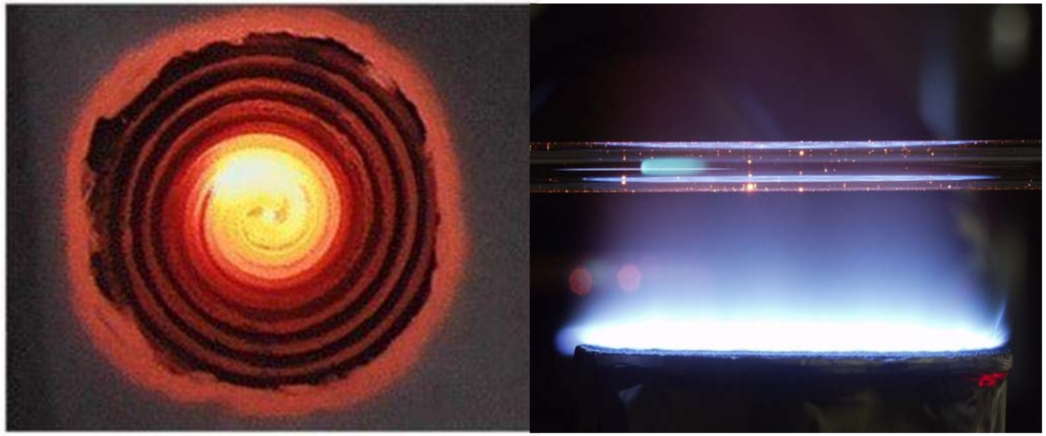
The First International Workshop on Flame Chemistry, July 28 - 29, 2012, Warsaw, Poland



Micro flow reactor with prescribed temperature profile

Toward fuel Indexing and kinetics study based on multiple weak flames

Kaoru Maruta, Tohoku Univ.

S. Minaev, N.I. Kim, T. Yokomori, H. Nakamura, S. Hasegawa, T. Tezuka
T. Kataoka, Y. Tsuboi, H. Oshibe, A. Yamamoto, R. Tanimoto, M. Hori,
K. Saruwatari, S. Suzuki, T. Kamada, X. Li, Y. Kizaki, T. Onishi and H. Takahashi

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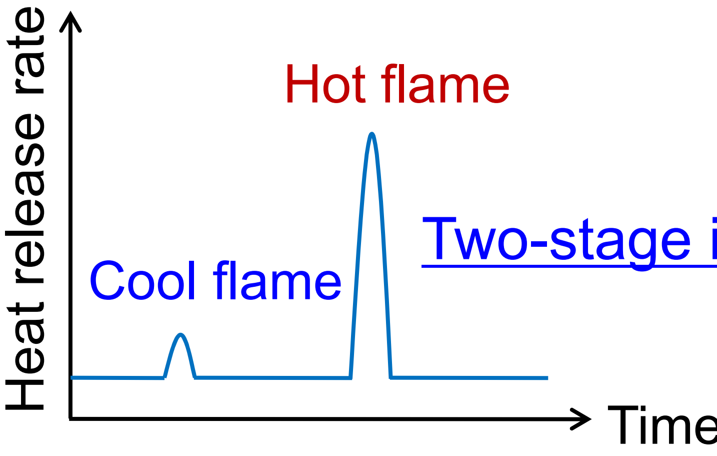
Background and objectives

