6	20	5	15.52	51.60	12.88	89.5	85.5	81.5	77.0
8	7	20	5	17.52	50.00	12.48	89.4	85.4	81.4	76.7
9	8	20	5	19.36	48.48	12.16	89.2	85.2	81.2	76.5
10	9	20	5	21.20	47.04	11.76	89.1	85.1	81.1	76.3
11	10	20	5	22.88	45.68	11.44	89.0	85.0	81.0	76.1

Simulation

- The simulation results were conducted by Chemkin Pro collection.
  - Equil-code
  - Premix-code
  - Oppdif-code

- The simulation was conducted at the equivalence ratio of 1 for air-fuel and oxy-fuel condition.

- The chemical reaction mechanism use is GRI-Mech 3.0(involves 53 species and 325 reactions).

Simulation

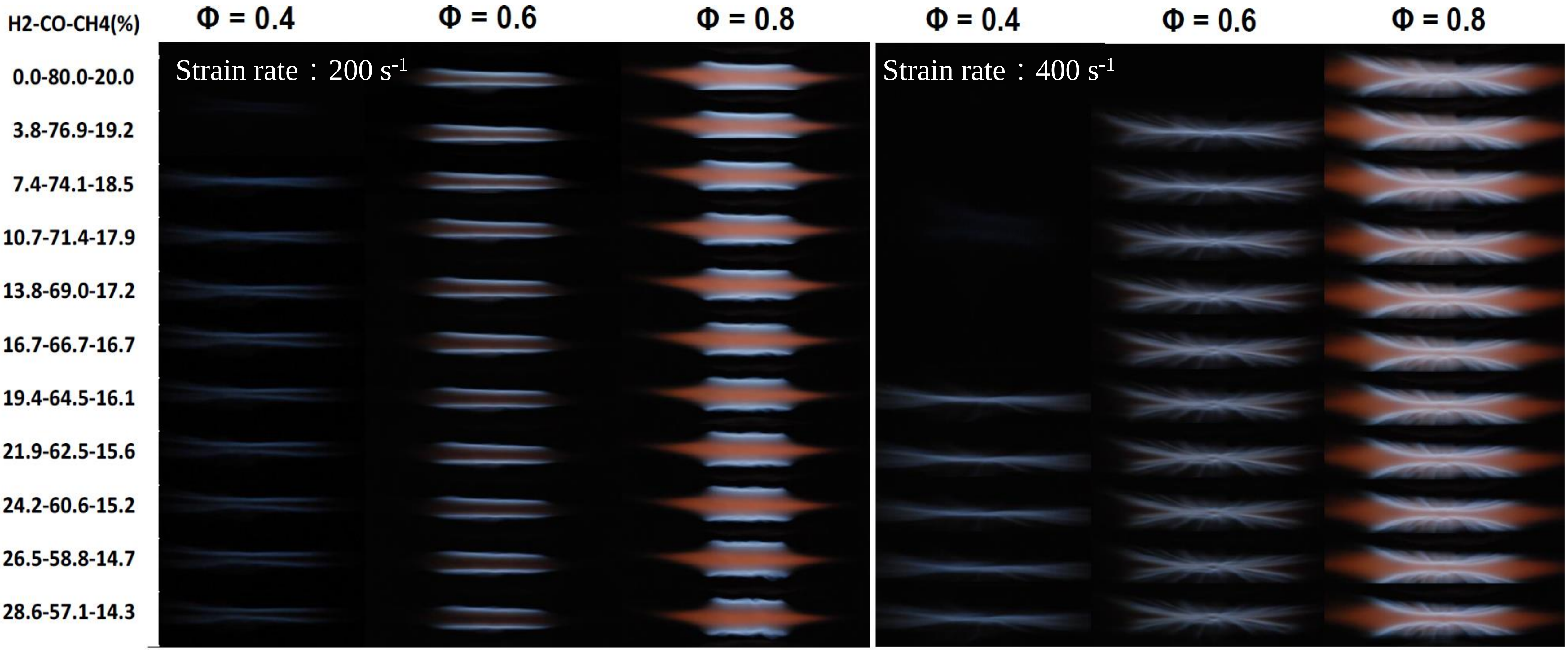
Mechanism	Species	Reactions	
GRI-mech 3.0	53	325	Methane combustion
USC mechII	111	784	H_2/CO/C1~C4 hydrocarbon combustion
Davis *et al.*	16	30	Specifically for H_2/CO combustion
Li	21	93	Be used in CO, CH_2O,CH_3OH and syngas oxidation
C2	87	367	Predicts a wide range of oxidation properties of H_2, CH_4, ethane, ethylene, acetylene and methanol

Simulation conditions

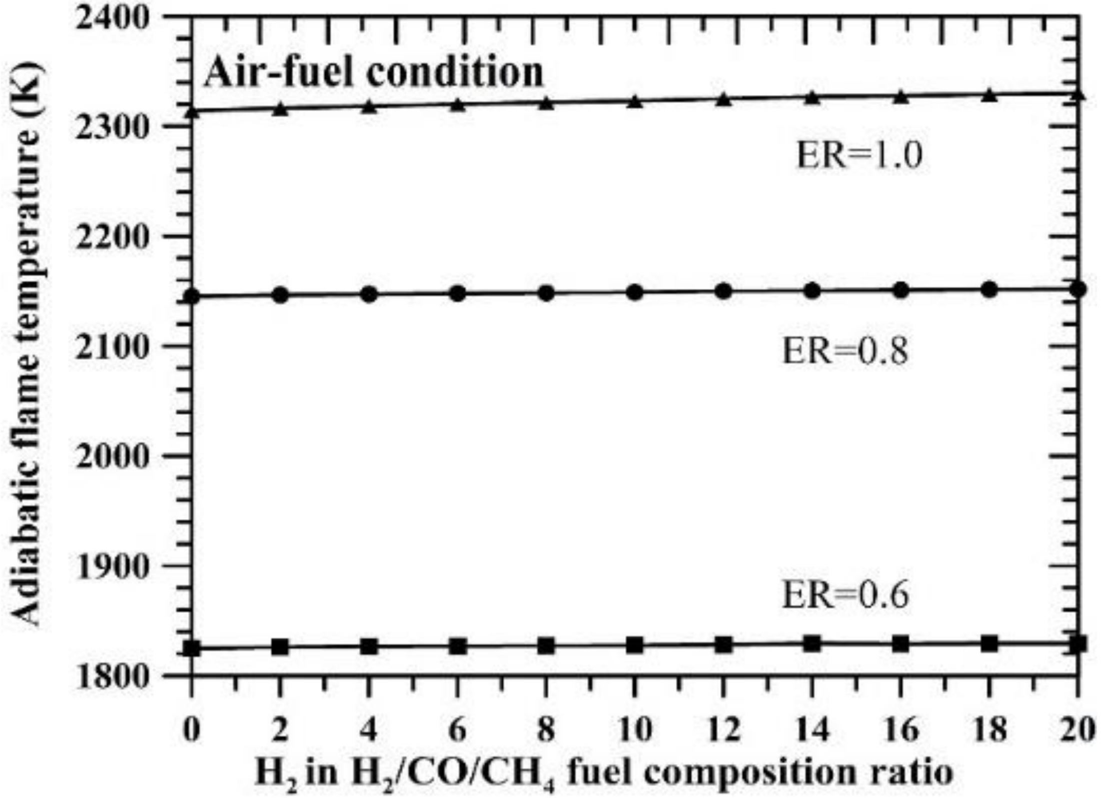
- The initial condition：**300** K and **1** atm.
- The oxy-fuel condition ：32%O_2 + 68%CO_2

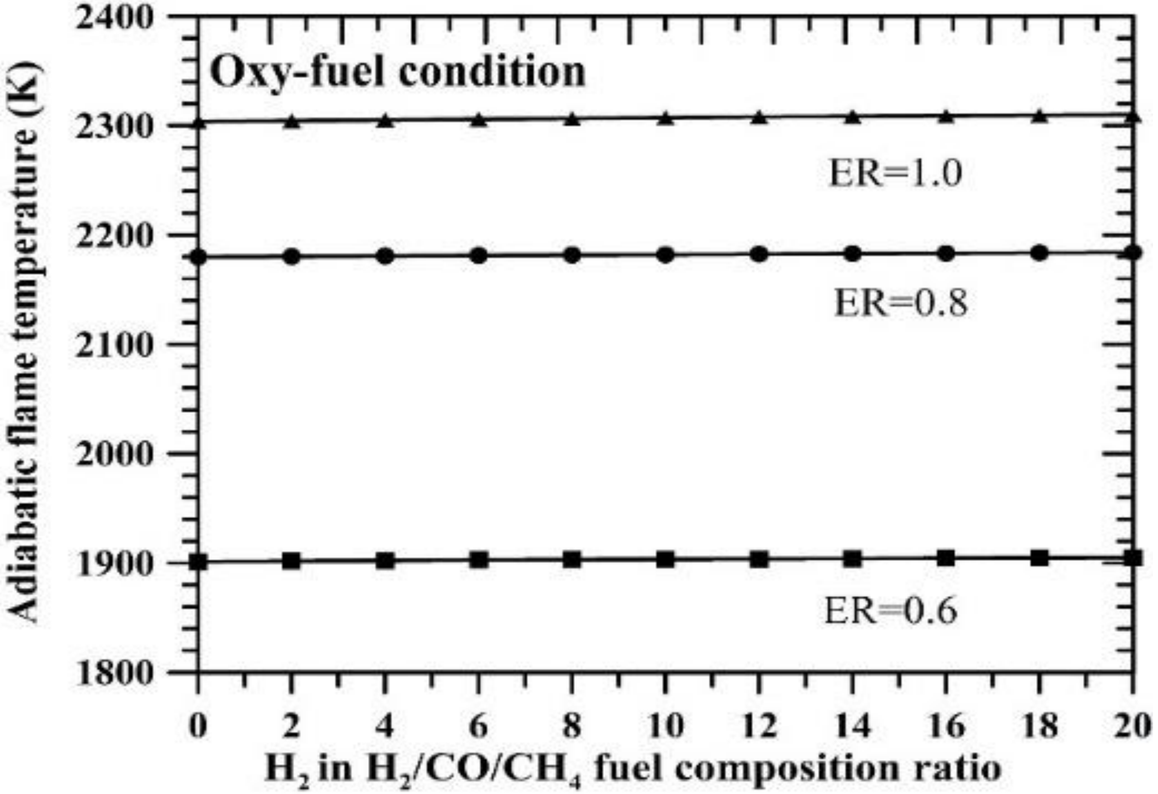
Flame NO.	H_2/CO/CH_4 Fuel composition ratio (%)			H_2/CO/CH_4 Mole fraction(vol%)			Air (vol%)	H_2/CO/CH_4 Mole fraction(vol%)			Oxy (vol%)
	H_2	CO	CH_4	H_2	CO	CH_4	ϕ= 1.0	H_2	CO	CH_4	ϕ= 1.0
1	0	20	5	0.00	16.63	4.16	79.21	0.00	22.86	5.71	71.43
2	2	20	5	1.57	15.75	3.94	78.74	2.16	21.59	5.40	70.85
3	4	20	5	2.99	14.95	3.74	78.32	4.09	20.46	5.12	70.33
4	6	20	5	4.27	14.23	3.56	77.94	5.83	19.44	4.86	69.87
5	8	20	5	5.43	13.58	3.39	77.59	7.41	18.52	4.63	69.44
6	10	20	5	6.49	12.98	3.25	77.28	8.84	17.68	4.42	69.06
7	12	20	5	7.46	12.44	3.11	76.99	10.15	16.91	4.23	68.71
8	14	20	5	8.35	11.94	2.98	76.73	11.35	16.21	4.05	68.39
9	16	20	5	9.18	11.47	2.87	76.48	12.45	15.56	3.89	68.09
10	18	20	5	9.94	11.04	2.76	76.26	13.47	14.97	3.74	67.82
11	20	20	5	10.65	10.65	2.66	76.05	14.41	14.41	3.60	67.57

