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Stabilized three-stage oxidation of gaseous n-heptane/air mixture in a micro flow reactor with a controlled temperature profile

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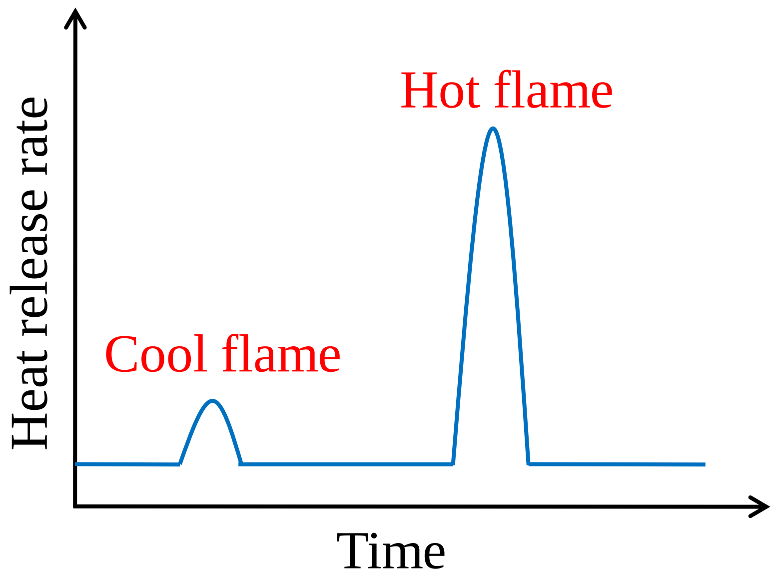
Background

It is important to know the ignition characteristics of various fuels.

⇒ Improvement of internal combustion engines.

- Spark ignition engines
- Compression ignition (Diesel, HCCI) engines
- Gas turbines   etc.

Typical ignition process of practical hydrocarbon fuels



Cool flame

- Low temperature oxidation (LTO)
- Small heat release

Hot flame

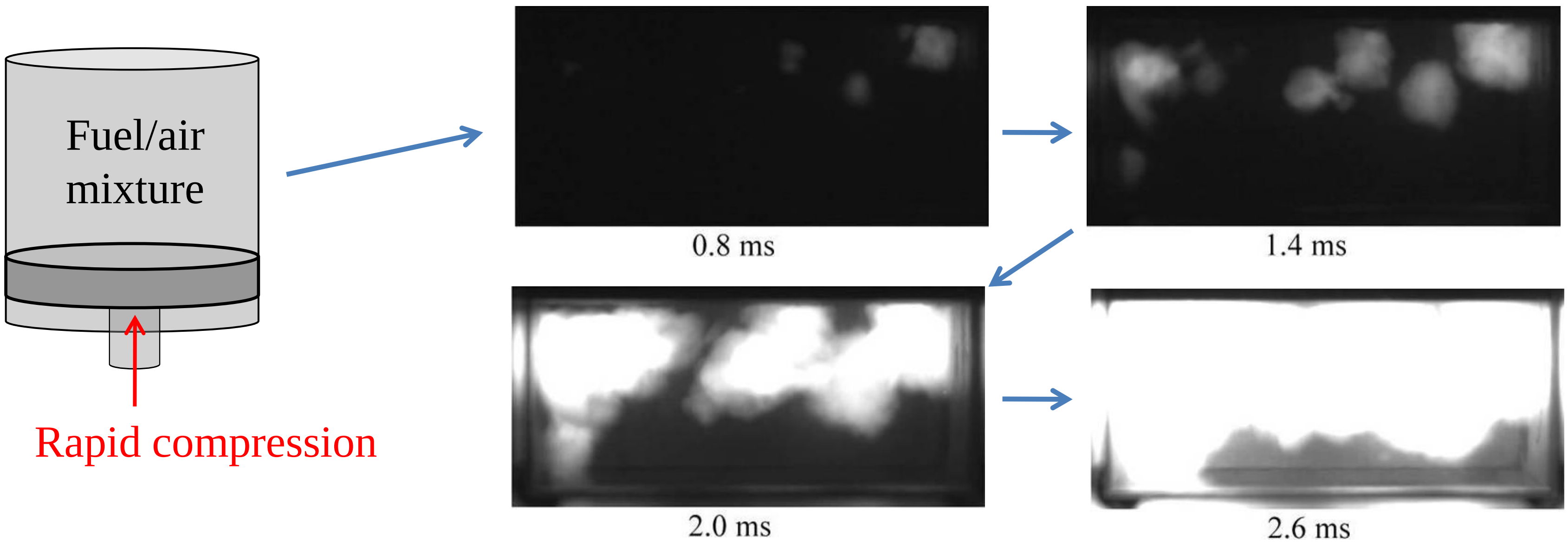
- High temperature oxidation (HTO)
- Main heat release

➡ Two-stage ignition at different temperature range

Two-stage ignition phenomena strongly affect the combustion control.

Approaches to investigate the ignition characteristics

Major approach: e.g., Rapid Compression Machines (RCMs)



Auto-ignition of methane/air mixture, Strozzi et al., CST 180 (2008)

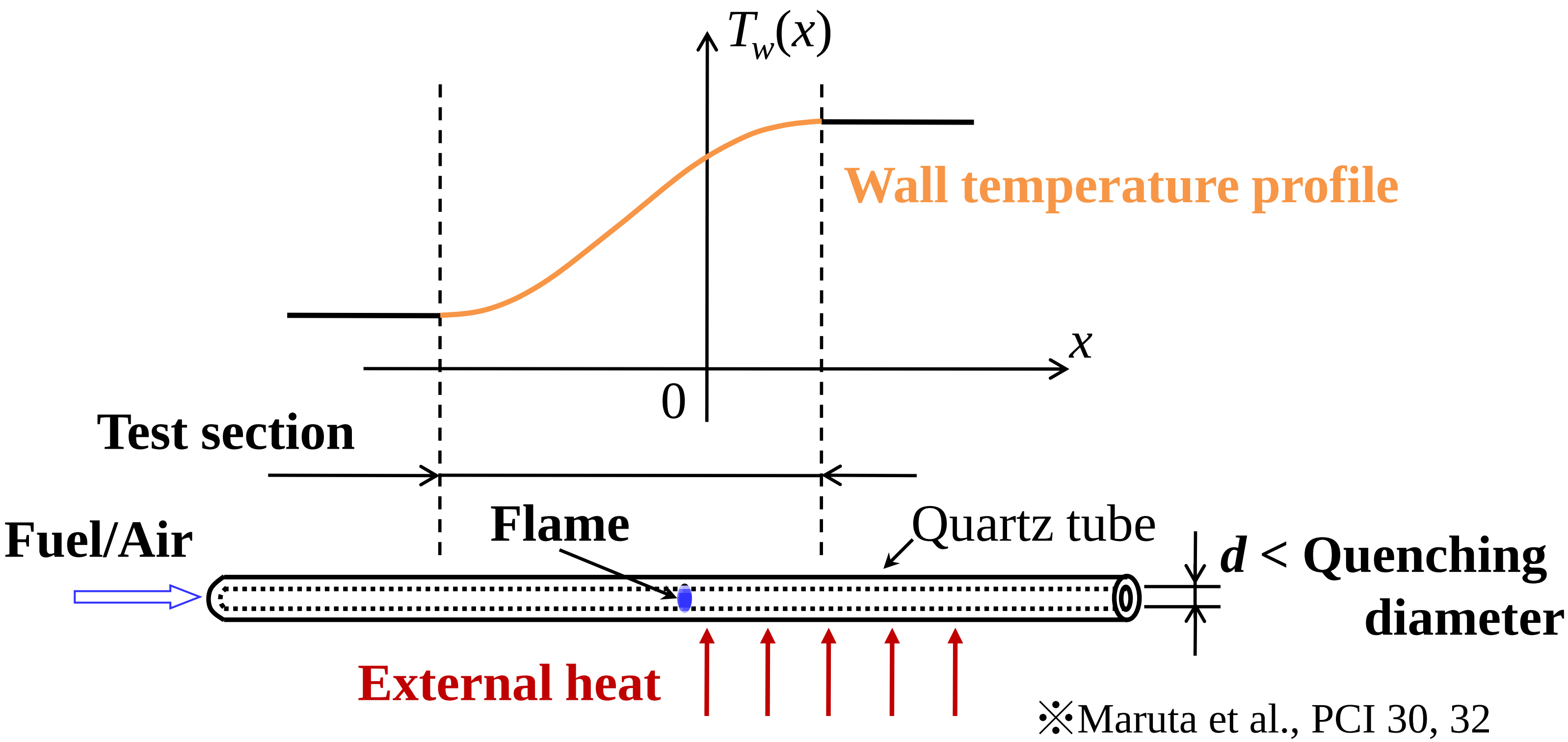
Difficulties in RCM experiments…

- Heat loss to chamber wall
- Roll-up vortices by piston motion
- Ignition in local spot → Propagation