For understandings ignition and combustion characteristics of practical fuels…

Data from
Shock tube and RCM
have been extensively used

Ignition delay



Micro flow reactor with prescribed temperature profile

Single or multiple weak flames

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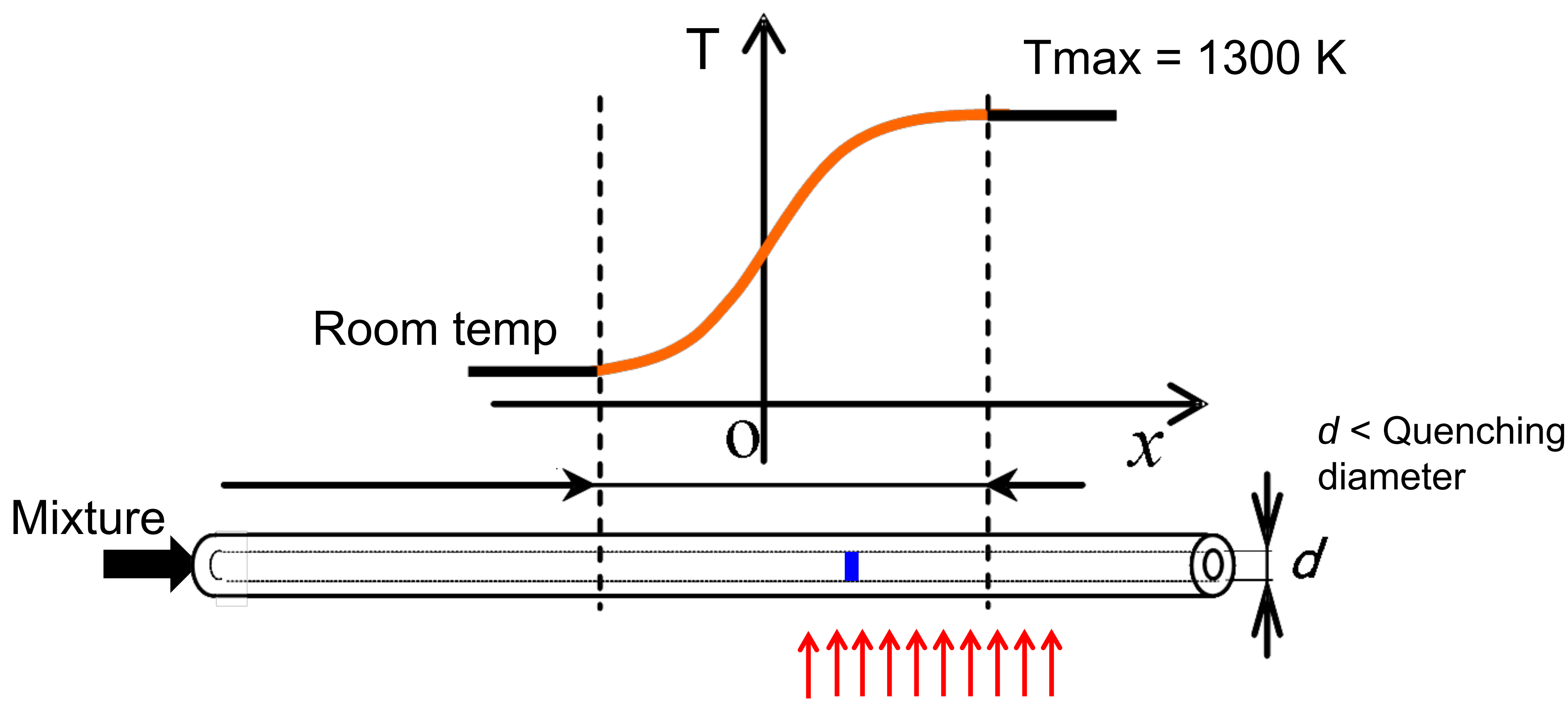
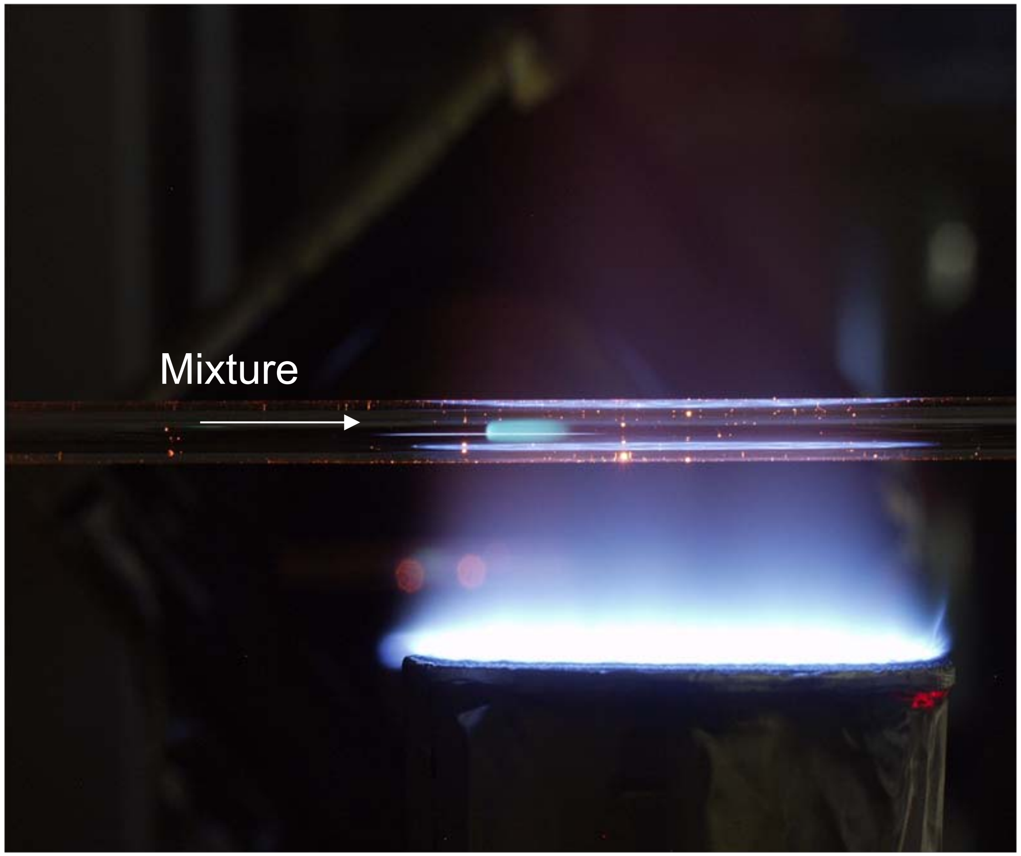
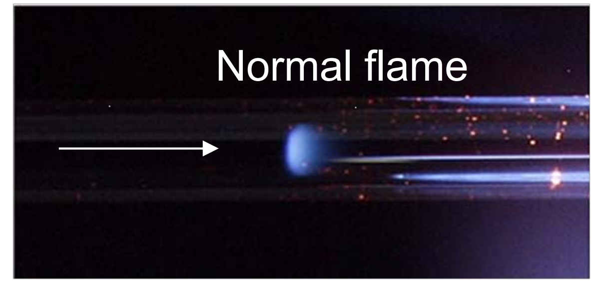
Micro flow reactor with prescribed temperature profile



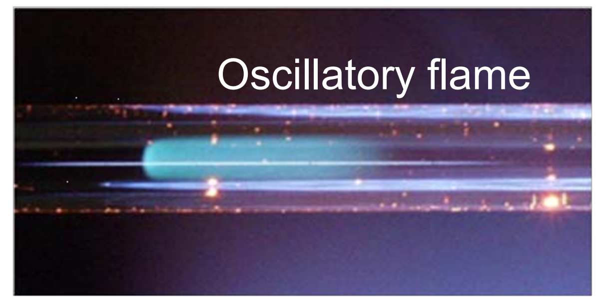
Stationary wall-temperature profile by an external heat source
Inner diameter of the tube < conventional quenching diameter
Gas phase temperature governed by wall temperature profile
Laminar flow and constant pressure