Results and discussion — Experiment



➢ Adiabatic Flame Temperature

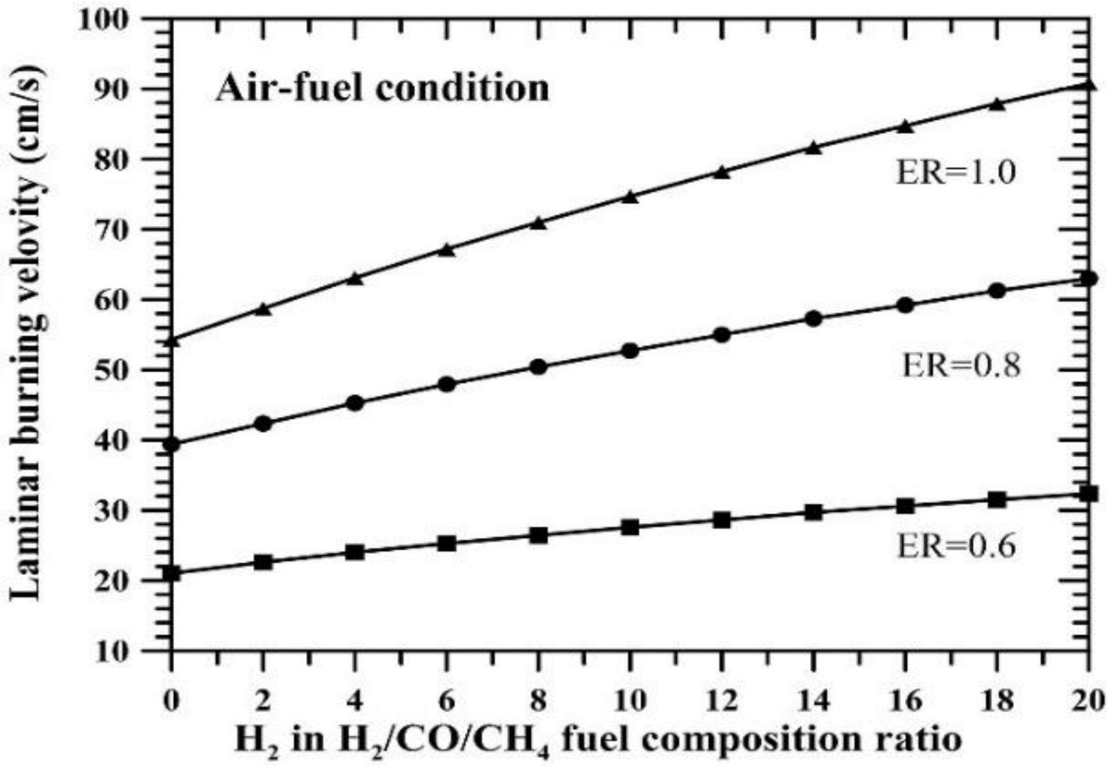


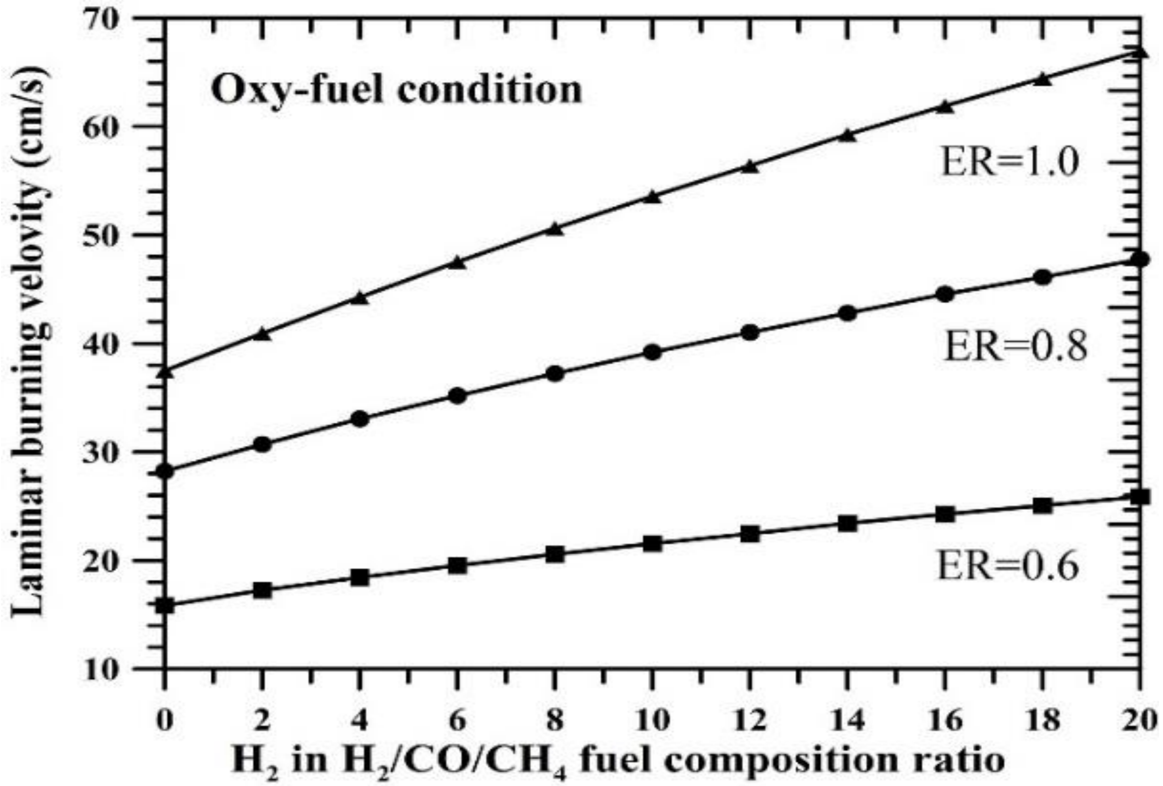


- The main characteristic for oxy-fuel condition is that the carbon oxide greatly affected the heat capacity.

Results and discussion — Num (2/13)