⇒ Disparities with the modeling that assumes homogeneous combustion

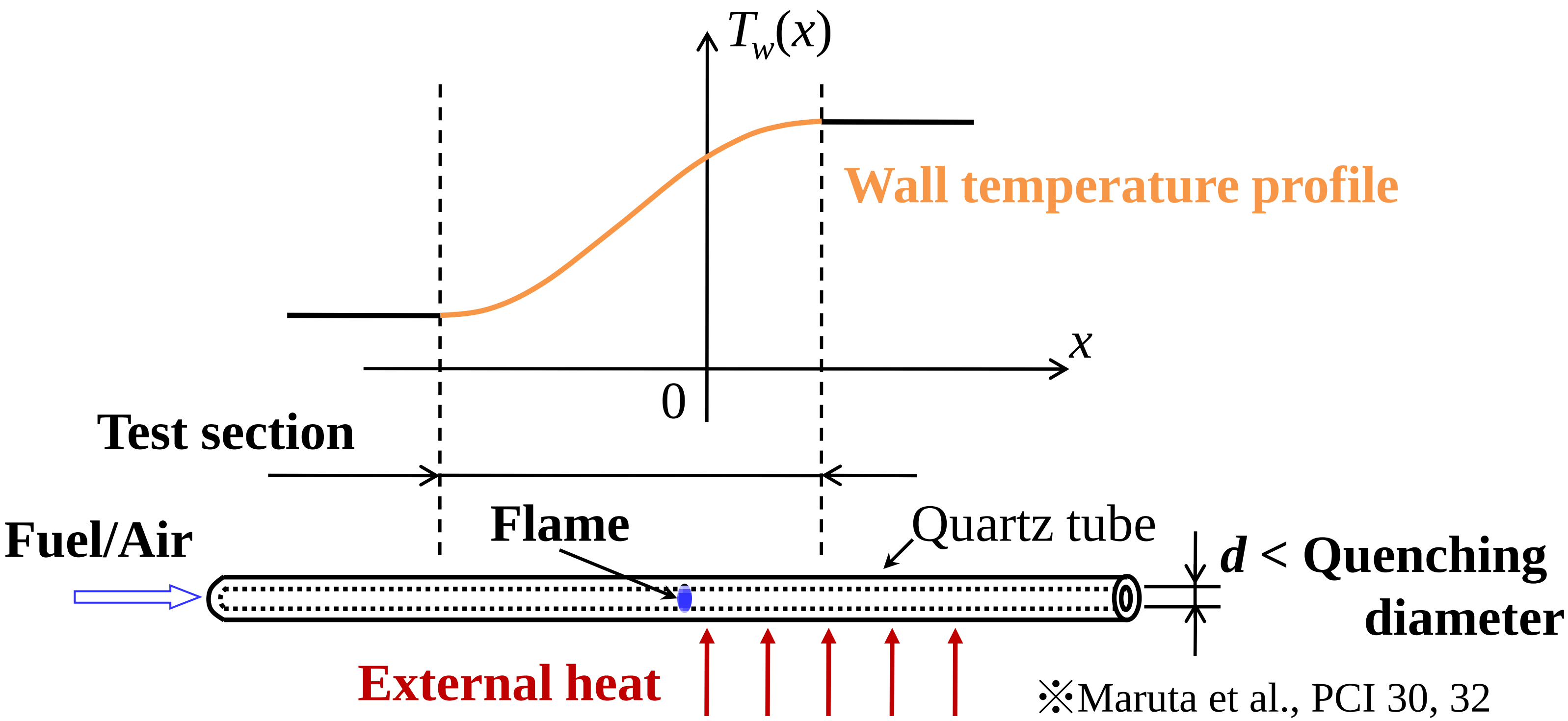
Multi-zone/dimensional model should be required to reproduce the experiments more accurately. But it needs higher computational cost.

Micro flow reactor with controlled temperature profile



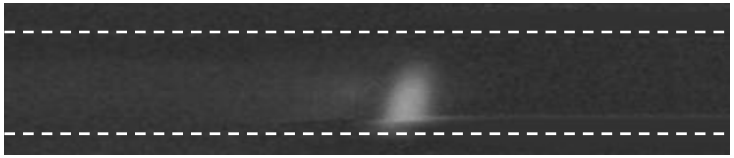
- Imposed wall-temperature profile in the flow direction
- Inner diameter of the tube < Ordinary quenching diameter
- Laminar flow ($Re \approx 1 \sim 100$)
- Constant pressure

Micro flow reactor with controlled temperature profile



※Maruta et al., PCI 30, 32

CH$_4$/air, 1atm, <u>U = 0.2 cm/s</u>
Tsuboi et al., PCI 32



At extremely low velocity ➡ Gas-phase temperature ≒ wall temperature

<u>Stable weak flames exist at certain positions in temperature profile.</u>

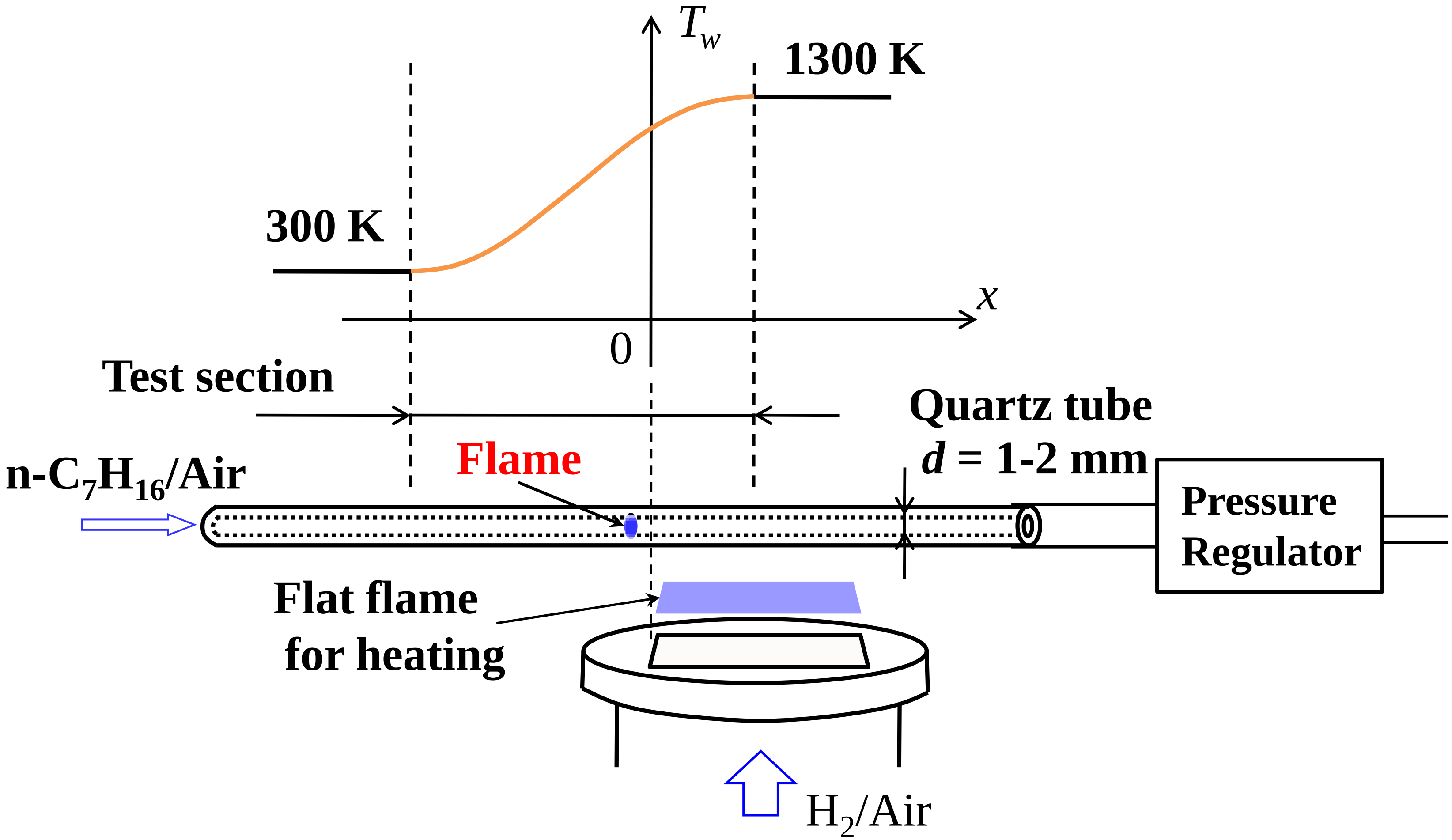
Objectives

n-Heptane ($n\text{-}C_7H_{16}$)

– A basic liquid hydrocarbon fuel that shows typical multi-stage ignition
– One of the primary reference fuel of automotive gasoline

Investigate ignition and combustion characteristics of gaseous n-heptane/air mixture using a micro flow reactor with a controlled temperature profile.