Flame behaviors in a micro flow reactor with a prescribed temperature profile

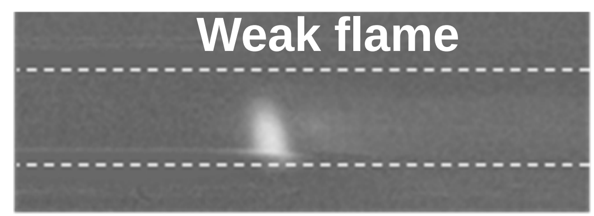




High velocity region



Intermediate velocity region



Low velocity region

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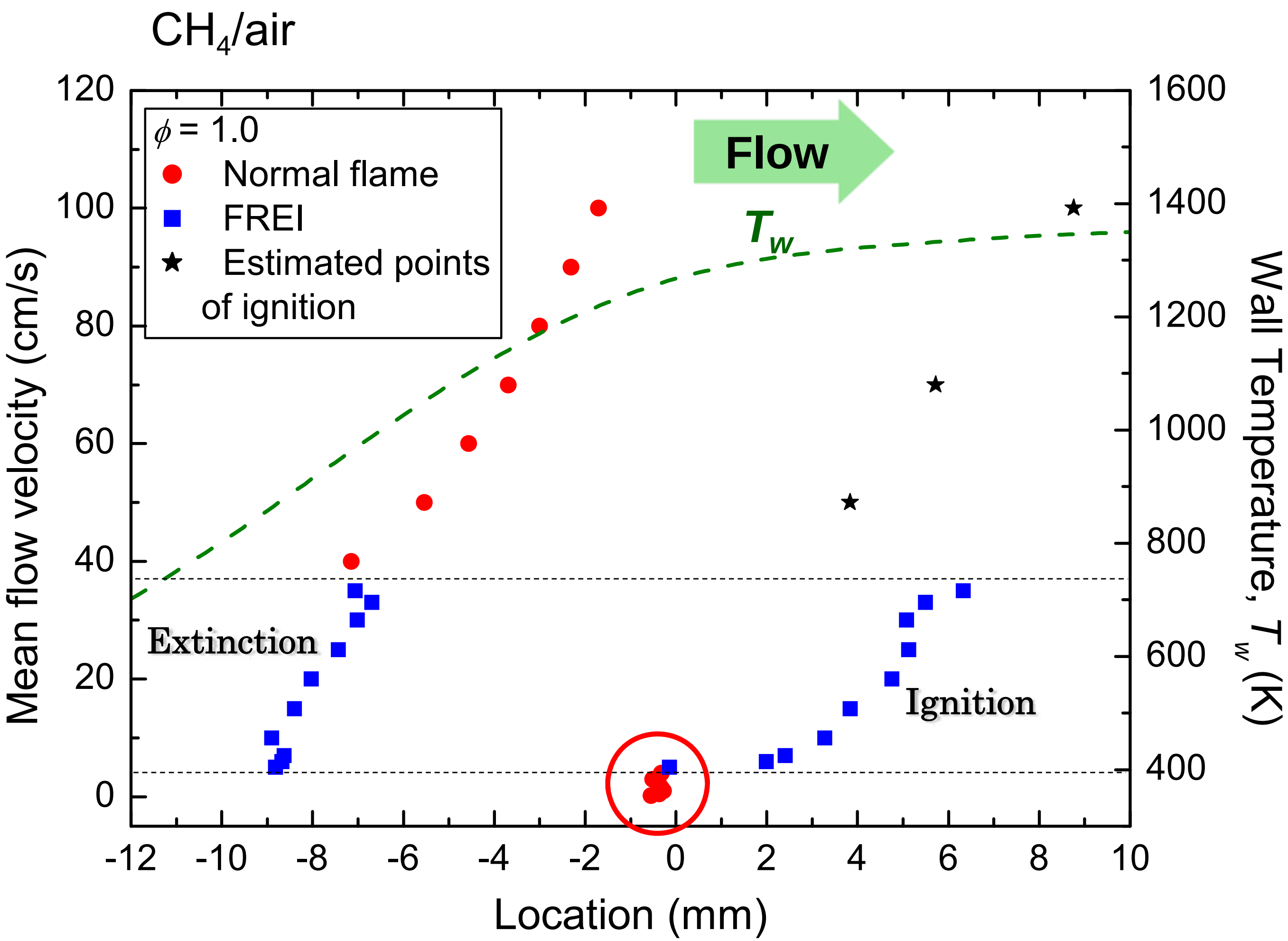
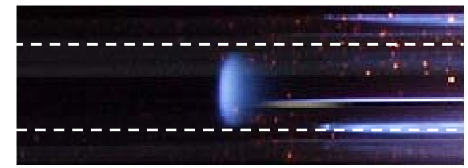
Three kinds of flame responses