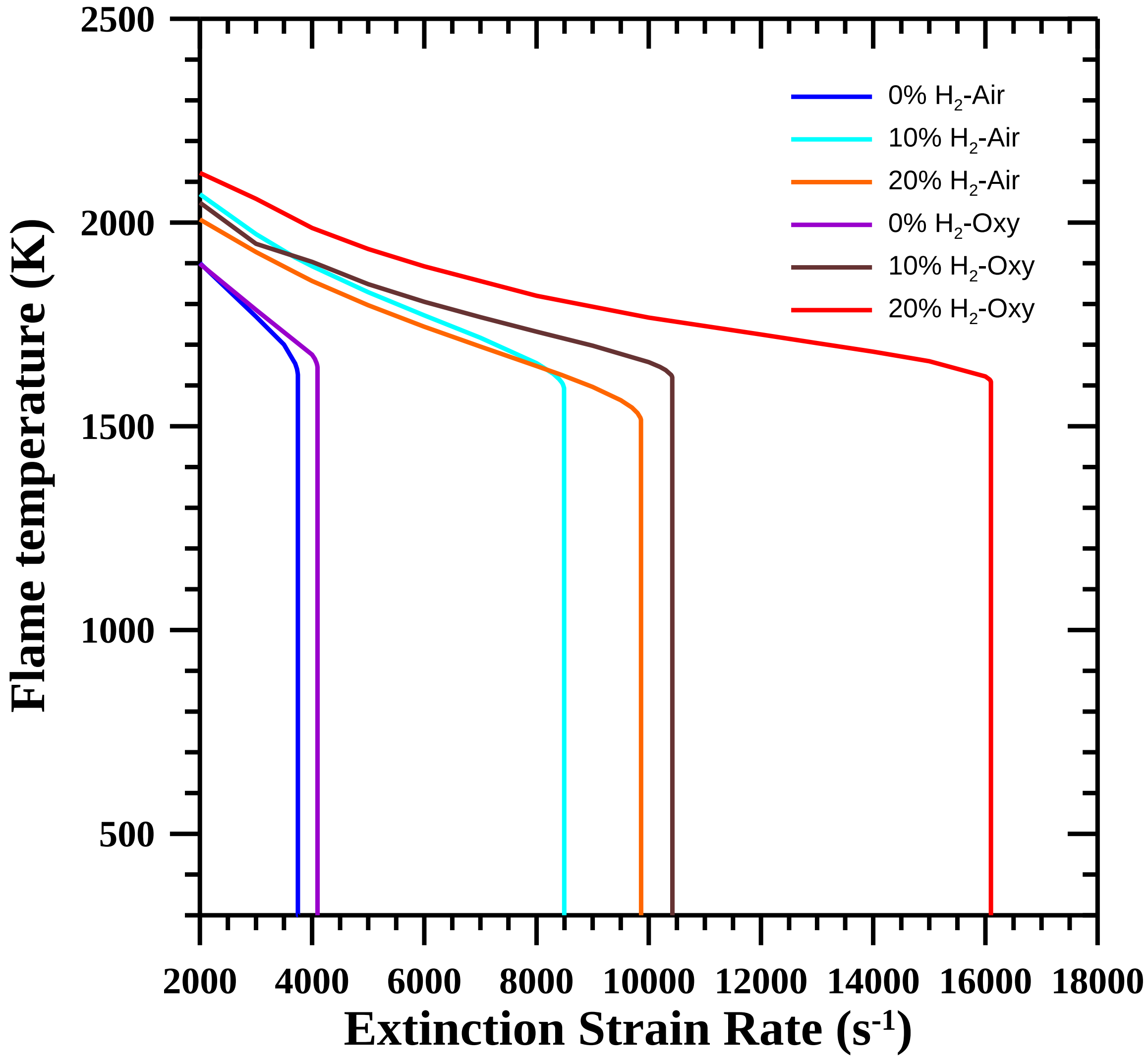
- Laminar Flame Velocity





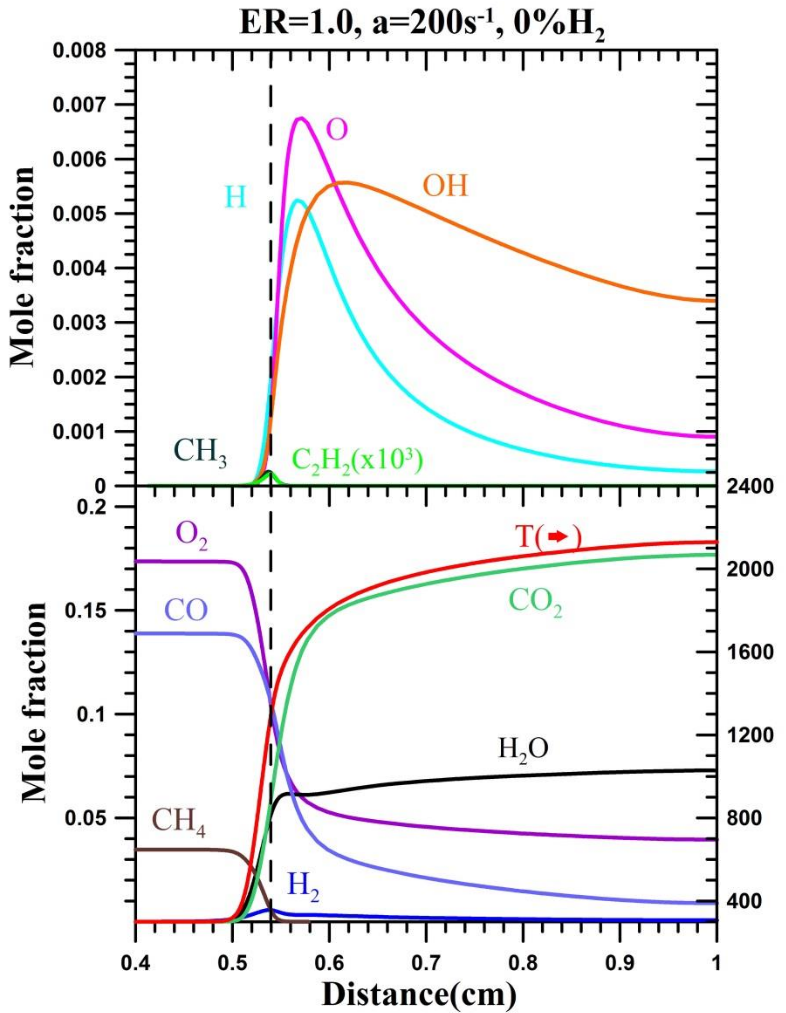
Extinction Strain Rate

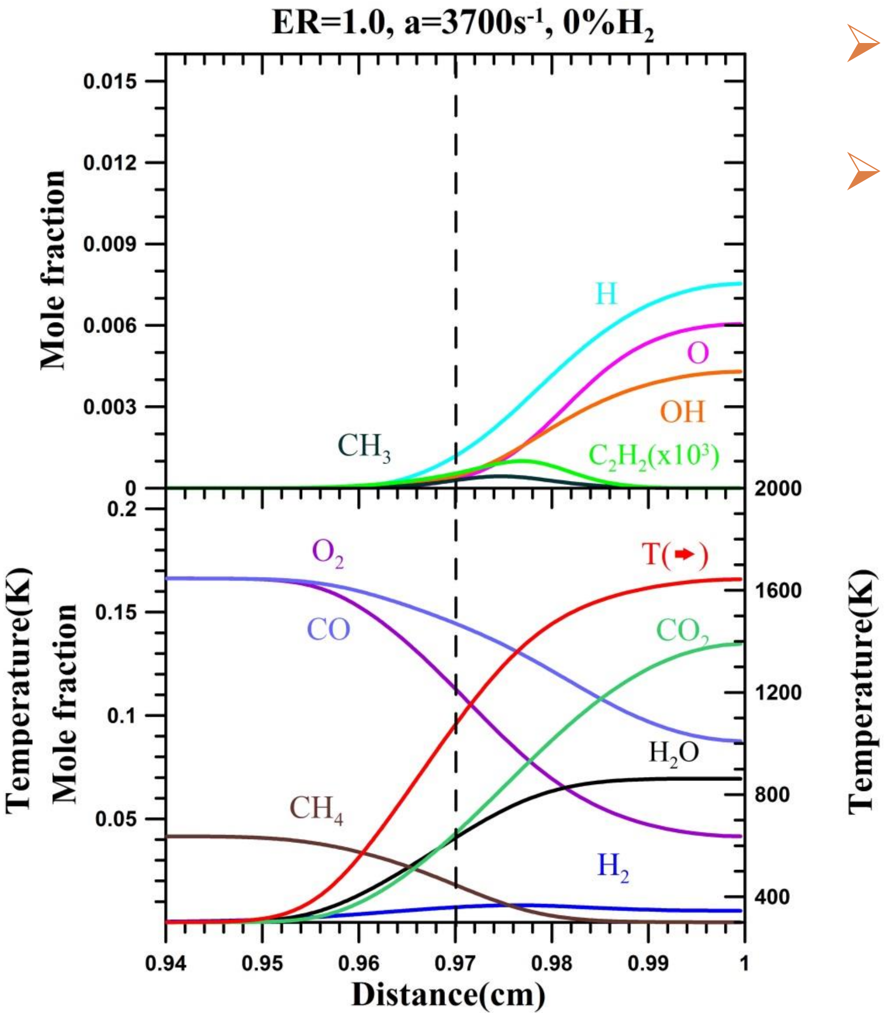
- The hydrogen addition would lead to an increase of higher extinction strain rate.



Results and discussion — Num (4/13)

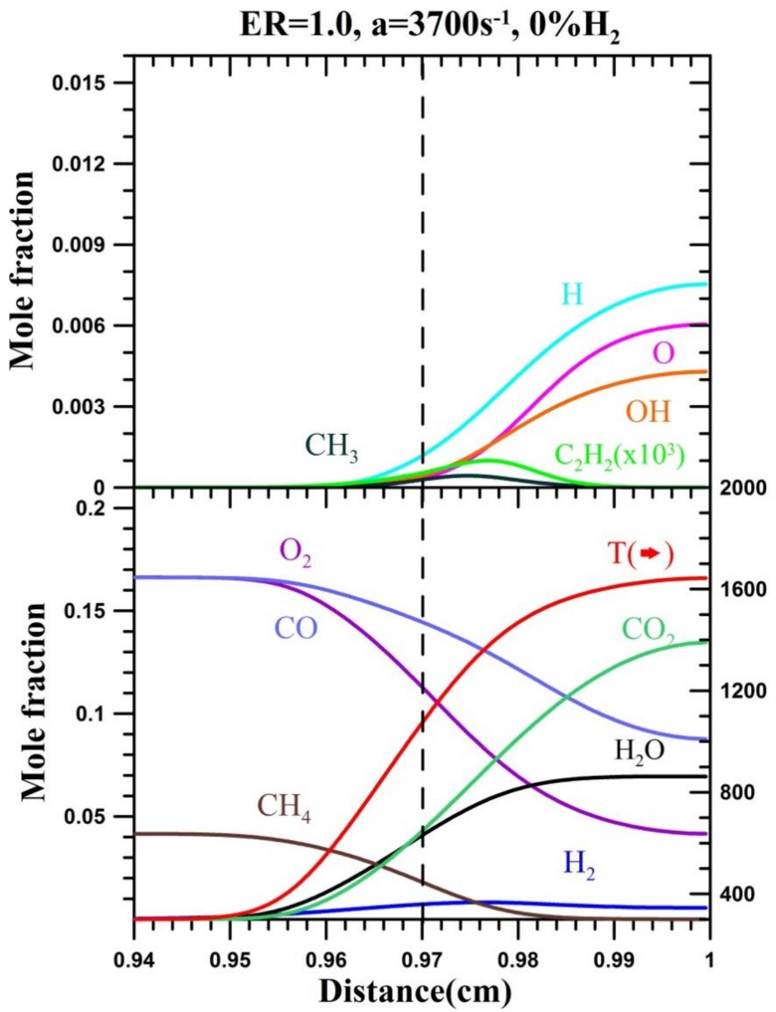
Concentration Distribution— Air-fuel condition