Experimental setup



- Stoichiometric gaseous n-heptane/air mixture, Pressure = 1-4 atm
- Flame images were taken by CH-filtered digital still camera
- Gas sampling analysis by GC

Computational method

Flame code PREMIX-based 1-D steady code

Gas-phase energy equation

$$\dot{M}\frac{dT}{dx}-\frac{1}{c_p}\frac{d}{dx}\left(\lambda A\frac{dT}{dx}\right)+\frac{A}{c_p}\sum_{k=1}^{K}\rho Y_k V_k c_{pk}\frac{dT}{dx}+\frac{A}{c_p}\sum_{k=1}^{K}\dot{\omega}_k h_k W_k \boxed{-\frac{A}{c_p}\frac{4\lambda Nu}{d^2}(T_w-T)}=0$$

Heat transfer with the wall

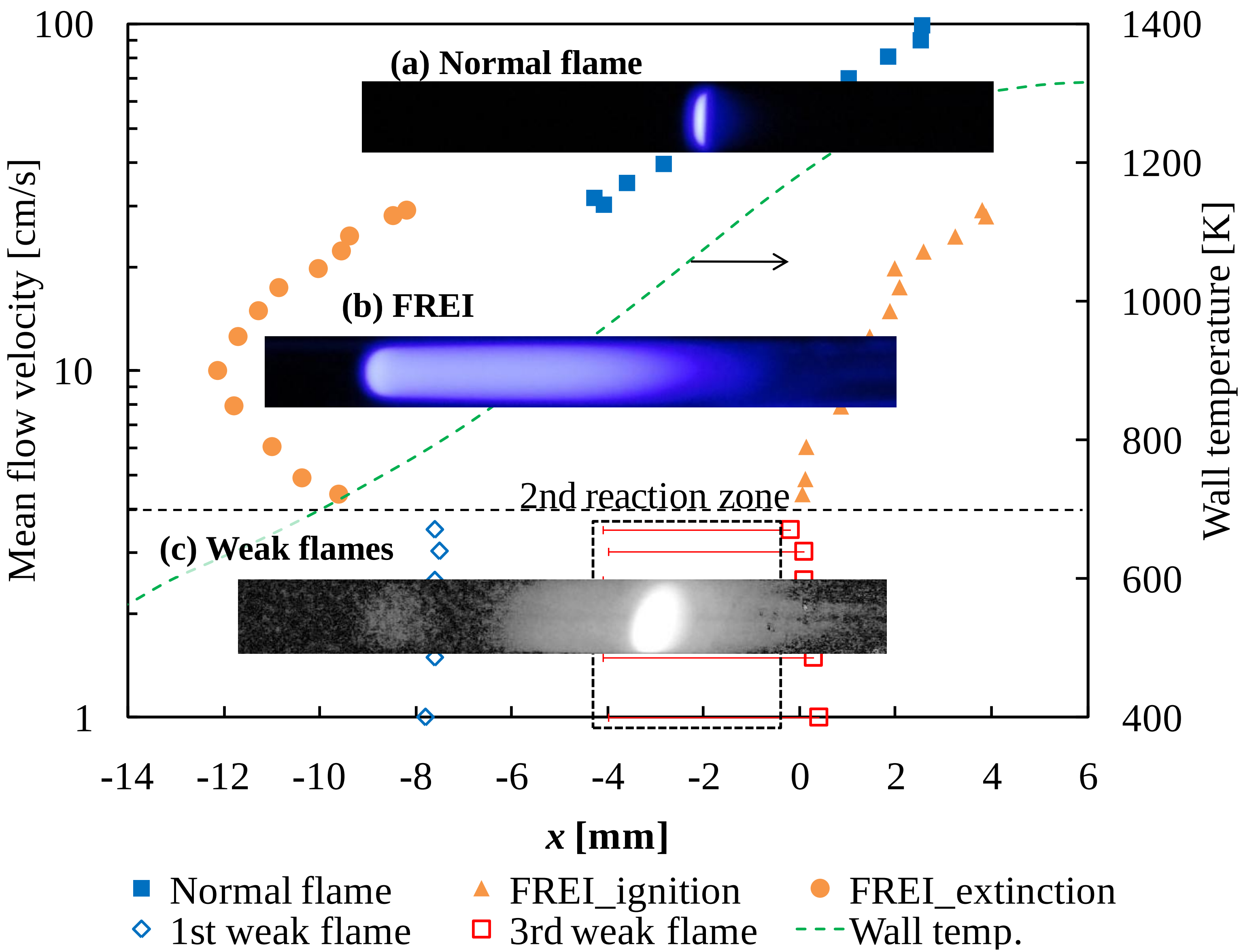
Reaction scheme n-Heptane, Reduced mechanism from LLNL (159 species, 1540 steps) ※Seiser et al., PCI 28 (2000)

Conditions
- Stoichiometric gaseous n-heptane/air mixture
- Experimentally measured wall-temperature profile as a boundary condition

Flame position Peaks in heat-release-rate (HRR) [W/cm^3] profile

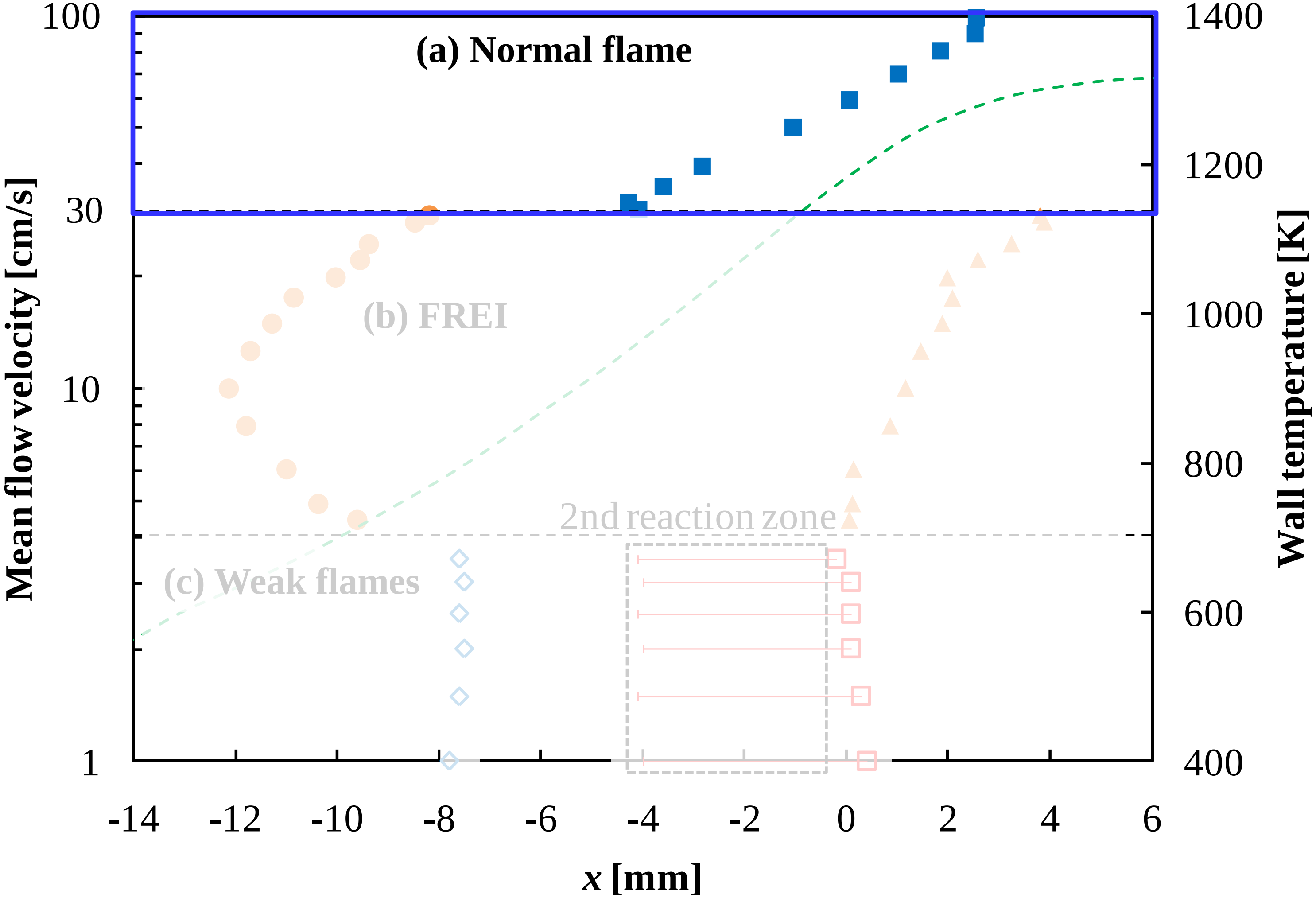
Combustion characteristics at atmospheric pressure

Experimental flame positions against various flow velocities



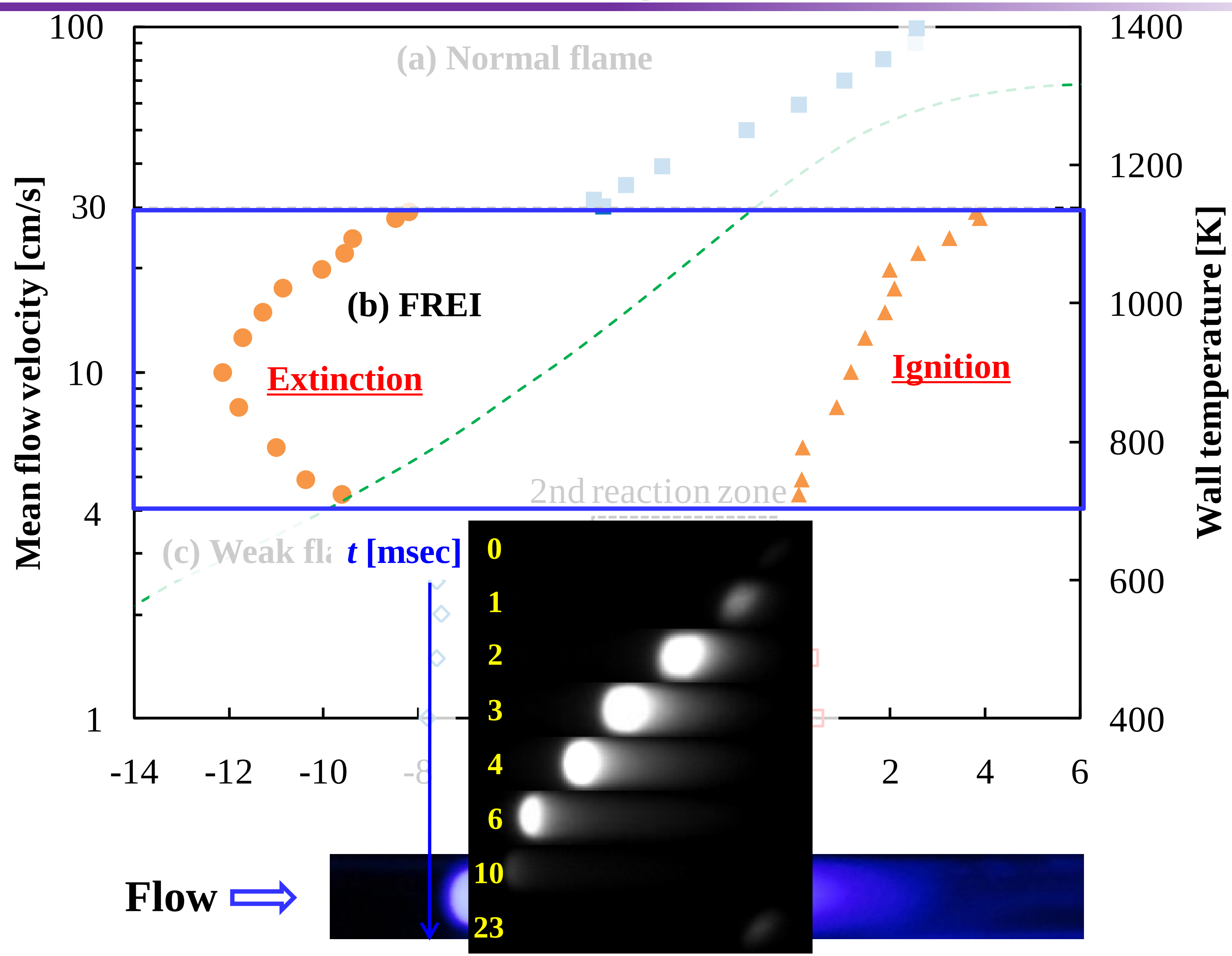
Three different flame responses were observed by changing inlet flow velocities.