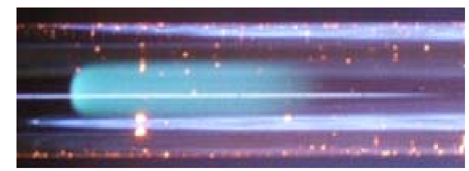


(1) Normal flame



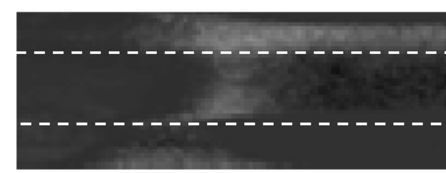
V=50cm/s

(2) Oscillatory flame



V=20cm/s

(3) Weak flame

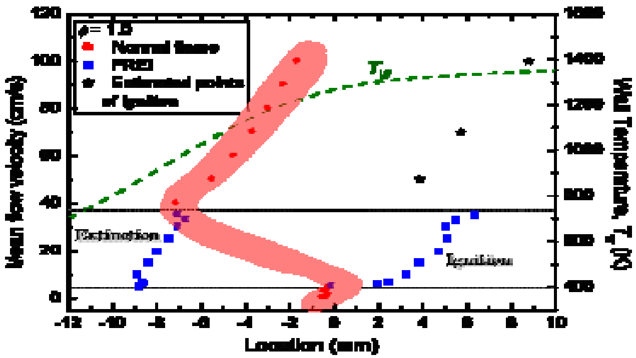


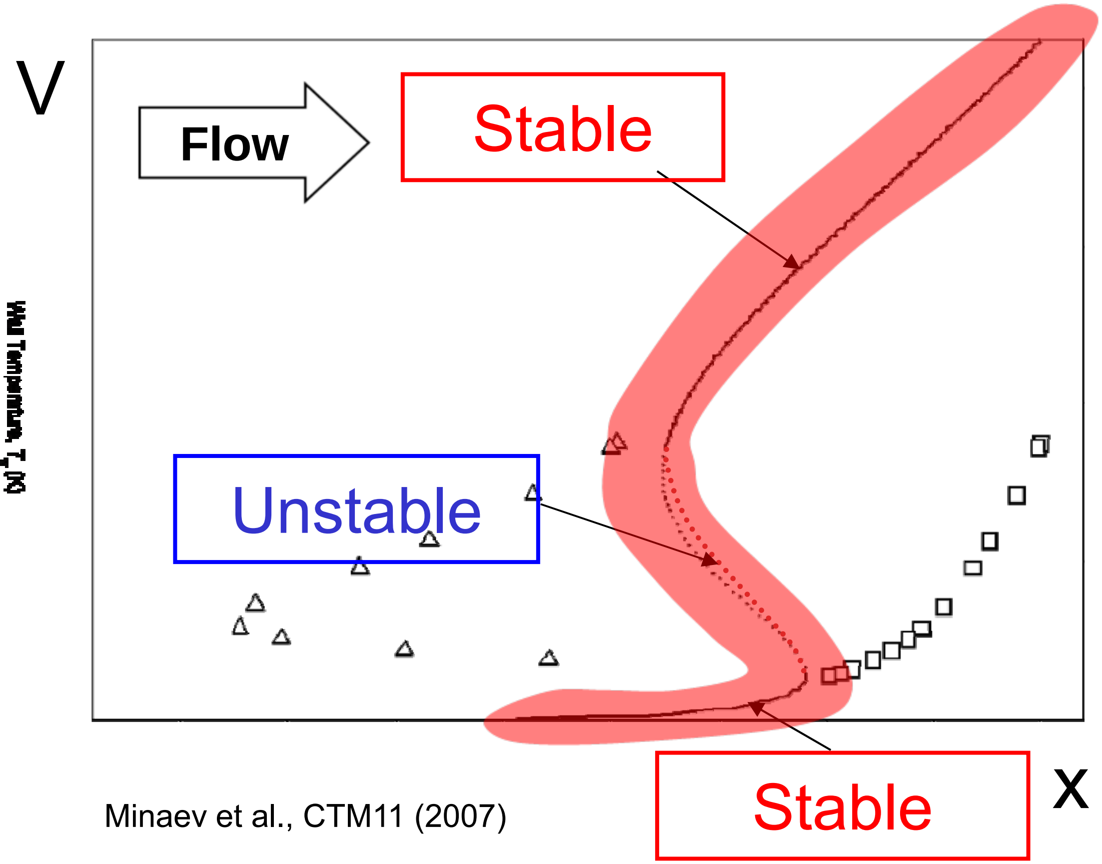
V=0.2cm/s

Normal flame, oscillatory flame, weak flame

Maruta et al., PCI30 (2005)

Theoretical S-shaped response

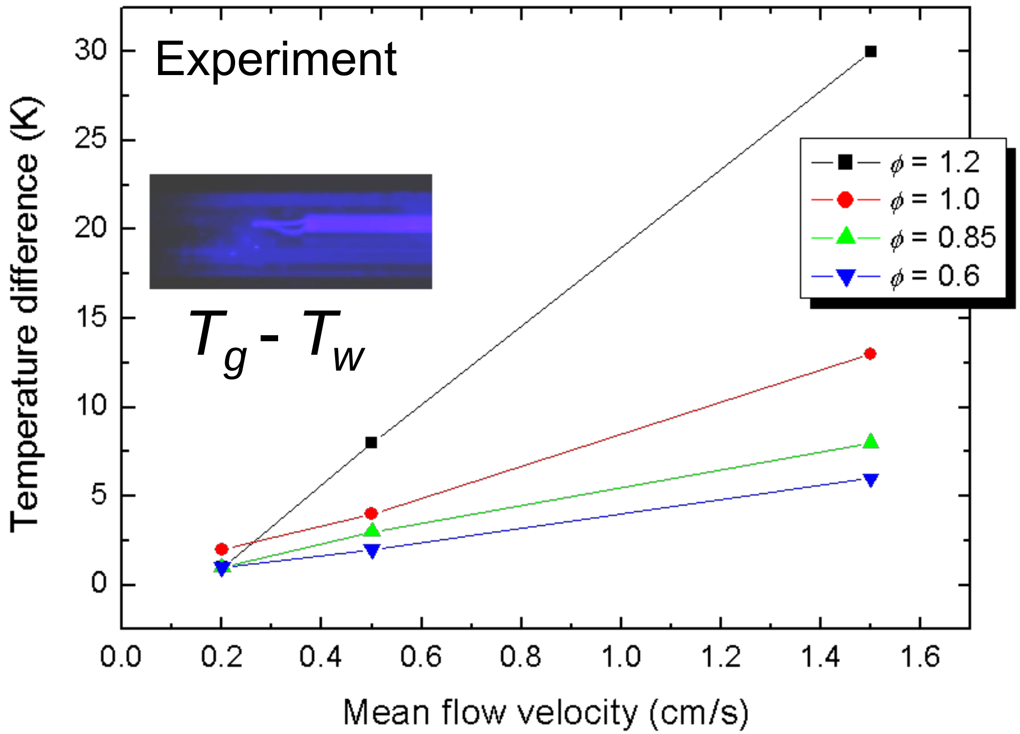




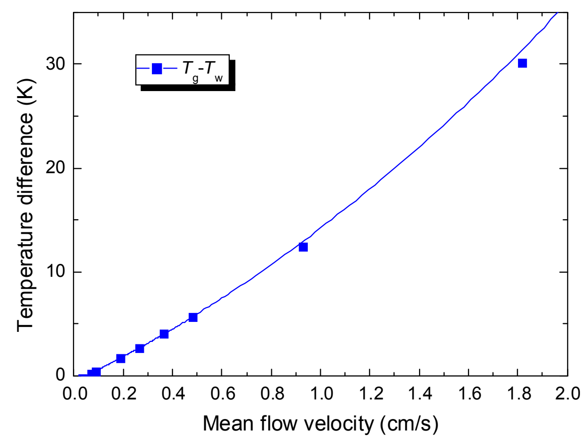
Minaev et al., CTM11 (2007)