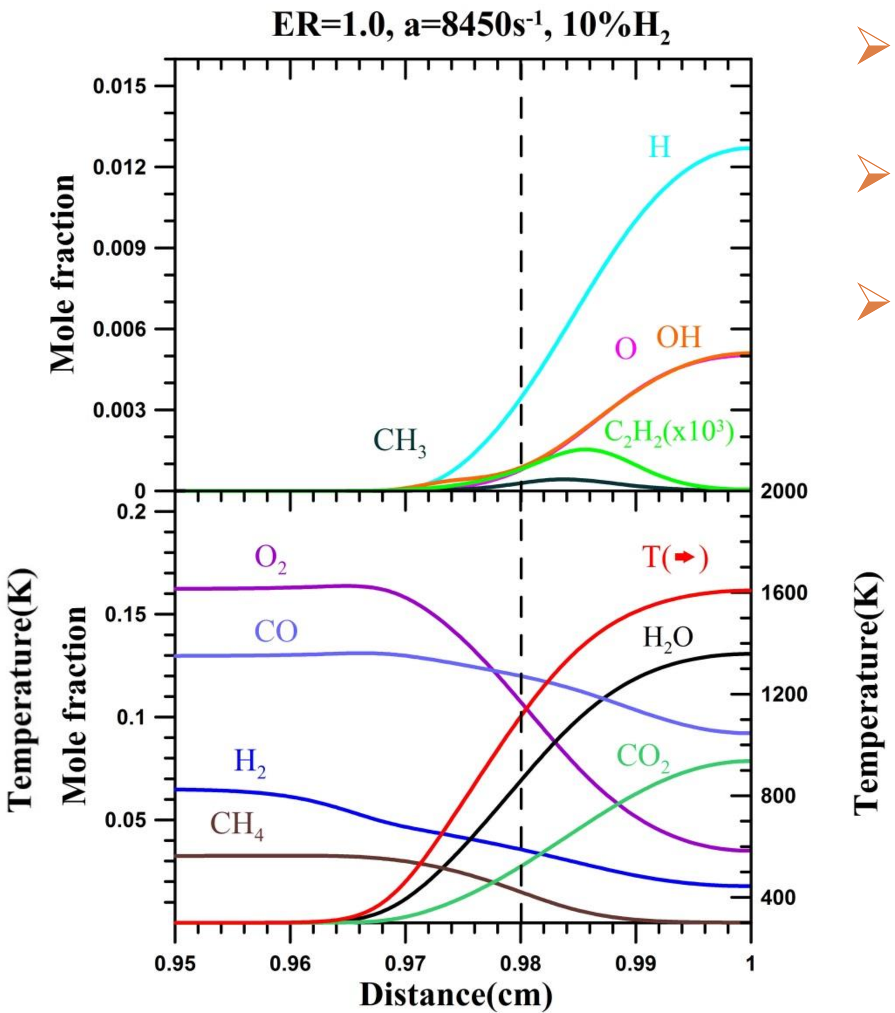




- Strain rate：200，3700s^{-1}
- Hydrogen：0%

➢ Concentration Distribution— Air-fuel condition



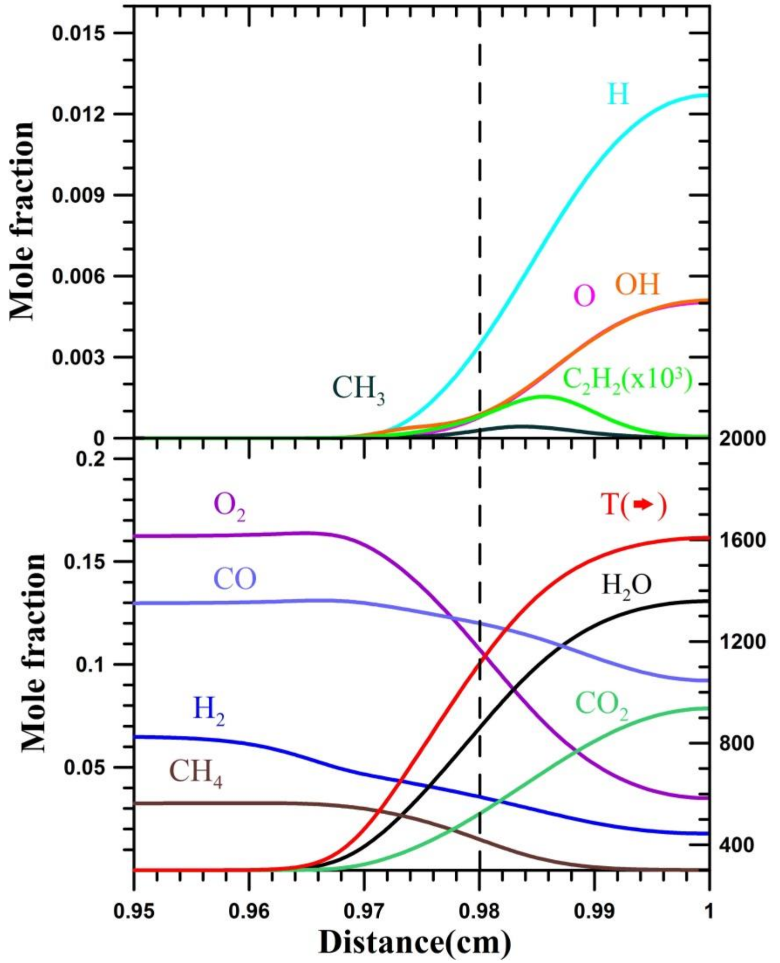


- Strain rate：near extinction
- Hydrogen：0%, 10%
- H radicals has increased dramatically along with the H_2 addition.

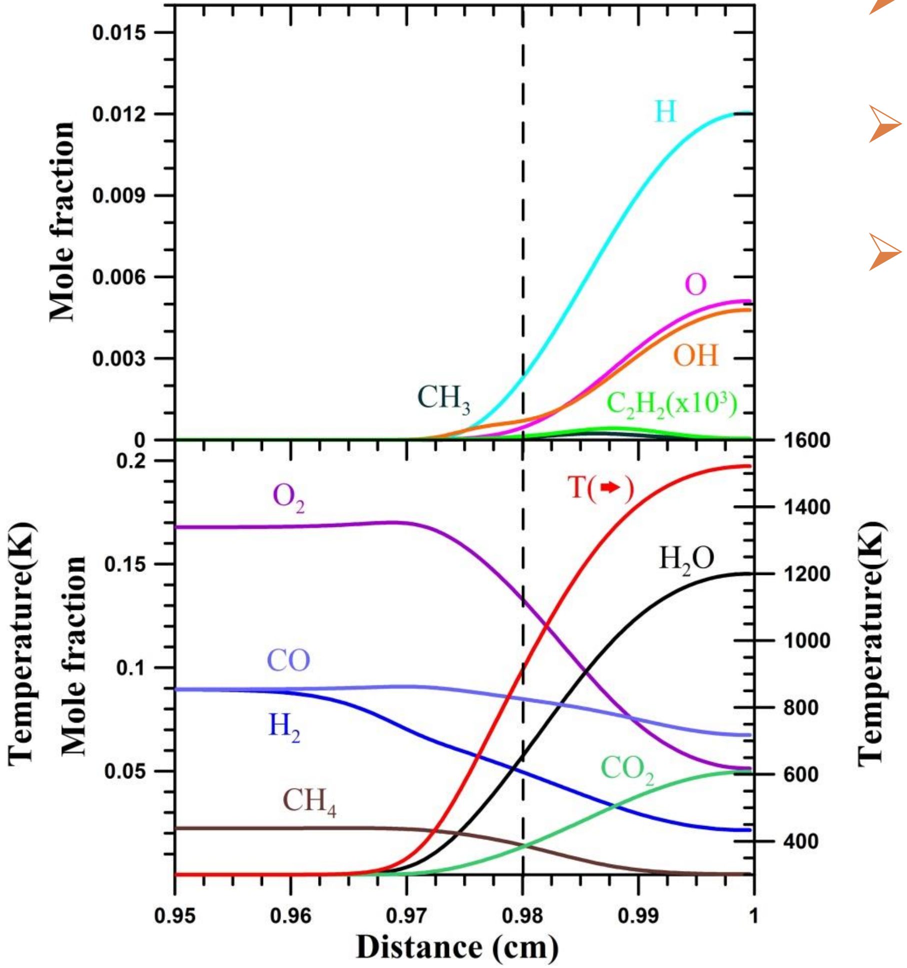
Results and discussion — Num (6/13)

Concentration Distribution— Air-fuel condition

ER=1.0, a=8450s^{-1}, 10%H_2



ER=1.0, a=9450s^{-1}, 20%H_2

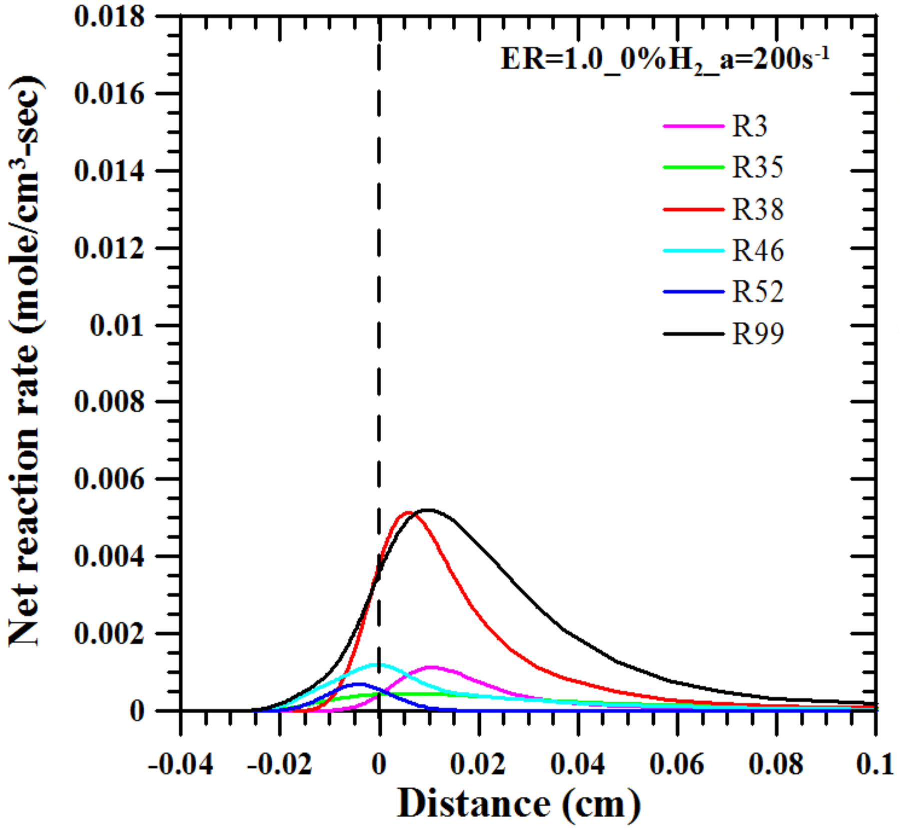


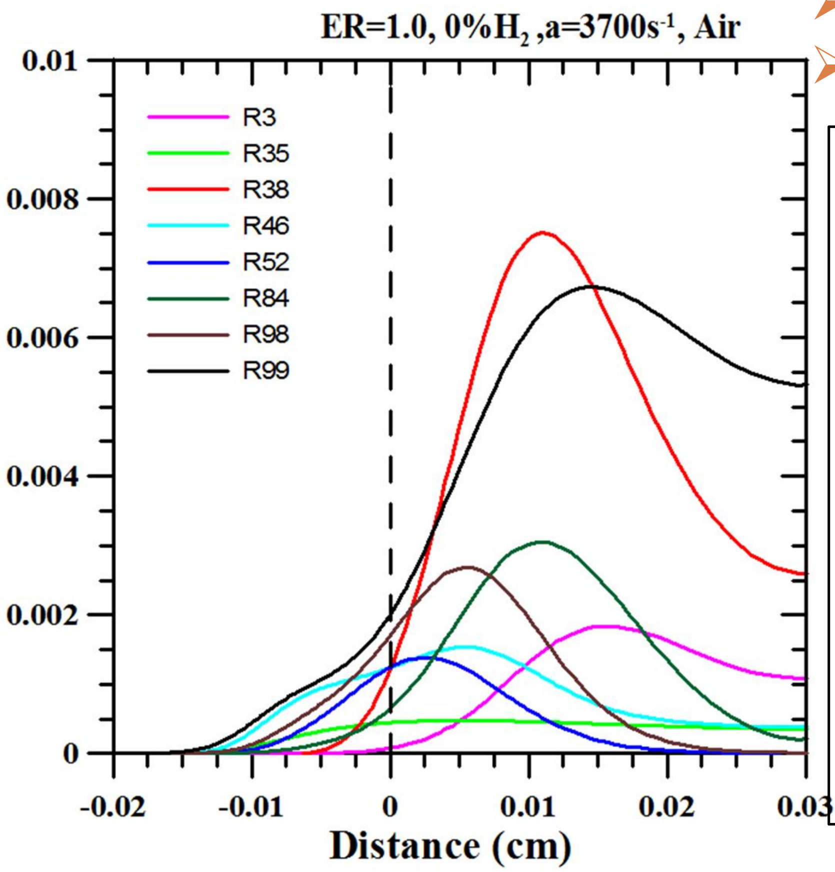
- Strain rate：near extinction
- Hydrogen：10%, 20%
- Compared 10% to 20% hydrogen addition, H radical both are similar in 0.012.