Normal flame in high velocity condition



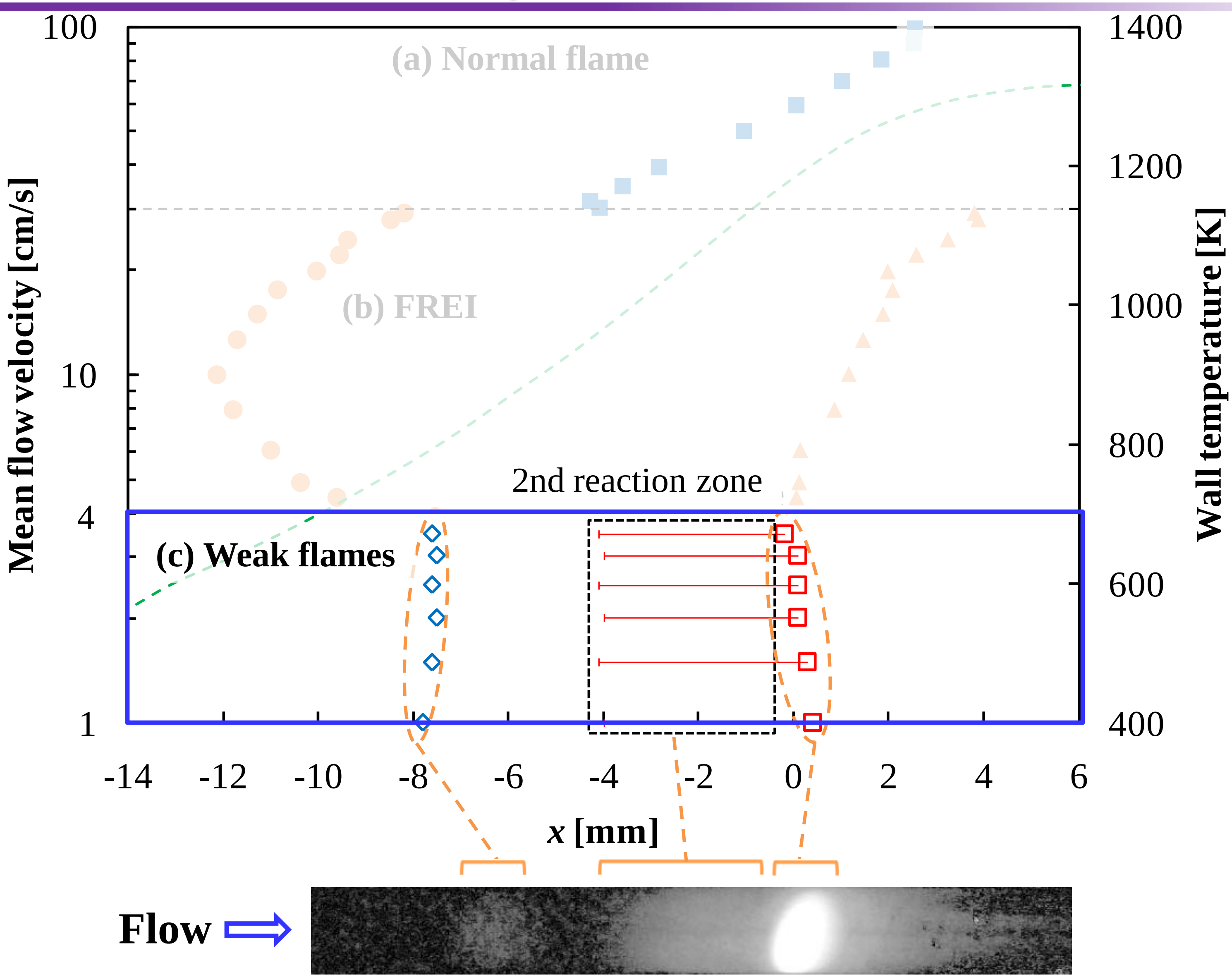
Normal flame Local mixture flow velocity = Flame propagating velocity

Unstable FREI in middle velocity condition



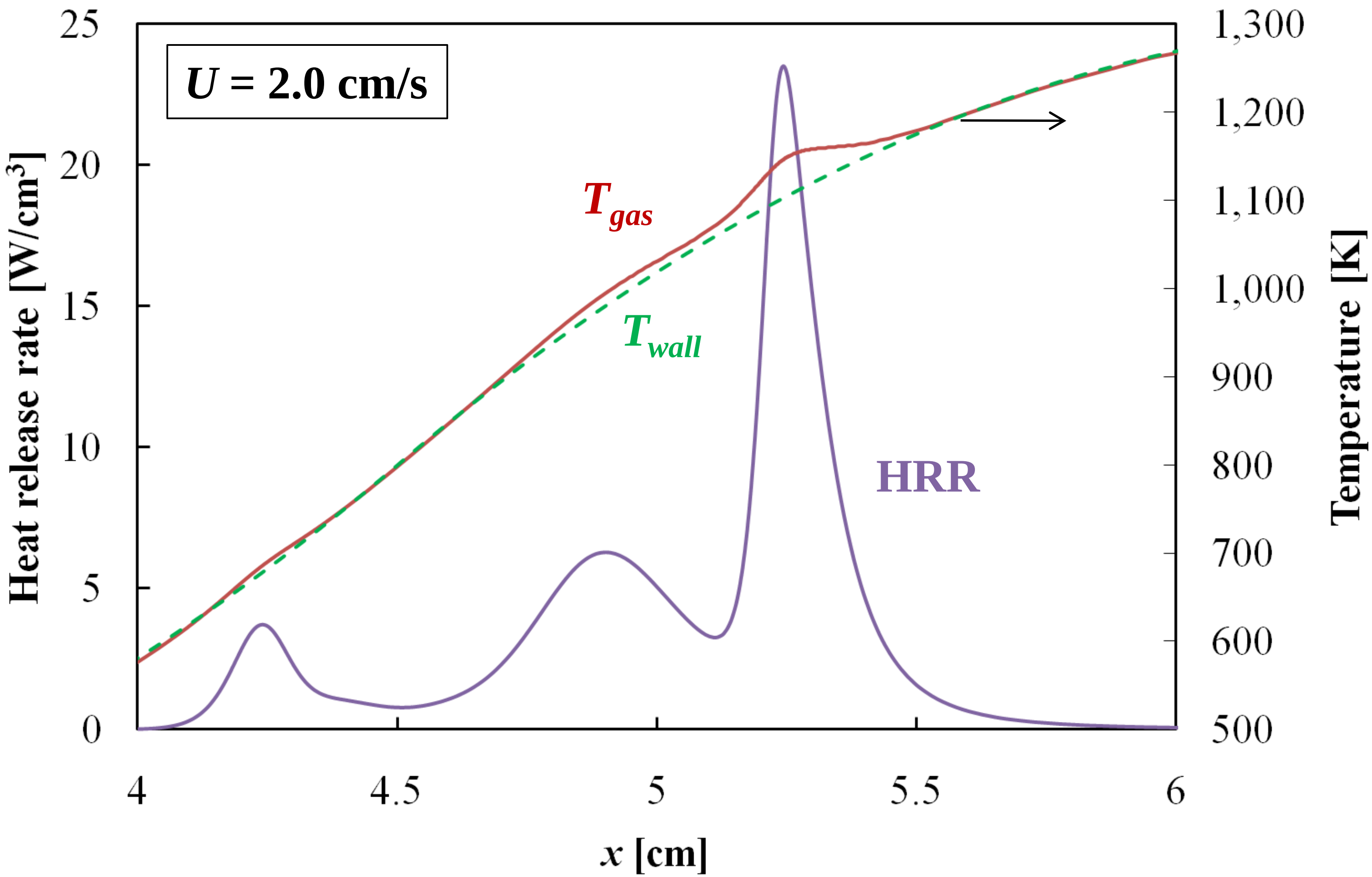
FREI Unstable Flames with Repetitive Extinction and Ignition