Two stable and one unstable solutions predicted theoretically →
Weak flame corresponds to ignition branch

Lower limit of weak flames identified



Computation



At V = 0.2 cm/s, T_w = 1225 K, T_g-T_w< 2 K for CH_4/air mixture

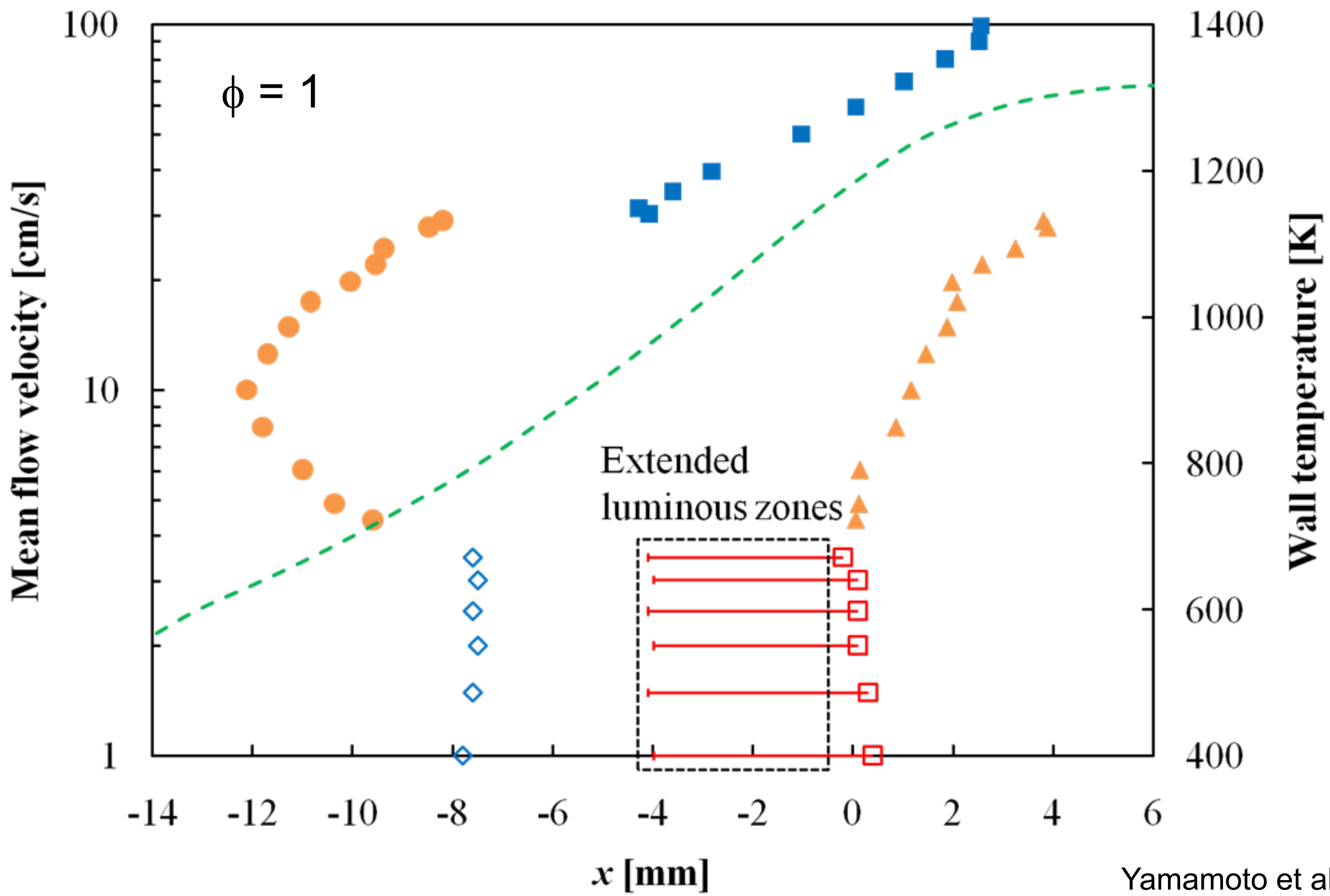
Extremely small temperature increase near lower limit

Flame position close to the ignition limit

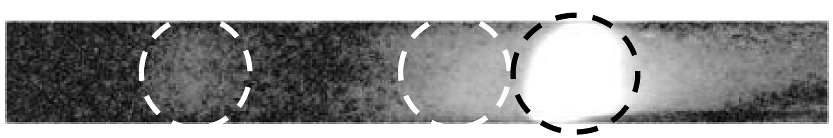
Weak flame location → Ignition temperature

Tsuboi et al., PCI32 (2009)

Triple weak flames, n-heptane



Yamamoto et al., PCI33 (2011)



U = 3 cm/s

Triple stationary weak flames observed
Weak flame location (temp.) insensitive to flow velocity

Computations (one-dimensional plug flow)