Results and discussion — Num (7/13)

Net reaction rate — Air-fuel condition

- Strain rate：200，3700s[-1]
- Hydrogen：0%





R3：$O+H_2 \leftrightarrow H+OH$

R35：$H+O_2+H_2O \leftrightarrow HO_2+H_2O$

R38： $H+O_2 \leftrightarrow O+OH$

R46： $H+HO_2 \leftrightarrow 2OH$

R52： $H+CH_3(+M) \leftrightarrow CH_4(+M)$

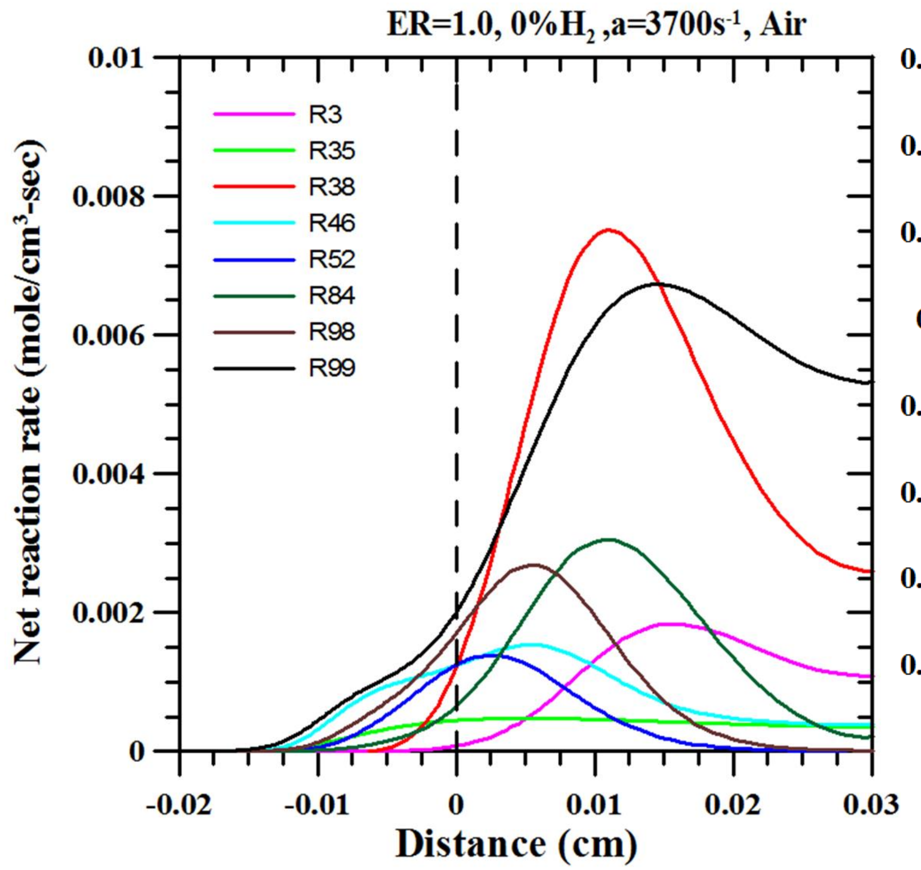
R84：$OH+H_2 \leftrightarrow H+H_2O$

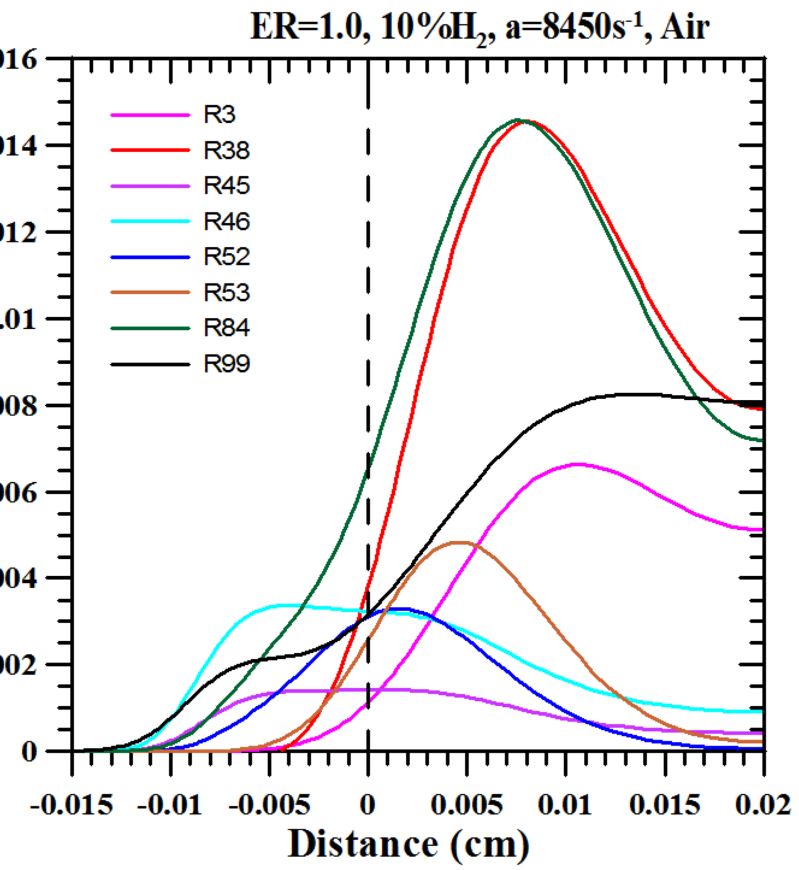
R98： $OH+CH_4 \leftrightarrow CH_3+H_2O$

R99： $OH+CO \leftrightarrow H+CO_2$

Results and discussion — Num (8/13)

➢ Net reaction rate — Air-fuel condition





- Strain rate：near extinction
- Hydrogen：0%, 10%

R3：$O+H_2 \leftrightarrow H+OH$

R35：$H+O_2+H_2O \leftrightarrow HO_2+H_2O$

R38： $H+O_2 \leftrightarrow O+OH$

R46： $H+HO_2 \leftrightarrow 2OH$

R52： $H+CH_3(+M) \leftrightarrow CH_4(+M)$

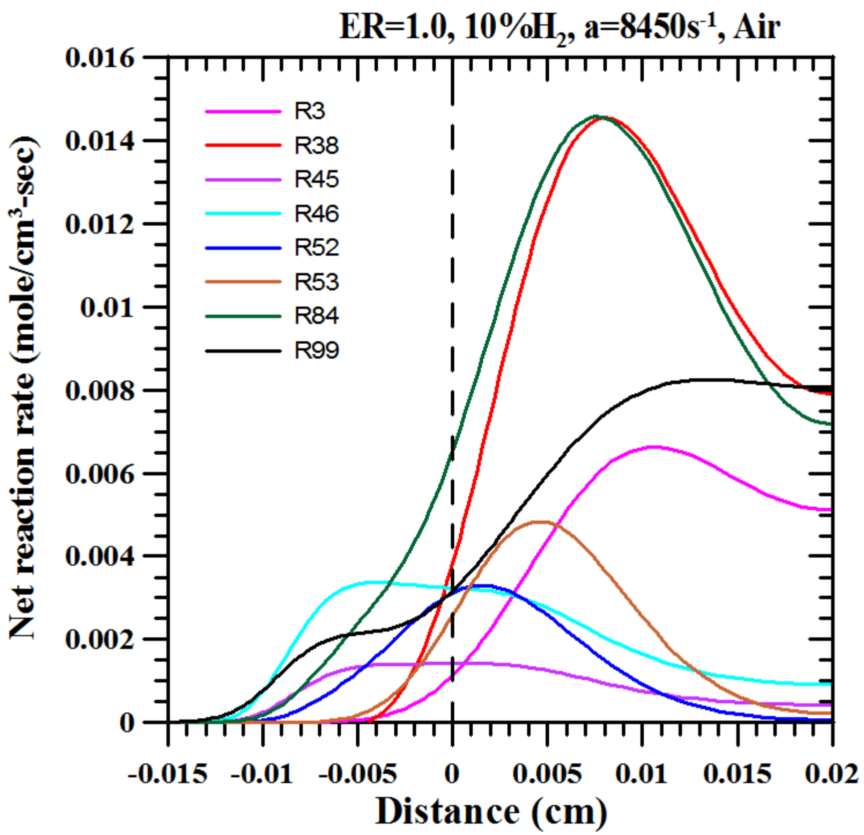
R84：$OH+H_2 \leftrightarrow H+H_2O$

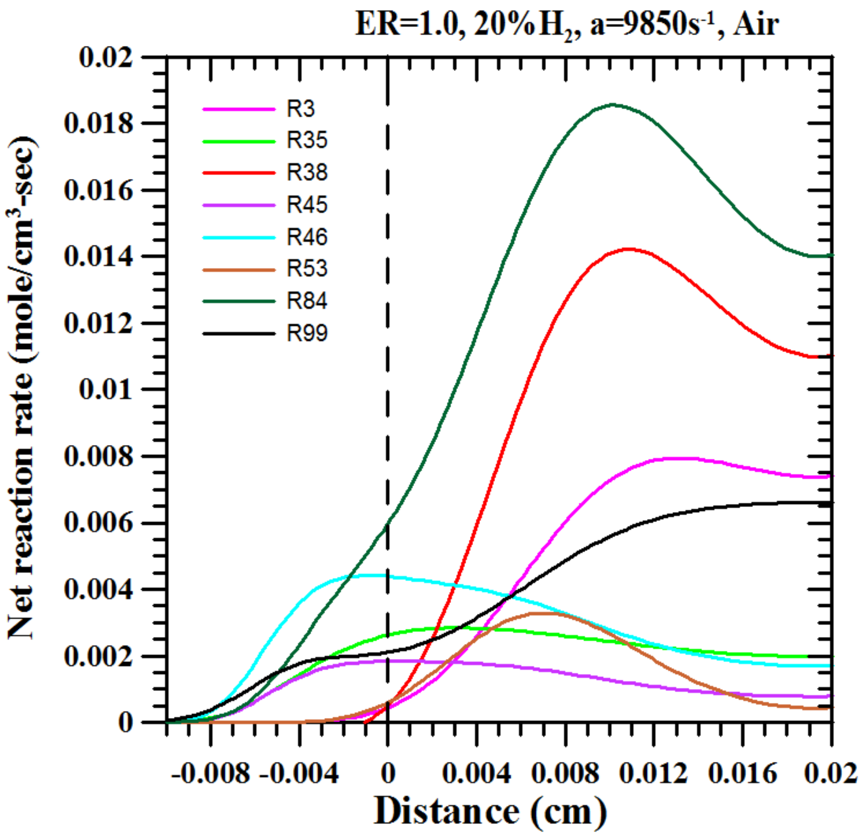
R98： $OH+CH_4 \leftrightarrow CH_3+H_2O$

R99： $OH+CO \leftrightarrow H+CO_2$

Results and discussion — Num (9/13)