Weak flames in low velocity condition



Stable weak flames Three reaction zones in the flow direction

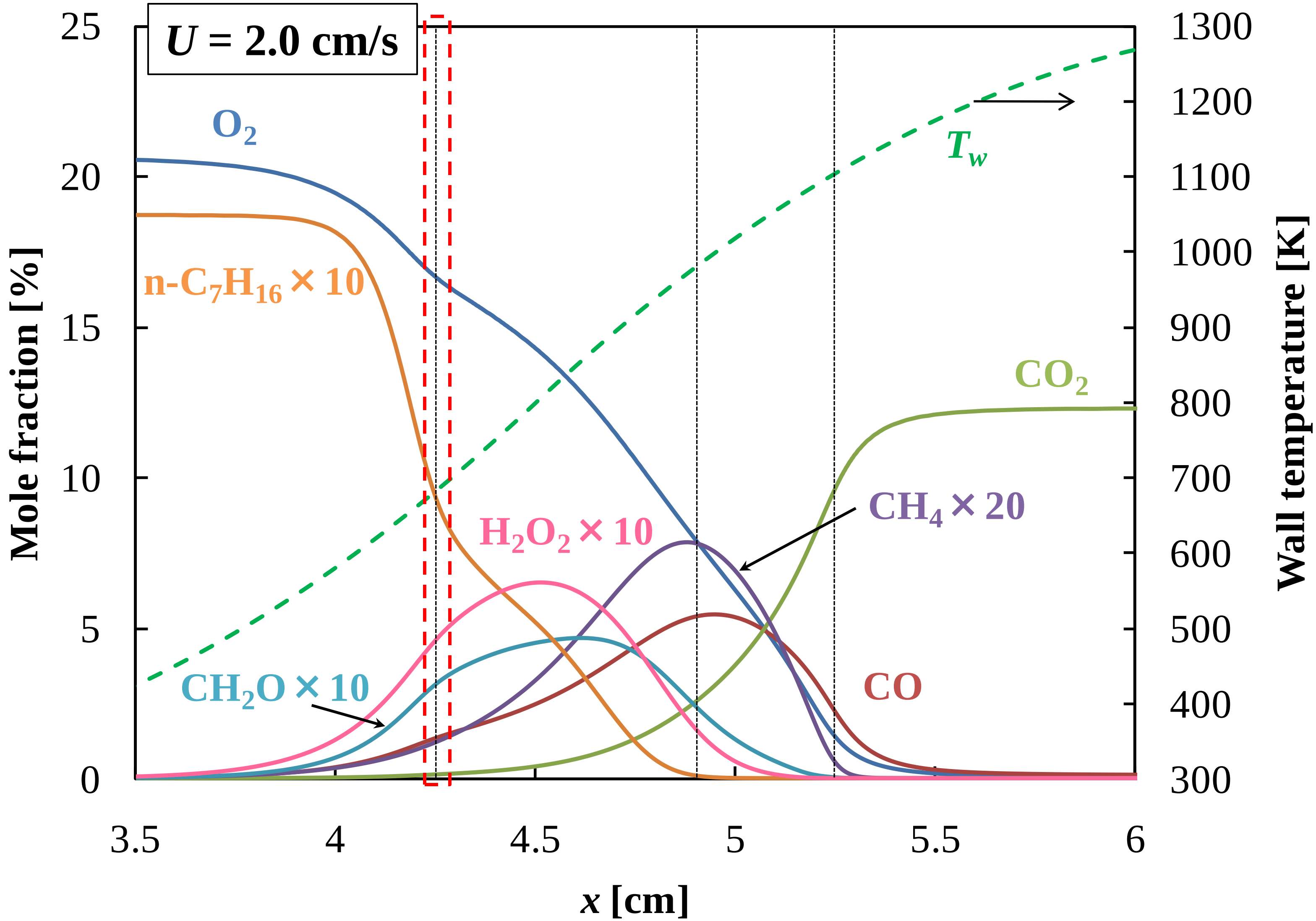
Computational profiles of T_g and HRR of weak flames



Three HRR peaks in the flow direction

➡ Observed three weak flames were reproduced.

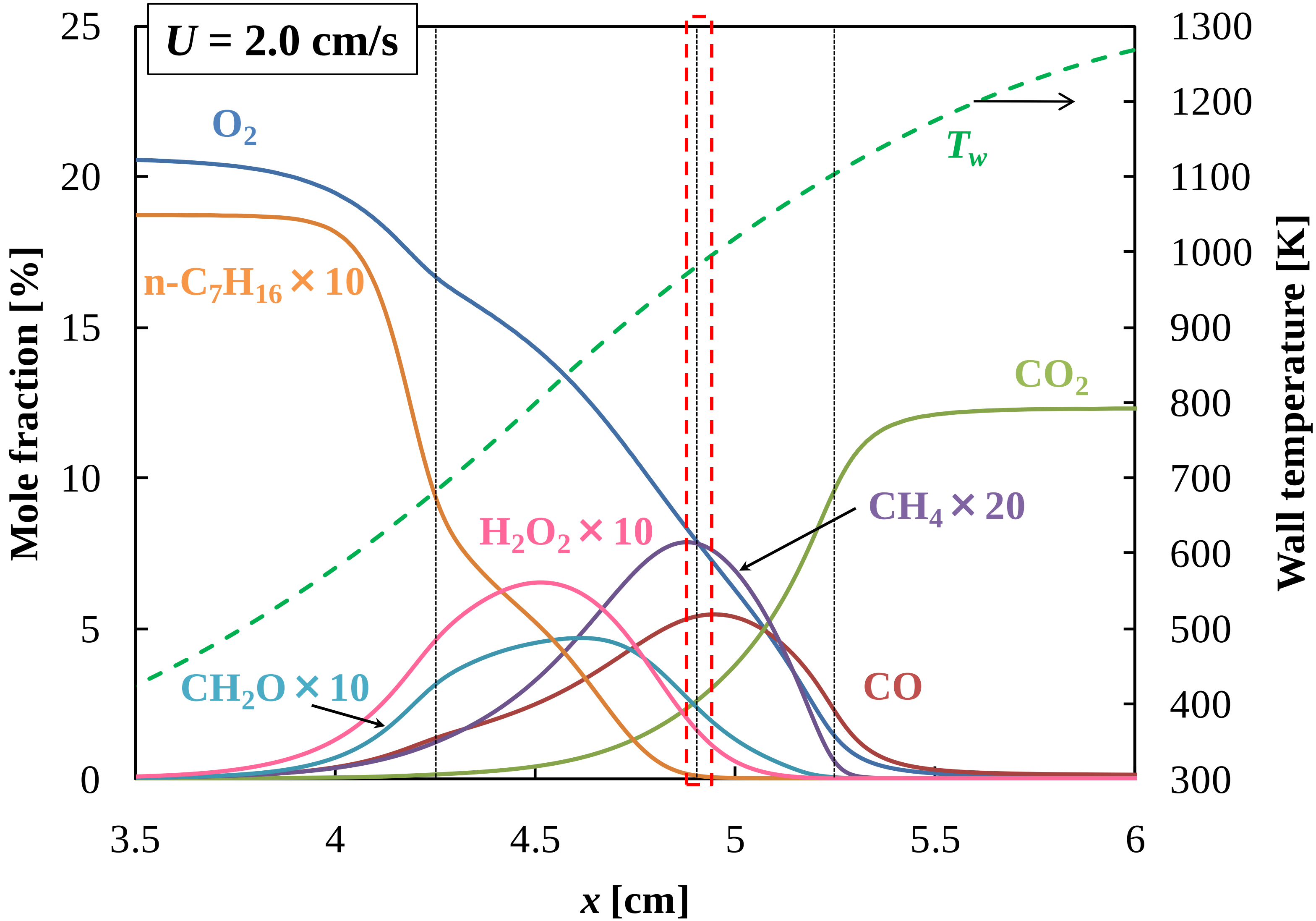
Computational species profiles -1st reaction-



Low temperature oxidation

Oxidation of fuel (n-C_7H_{16}) → Form CH_2O, H_2O_2, CO, CH_4 etc.