Code PREMIX with small modification

Gas-phase energy equation

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

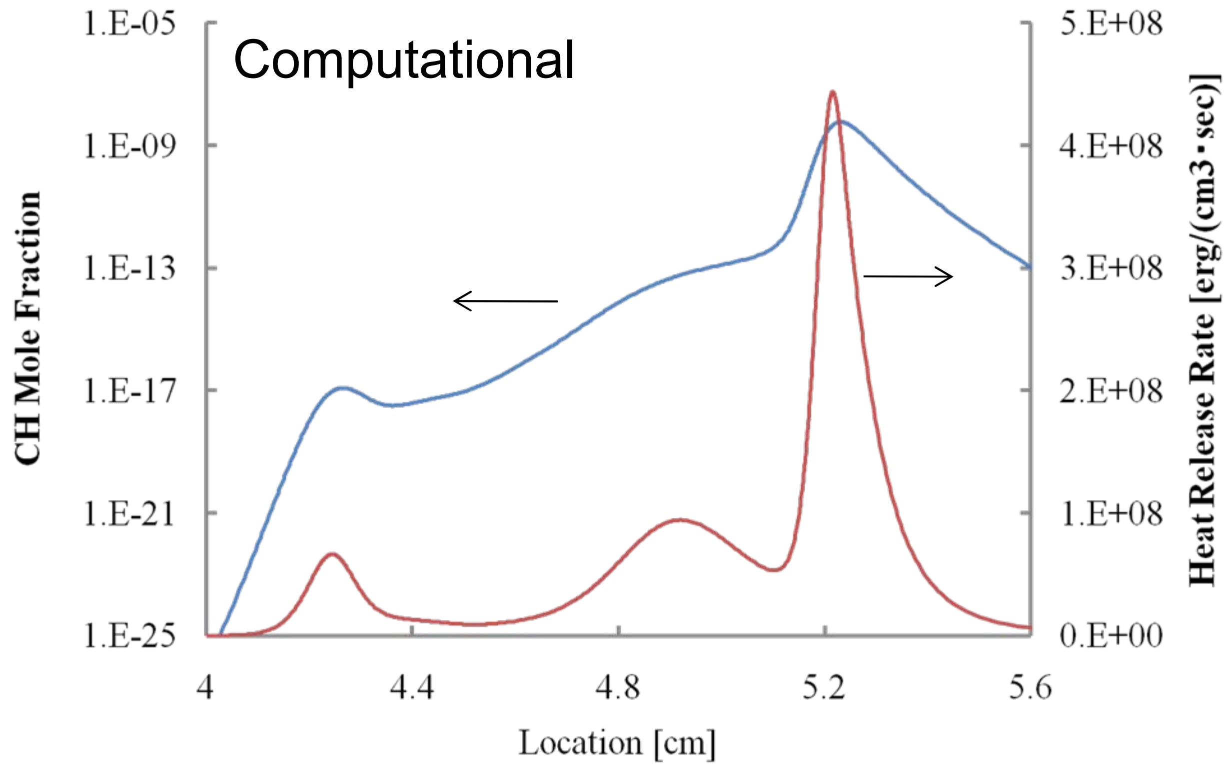
Heat transfer with the wall

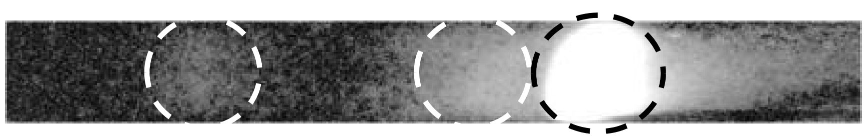
Reaction scheme *n*-heptane, reduced mechanism from LLNL
(159 species, 1540 steps) Seiser et al., PCI 28 (2000)

Conditions Stoichiometric gaseous *n*-heptane/air mixture
Experimental wall temperature profile was provided as Tw(x)