➢ Net reaction rate — Air-fuel condition





- ➢ Strain rate：near extinction
- ➢ Hydrogen：10, 20%

R3：$O+H_2 \leftrightarrow H+OH$

R35：$H+O_2+H_2O \leftrightarrow HO_2+H_2O$

R38： $H+O_2 \leftrightarrow O+OH$

R46： $H+HO_2 \leftrightarrow 2OH$

R53： $H+CH_4 \leftrightarrow CH_3+H_2$

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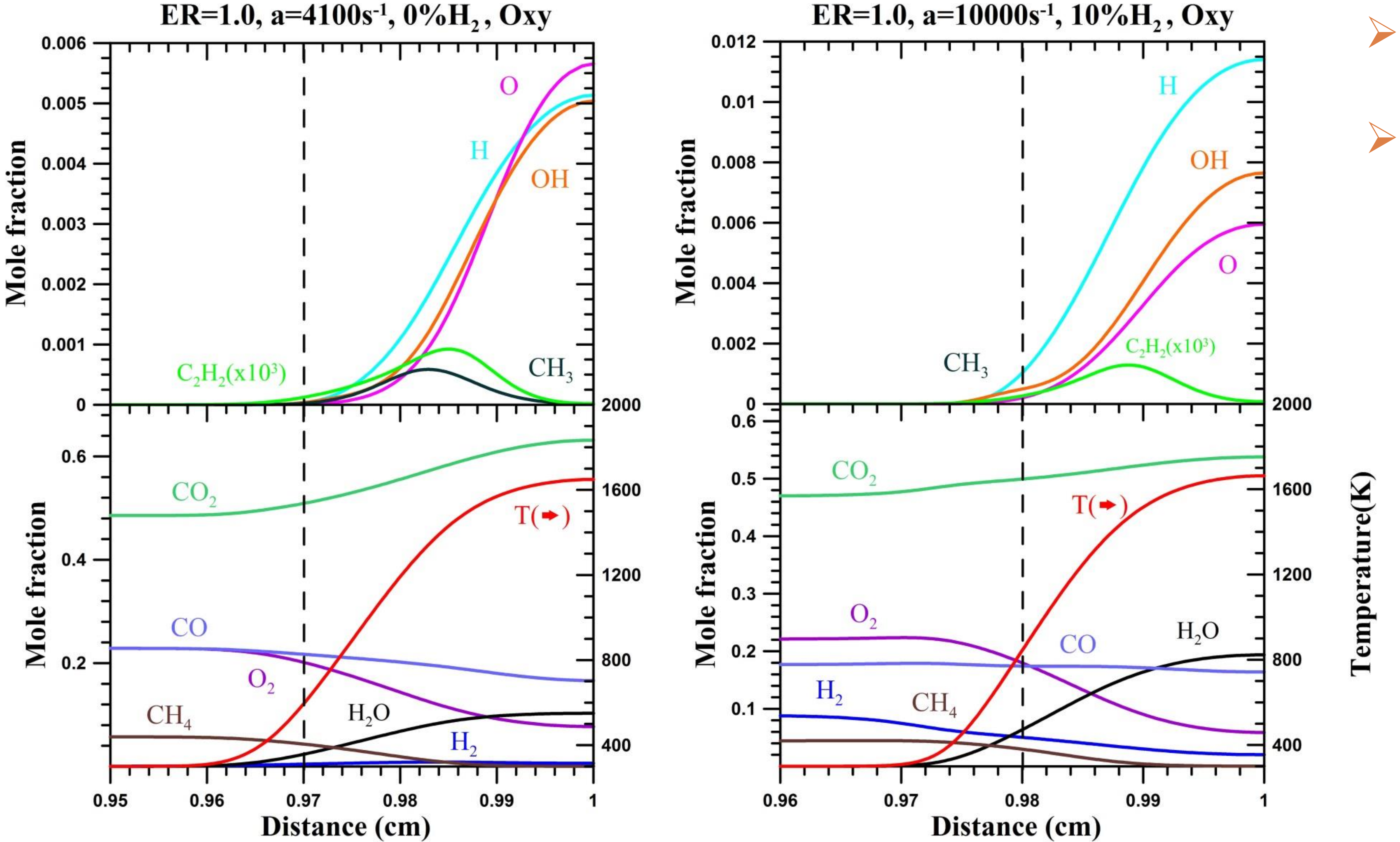
R98： $OH+CH_4 \leftrightarrow CH_3+H_2O$

R99： $OH+CO \leftrightarrow H+CO_2$

Results and discussion — Num (10/13)

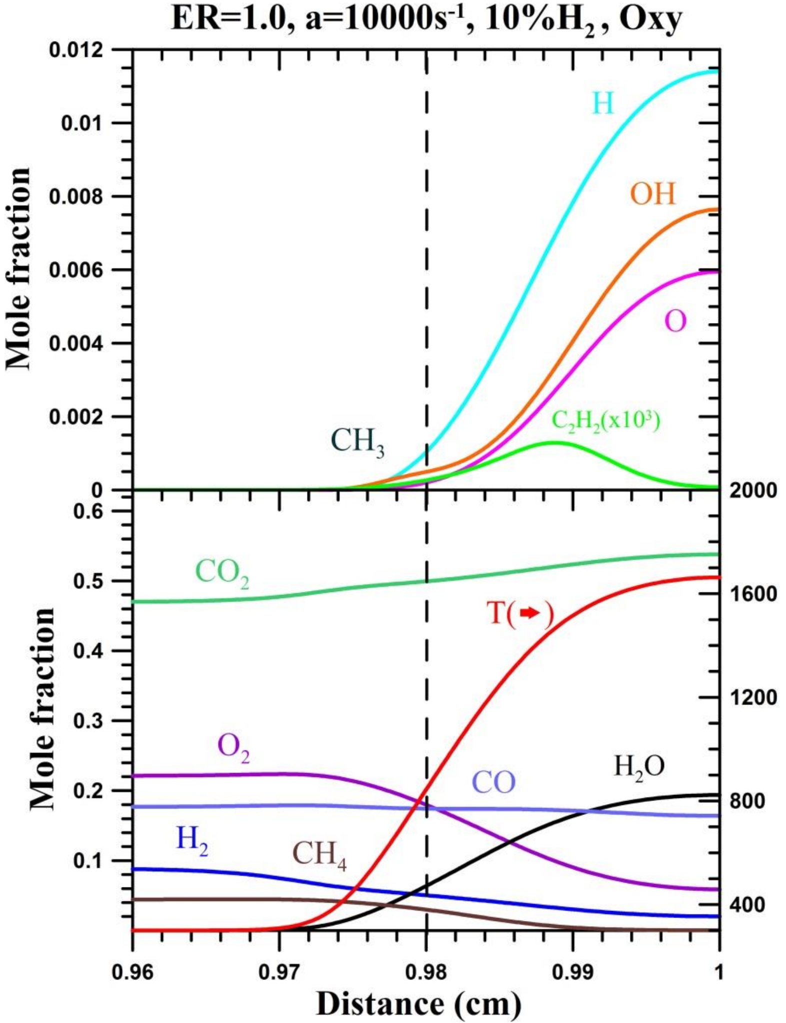
➢ Concentration Distribution — Oxy-fuel condition

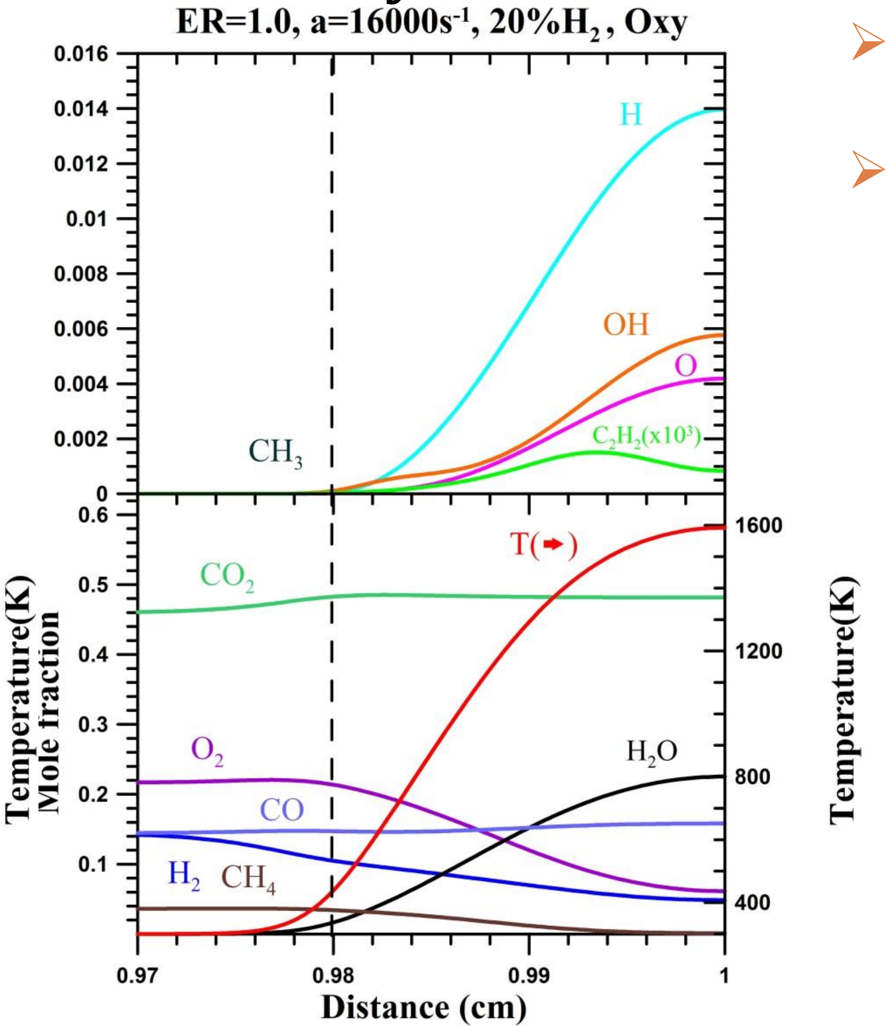


- Strain rate：near extinction
- Hydrogen：0%, 10%

Results and discussion — Num (11/13)