Computational species profiles -2nd reaction-



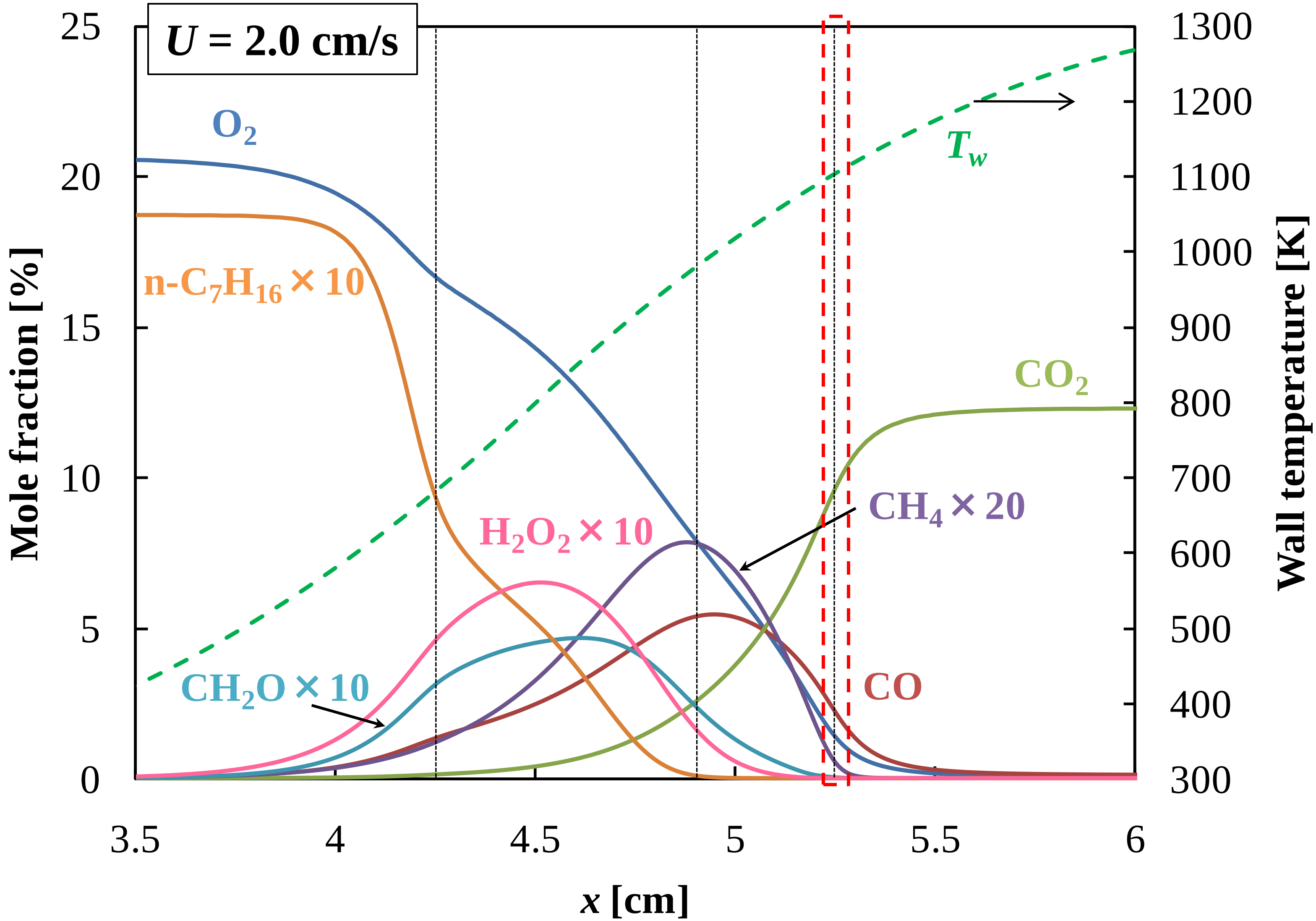
<u>H_2O_2 decomposition</u>

H_2O_2 (+M) ⇒ 2OH (+M)

CH_2O + OH ⇒ <u>HCO</u> + H_2O

<u>HCO</u> + O_2 ⇒ CO + HO_2

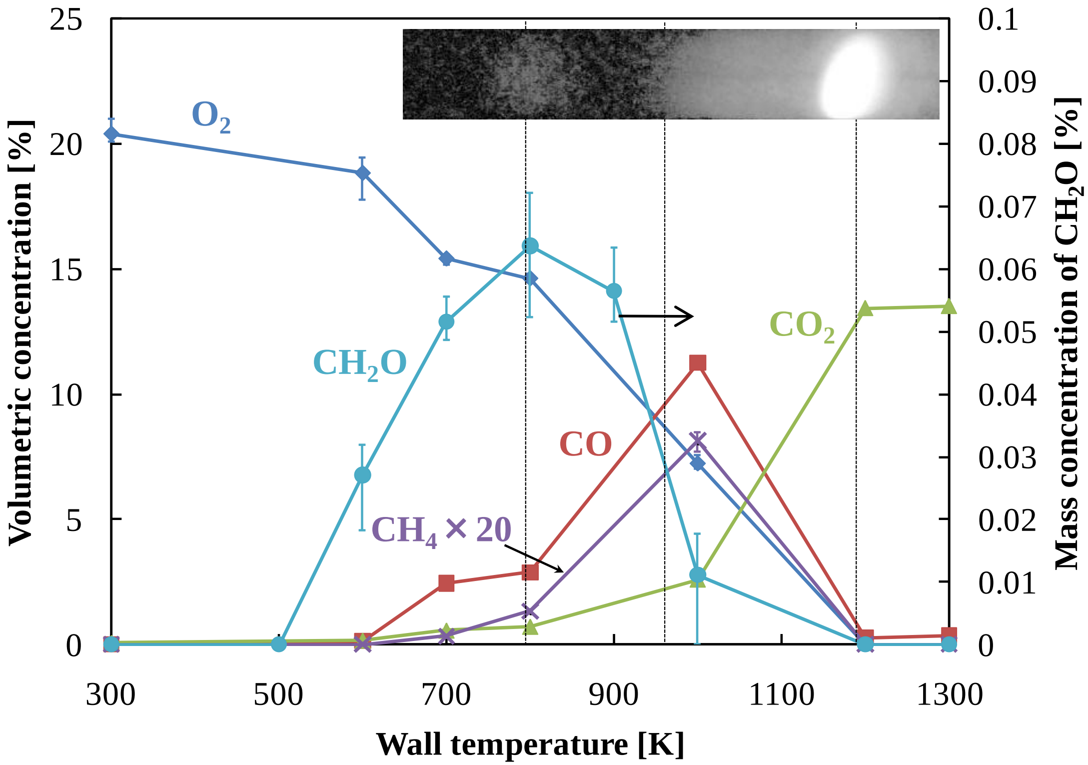
Computational species profiles -3rd reaction-



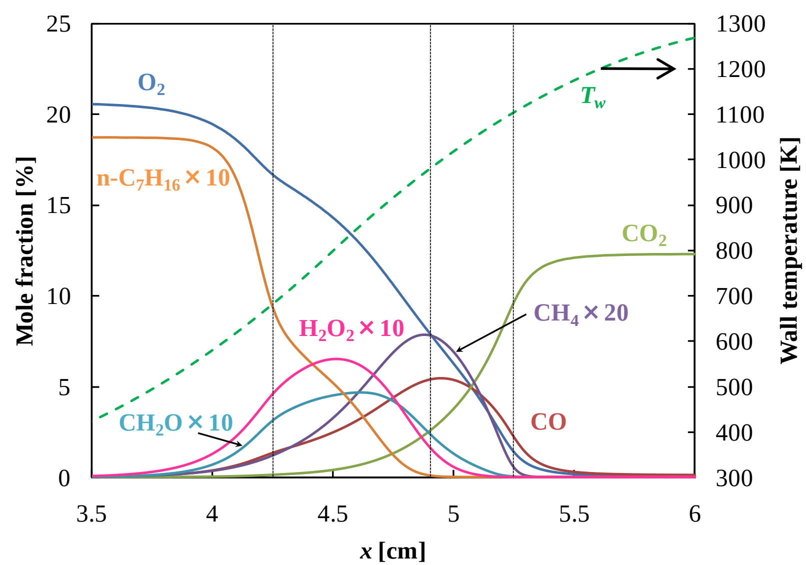
<u>Oxidation of CH_4 & CO to CO_2:</u> $CO + OH \Rightarrow CO_2 + H$

Comparison of experimental & computational species profiles

Measurement with GC (U = 2.0 cm/s)



Computation (U = 2.0 cm/s)

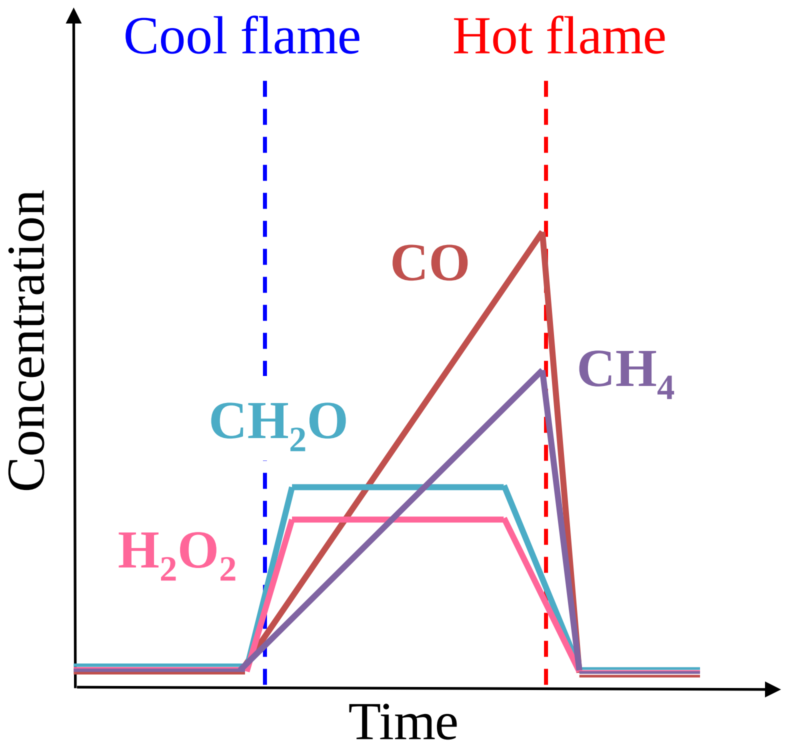


Three-stage oxidation process was experimentally confirmed by gas sampling analysis with GC.