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

Triple weak flames, n-heptane

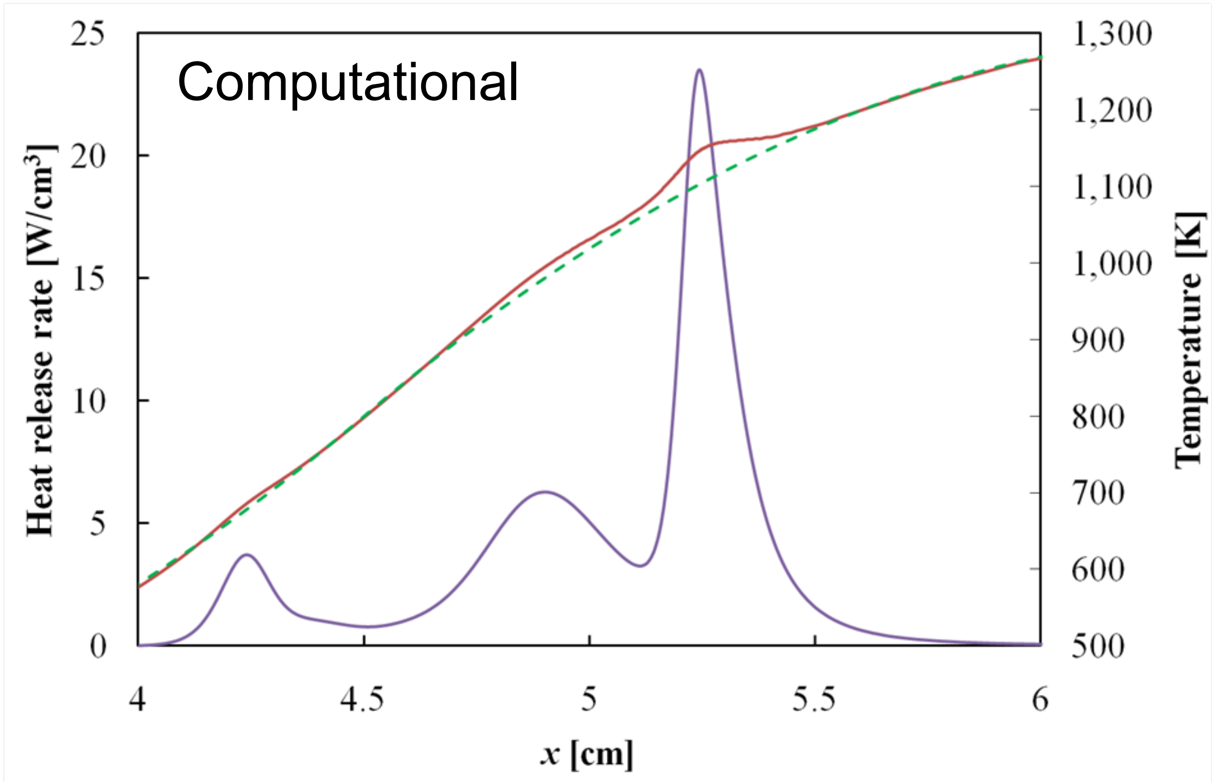


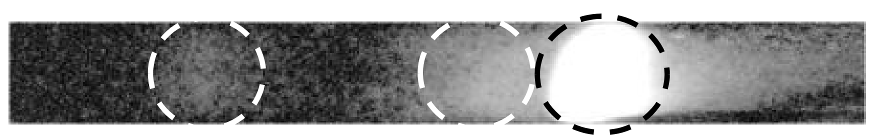


U = 3 cm/s

Three-stage heat release

Triple weak flames, n-heptane

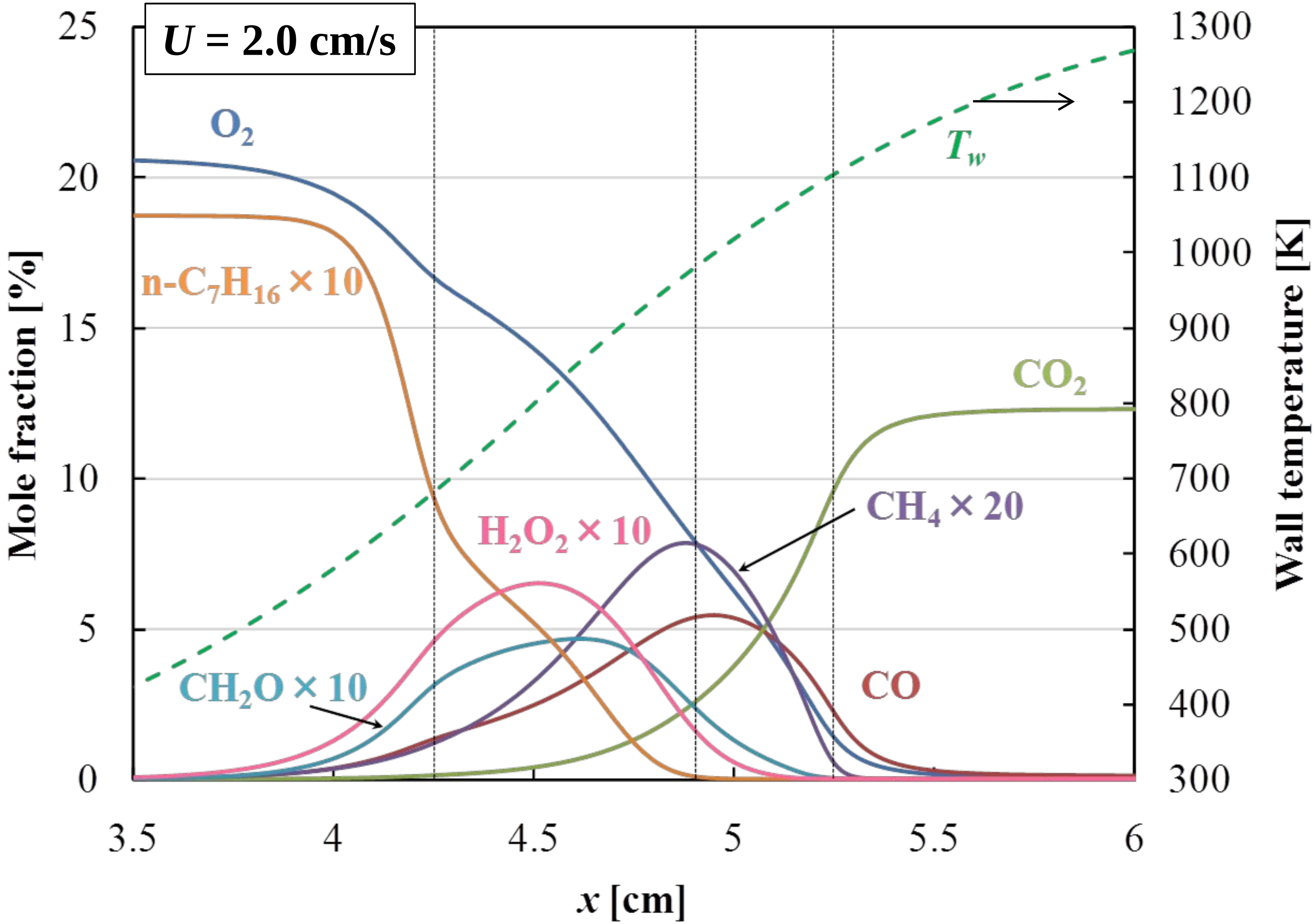




U = 3 cm/s

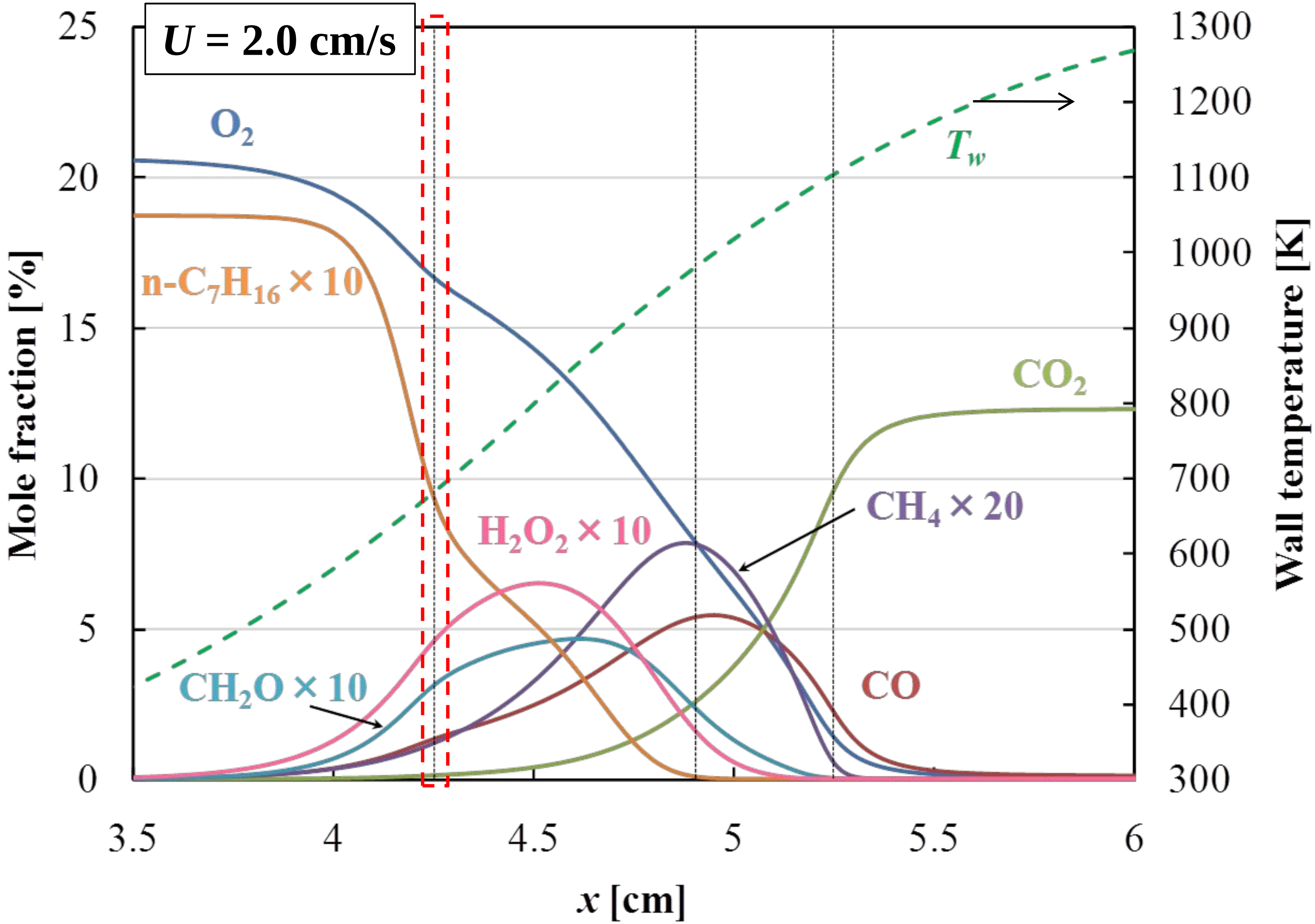