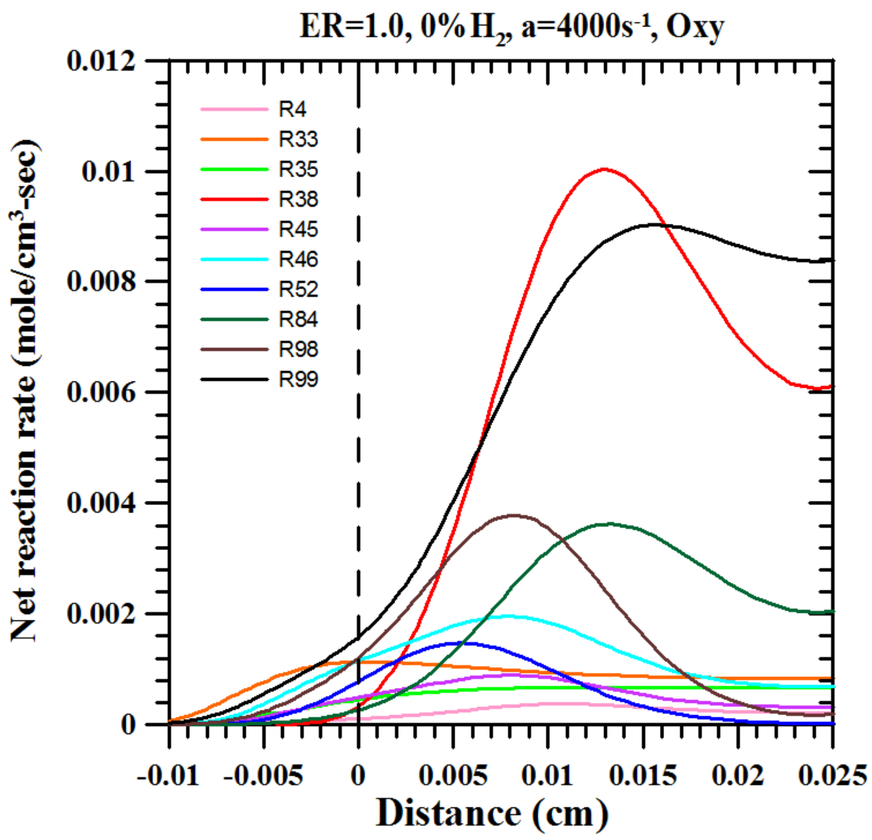
- **Concentration Distribution — Oxy-fuel condition**

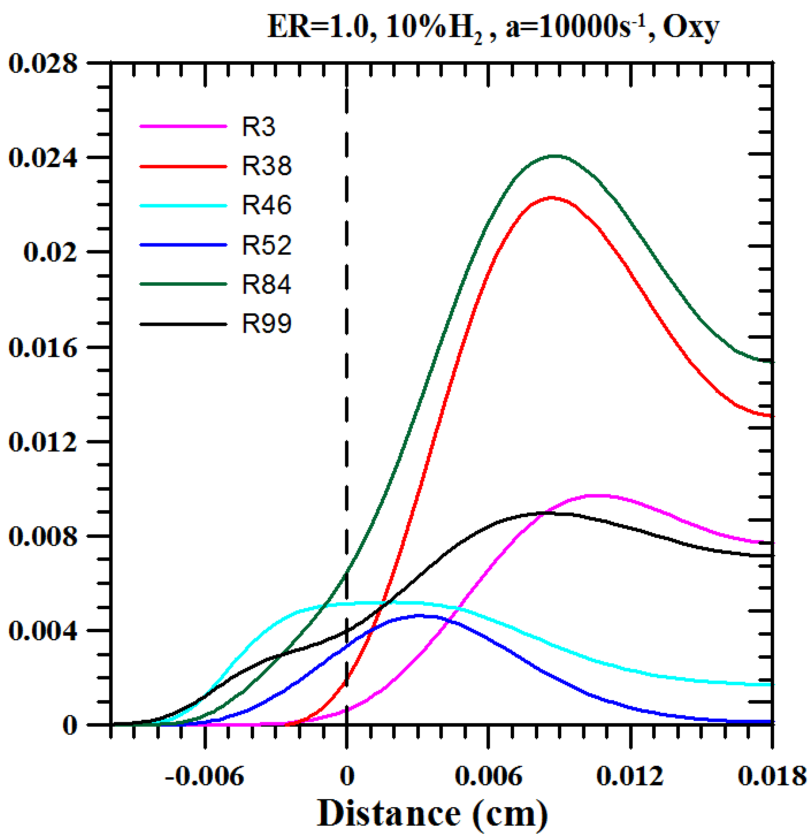




- Strain rate：near extinction
- Hydrogen：10%, 20%

- **Net reaction rate — Oxy-fuel condition**





- Strain rate：near extinction
- Hydrogen：0, 10%

R3：$O+H_2 \leftrightarrow H+OH$

R35：$H+O_2+H_2O \leftrightarrow HO_2+H_2O$

R38： $H+O_2 \leftrightarrow O+OH$

R46： $H+HO_2 \leftrightarrow 2OH$

R52： $H+CH_3(+M) \leftrightarrow CH_4(+M)$

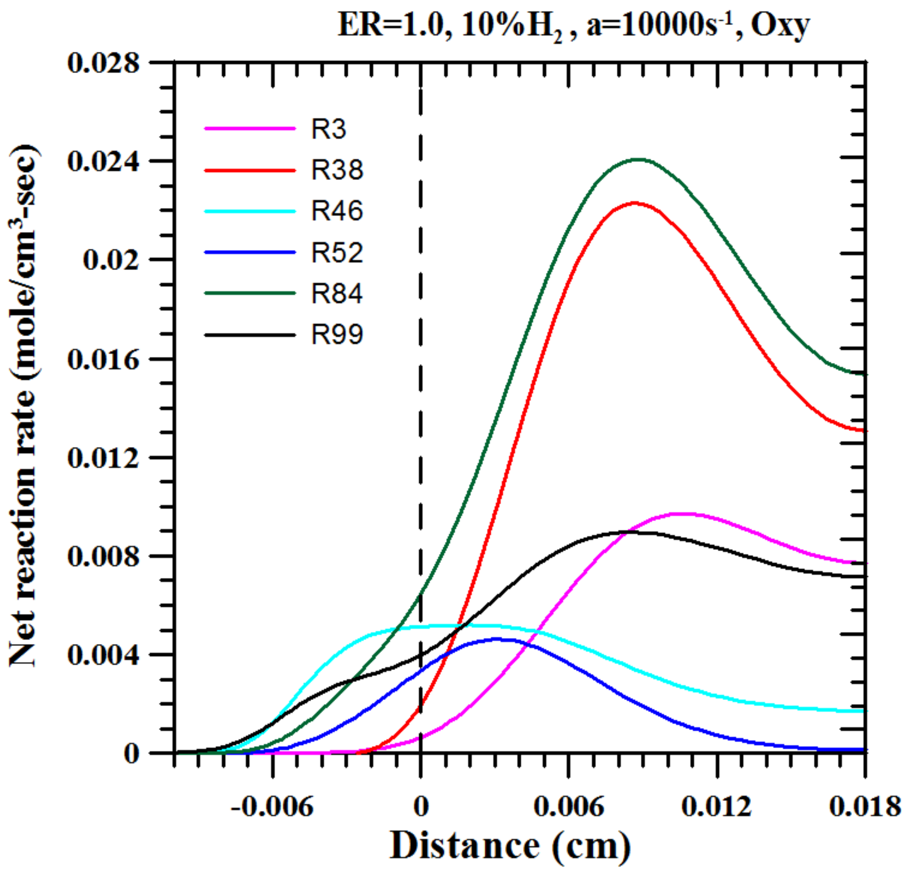
R84：$OH+H_2 \leftrightarrow H+H_2O$

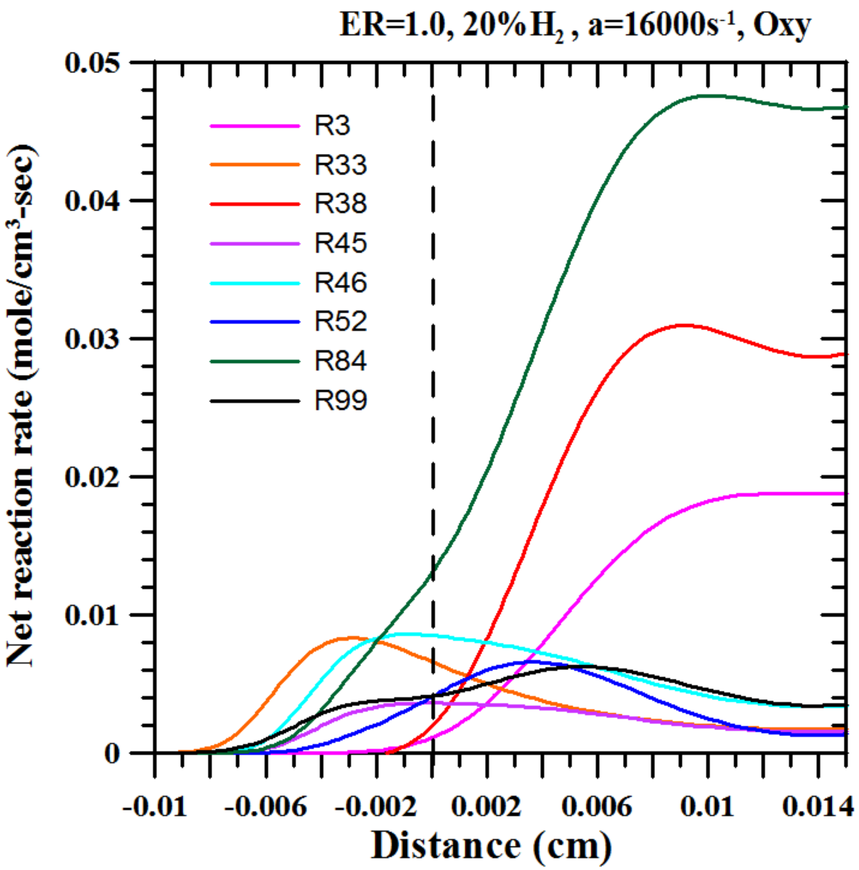
R98： $OH+CH_4 \leftrightarrow CH_3+H_2O$

R99： $OH+CO \leftrightarrow H+CO_2$

Results and discussion — Num (13/13)