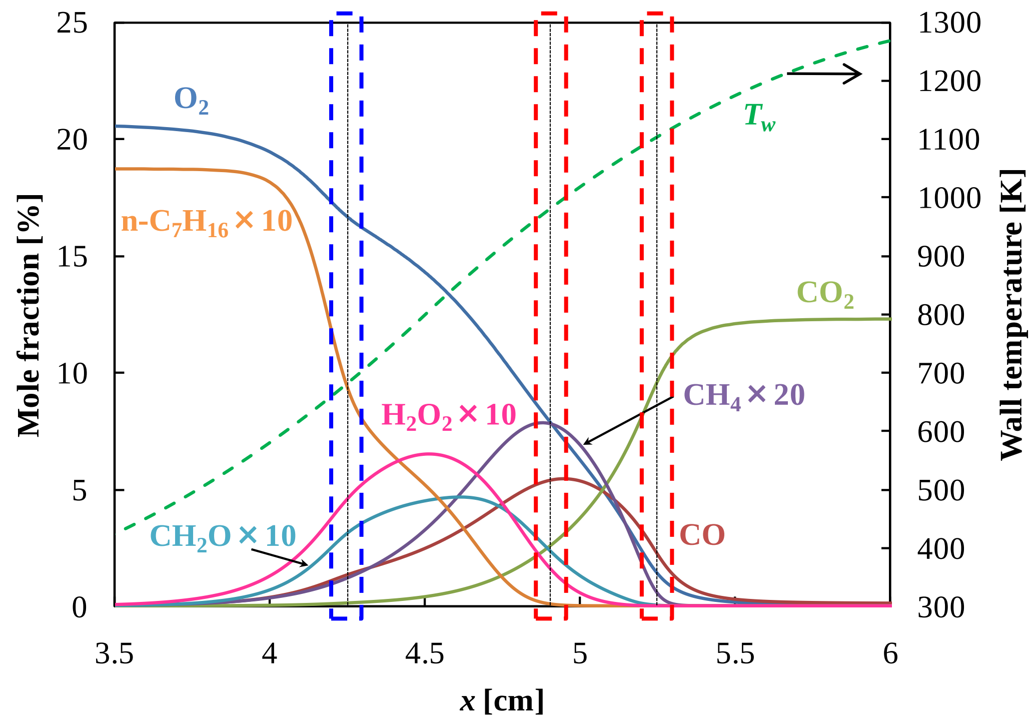
Profile of each species qualitatively agreed well.

Interpretation of the three-stage oxidation

Typical two-stage oxidation



Present three-stage oxidation



From the species profiles…

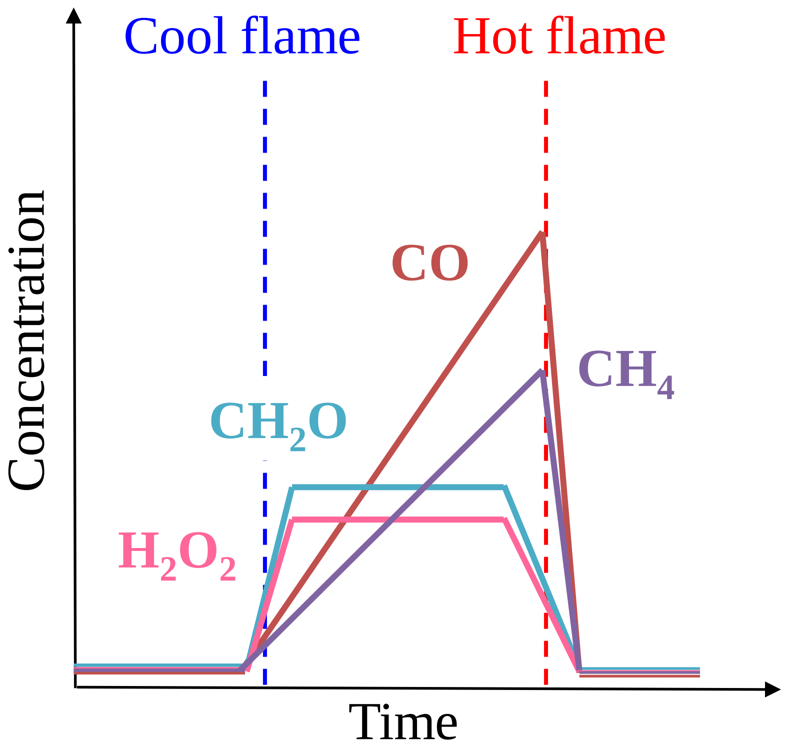
Typical two-stage oxidation: Cool flame + Hot flame

Present three-stage oxidation: Cool flame + Separated hot flames

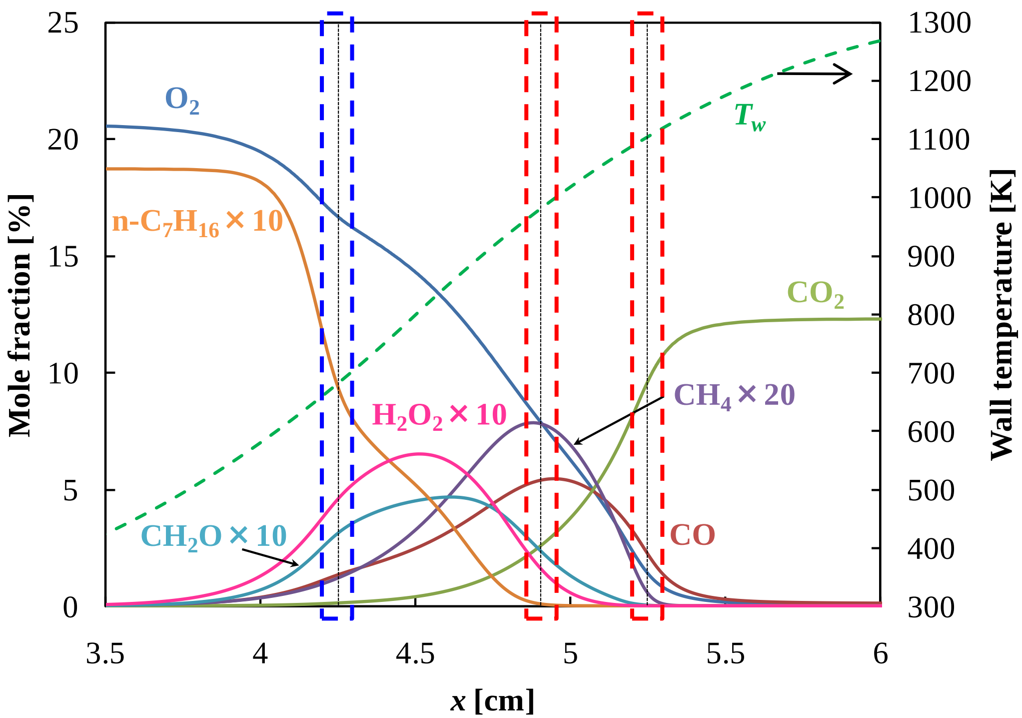
(Blue flame & Hot flame)

Interpretation of the three-stage oxidation

Typical two-stage oxidation



Present three-stage oxidation



Ordinary approach

Strongly transient ignition

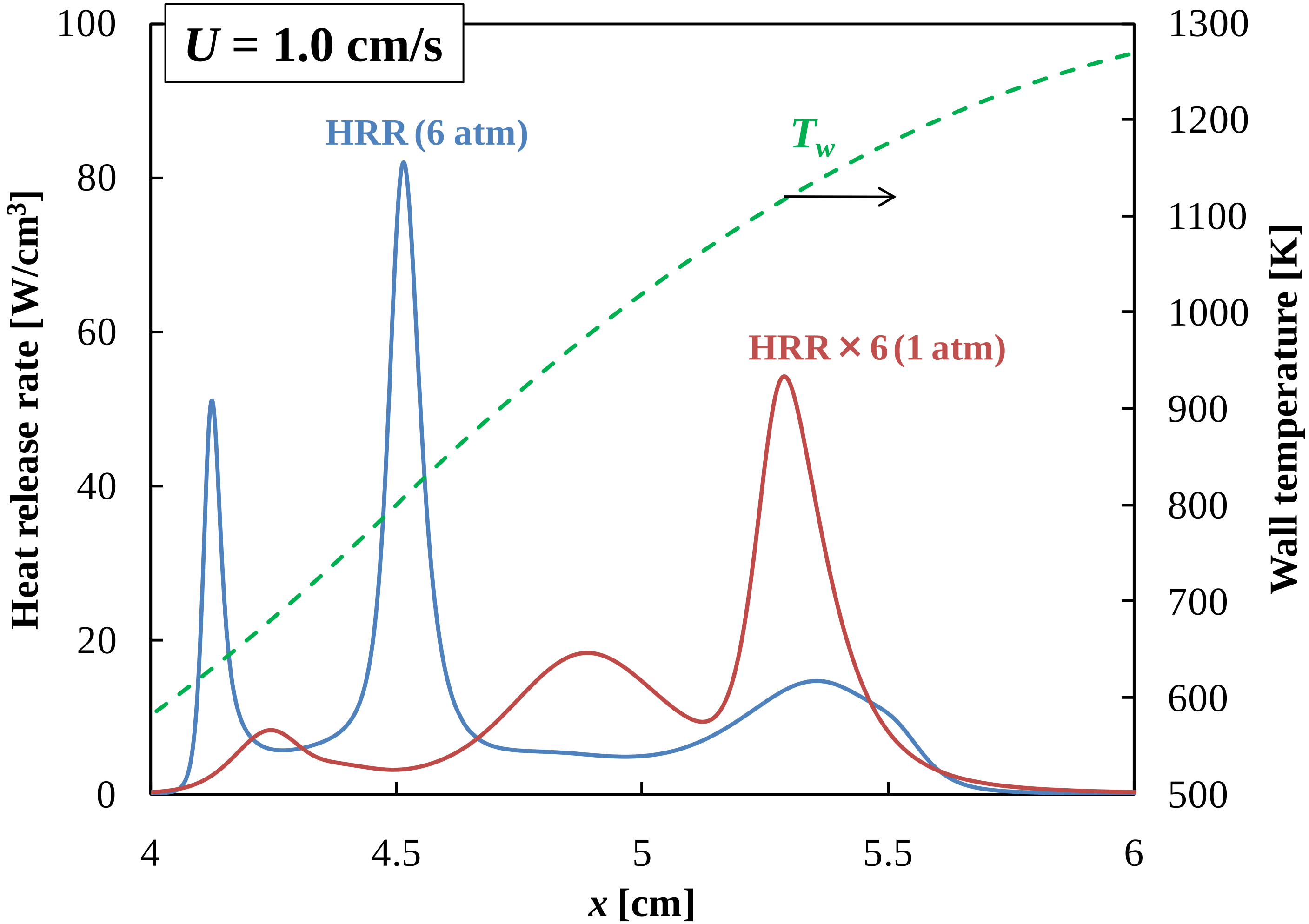
Micro flow reactor

Stabilized spatial profile

Micro flow reactor can contribute to chemical kinetic studies.

Pressure dependence of three-stage oxidation

Pressure dependence of HRR profile (Computation)

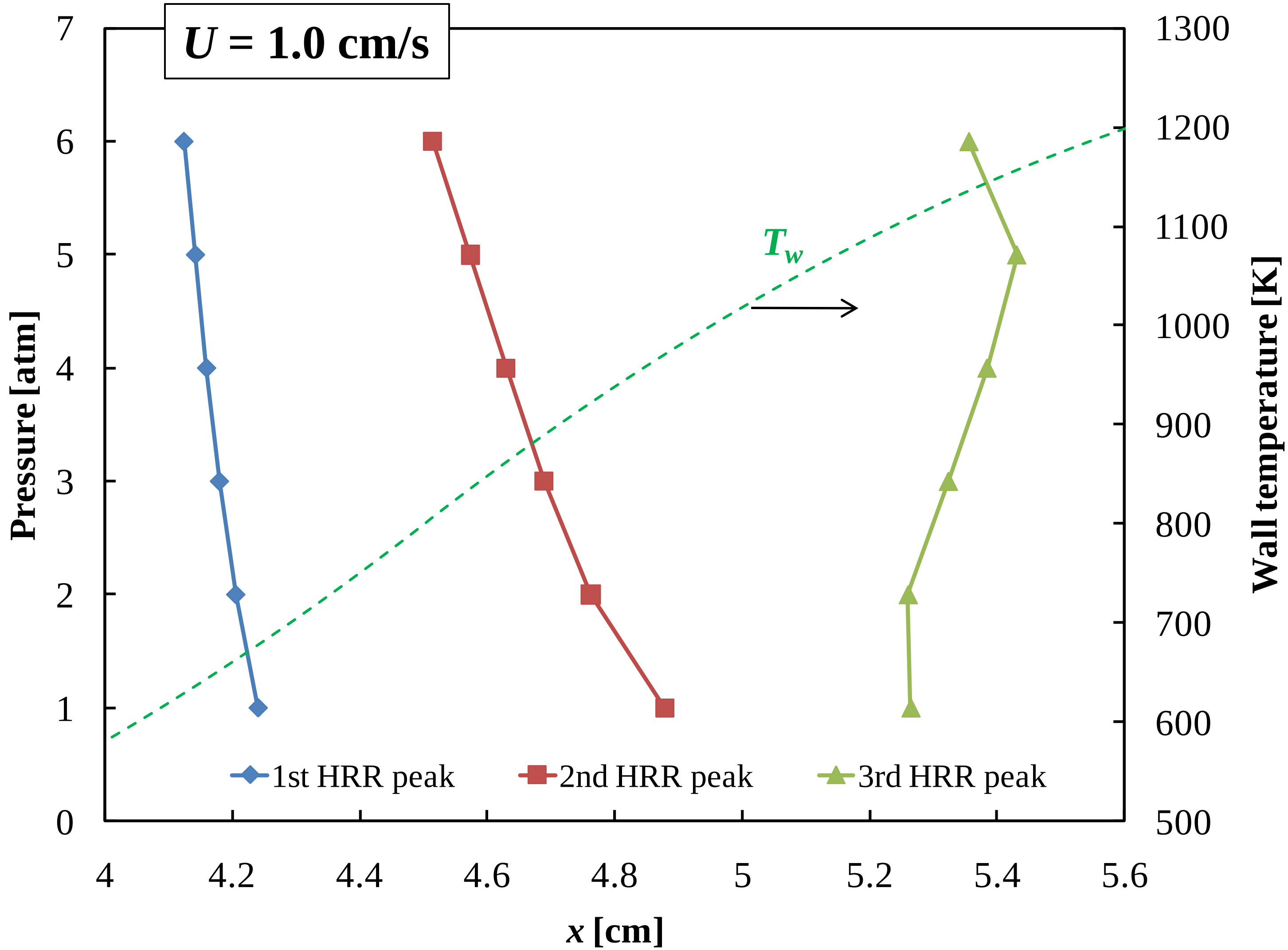


1 atm: 3rd HRR peak is the strongest.

→ 6 atm: 1st and 2nd HRR peaks are stronger than 3rd peak.

Main heat release shift to the lower temperature side at high pressure.

Pressure dependence of HRR peak positions (Computation)



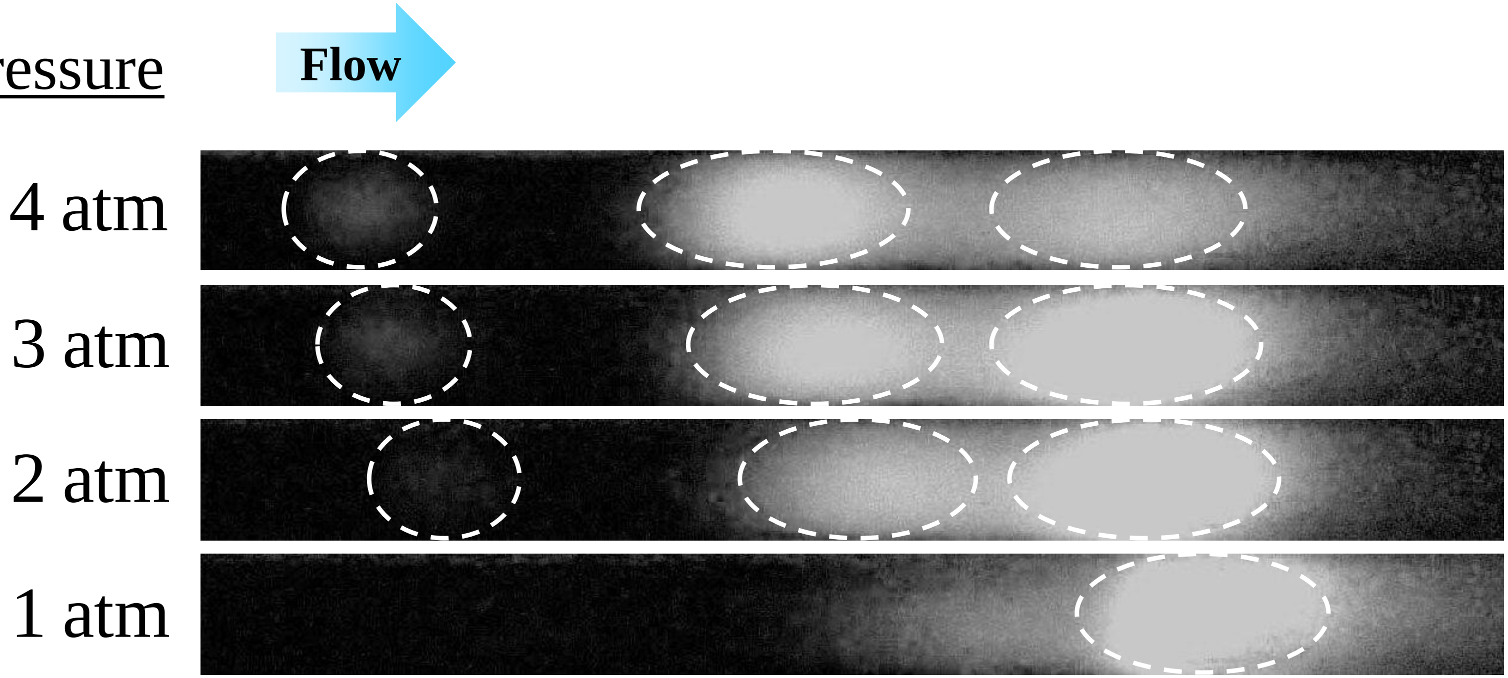
Increase of pressure →

- 1st & 2nd peak shift to lower temperature side.
- 3rd peak shifts to higher temperature side at 2-5 atm.

Weak flame images at high pressures

***U* = 3.0 cm/s, *d* = 1 mm**

Pressure



As increasing pressure from 1 to 4 atm…

- 1st and 2nd flames become strong, 3rd flame becomes weakened.
- 2nd and 3rd flames are clearly separated.

Low and middle temperature reactions affect the whole ignition process more significantly at higher pressure conditon.

Conclusions

Ignition and combustion characteristics of a gaseous n-heptane/air mixture were examined using a micro flow reactor with a controlled temperature profile.

- Three different flame responses were observed by changing an inlet mean flow velocity. Especially at the low velocity condition, three reaction zones were observed in the flow direction.

- Three peaks of heat release rate in the flow direction were obtained in the computation. Computational species concentration profiles agreed well with the results of gas sampling analysis.

- Under the high pressure condition, 1st and 2nd flames become stronger, and 3rd flame becomes weakened. This indicates that low and middle temperature reactions affect the whole ignition process more significantly at higher pressure condition.

Thank you for your kind attention!