Net reaction rate — Oxy-fuel condition





- Strain rate：near extinction
- Hydrogen：10, 20%

R3：$O+H_2 \leftrightarrow H+OH$

R33：$H+O_2+M \leftrightarrow HO_2+M$

R35：$H+O_2+H_2O \leftrightarrow HO_2+H_2O$

R38： $H+O_2 \leftrightarrow O+OH$

R46： $H+HO_2 \leftrightarrow 2OH$

R52： $H+CH_3(+M) \leftrightarrow CH_4(+M)$

R84：$OH+H_2 \leftrightarrow H+H_2O$

R98： $OH+CH_4 \leftrightarrow CH_3+H_2O$

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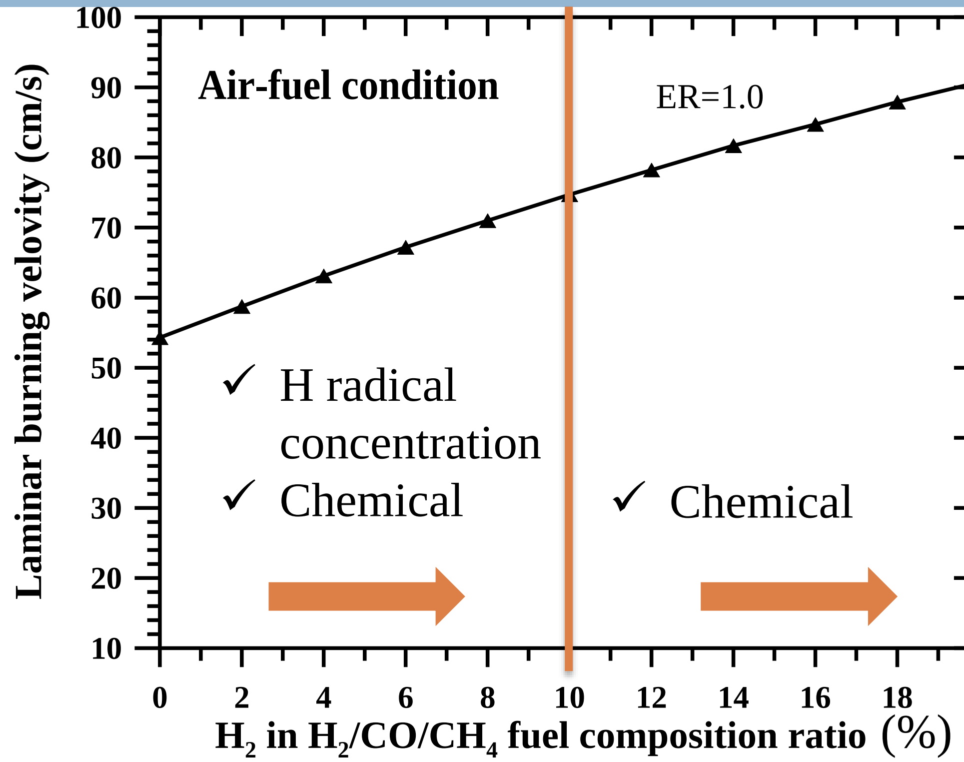
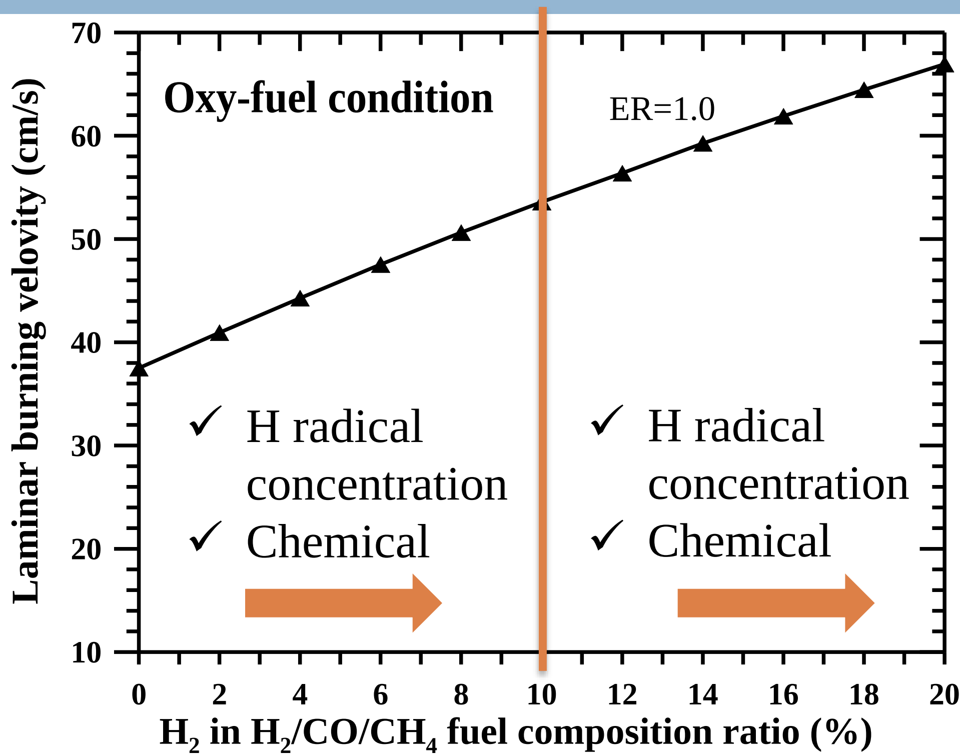
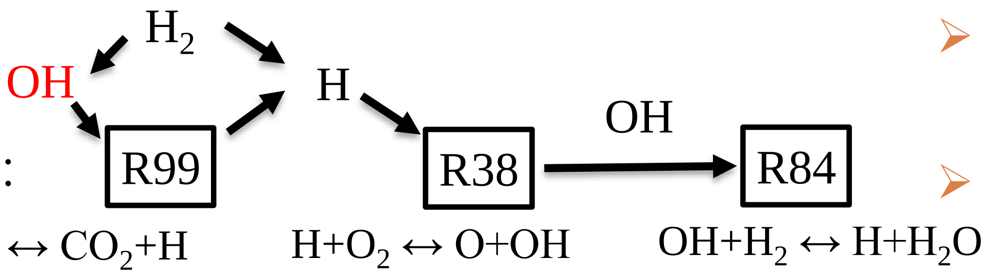
Conclusions

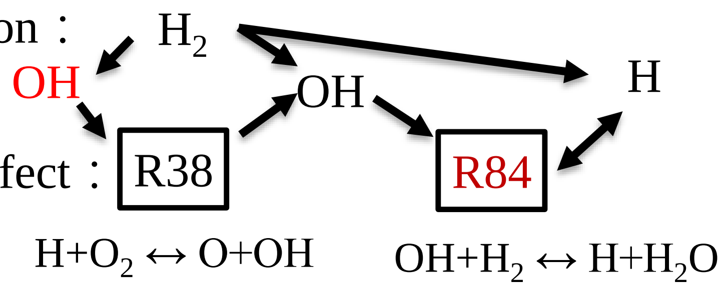




- Concentration :
- Chemical effect :



- Concentration :
- Chemical effect :



Conclusions

Extinction strain rate issue

- Air-fuel condition：
  - Strain rate =200~3700s^{-1} → Chemical effect
  - Strain rate =3700~8450s^{-1} → Concentration, Chemical effect
  - Strain rate =8450~9850s^{-1} → Chemical effect

Strain rate =200~3700 s^{-1}

R46 ($H+HO_2 \leftrightarrow 2OH$)

→ R84 ($OH+H_2 \leftrightarrow H+H_2O$) → R38 ($H+O_2 \leftrightarrow O+OH$)

→ R99 ($CO+OH \leftrightarrow CO_2+H$)

Strain rate =3700~8450 s^{-1}

R3 ($O+H_2 \leftrightarrow H+OH$)

↓

R99 ($CO+OH \leftrightarrow CO_2+H$)

↓

R38 ($H+O_2 \leftrightarrow O+OH$)

R84 ($OH+H_2 \leftrightarrow H+H_2O$)

Strain rate =8450~9850 s^{-1}

R3 ($O+H_2 \leftrightarrow H+OH$)

↓

R99 ($CO+OH \leftrightarrow CO_2+H$)

↓

R38 ($H+O_2 \leftrightarrow O+OH$)

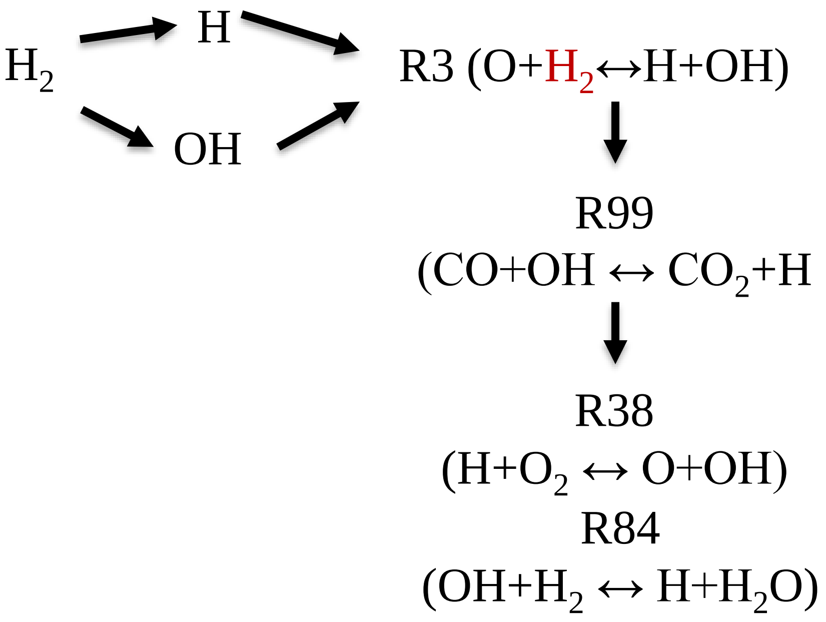
↓

R84 ($OH+H_2 \leftrightarrow H+H_2O$)

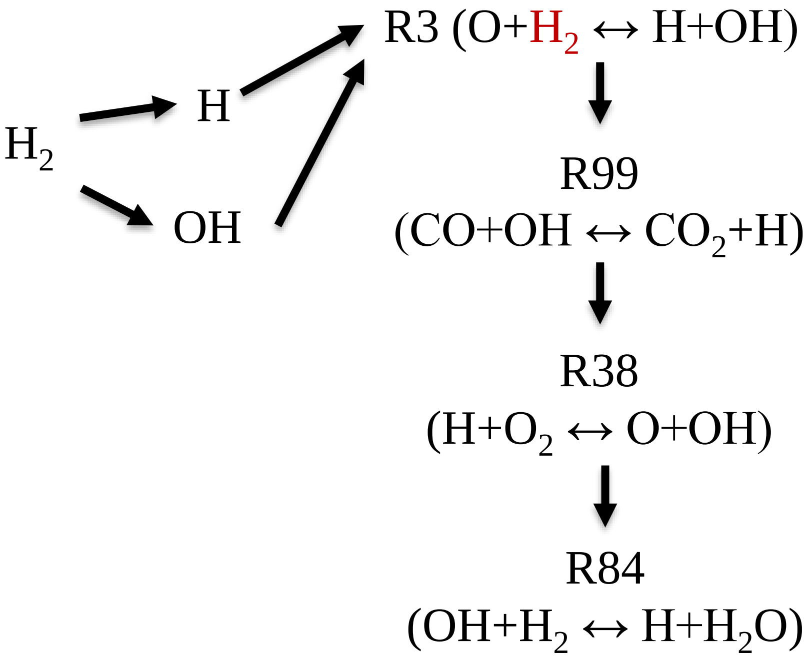
Conclusions

- Extinction strain rate issue
  - Oxy-fuel condition：
    - Strain rate =4100~10000s^{-1} → Concentration, Chemical effect
    - Strain rate =10000~16000s^{-1} → Concentration, Chemical effect

- Strain rate =4100~10000s^{-1}



- Strain rate =10000~16000s^{-1}



Thank you for attention

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