Three-stage heat release

Computational species profiles



Yamamoto et al., PCI33 (2011)

Computational species profiles -1st weak flame-



LTO: CH_2O, H_2O_2, CO, CH_4 produced

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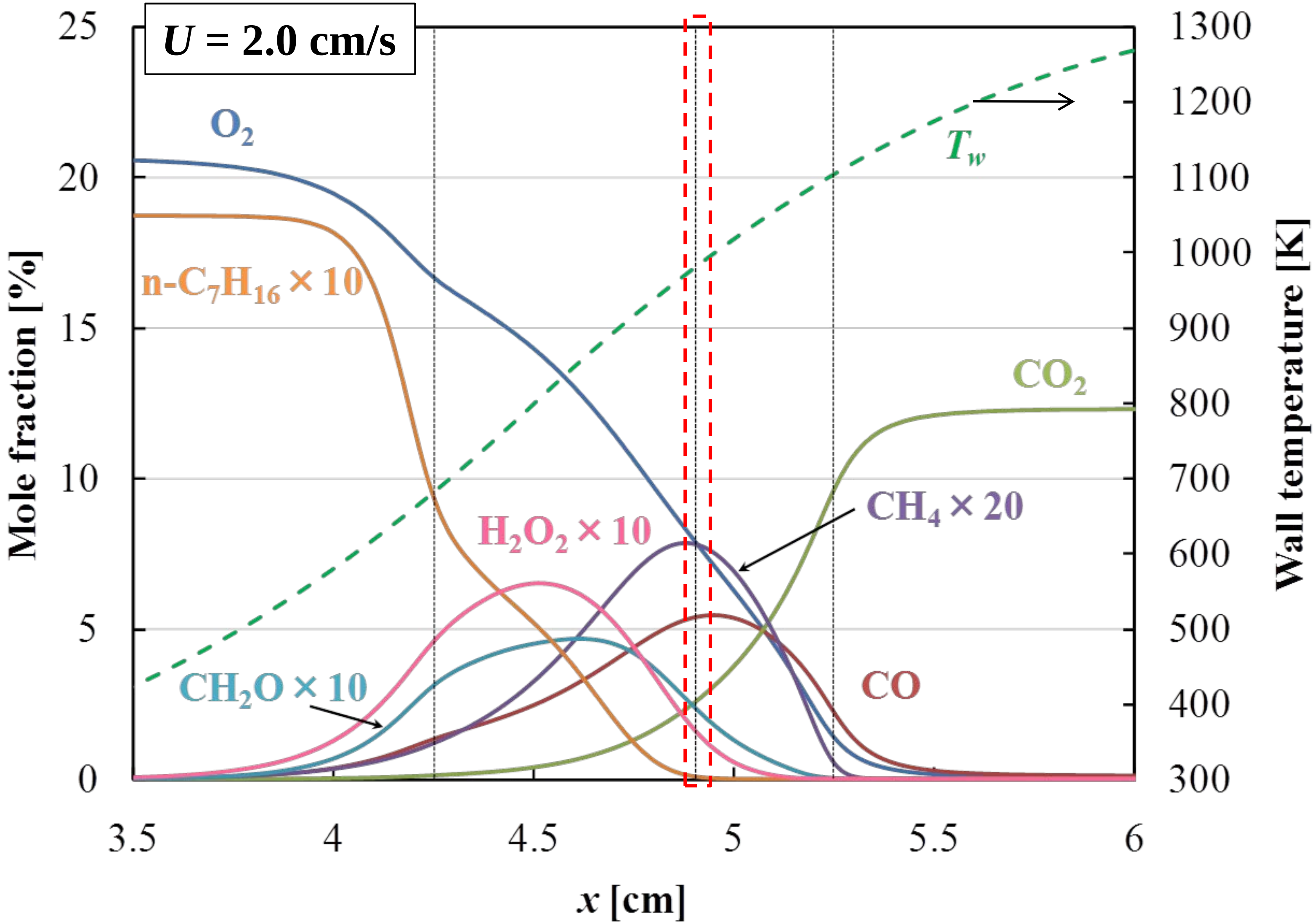
Computational species profiles -2nd weak flame-



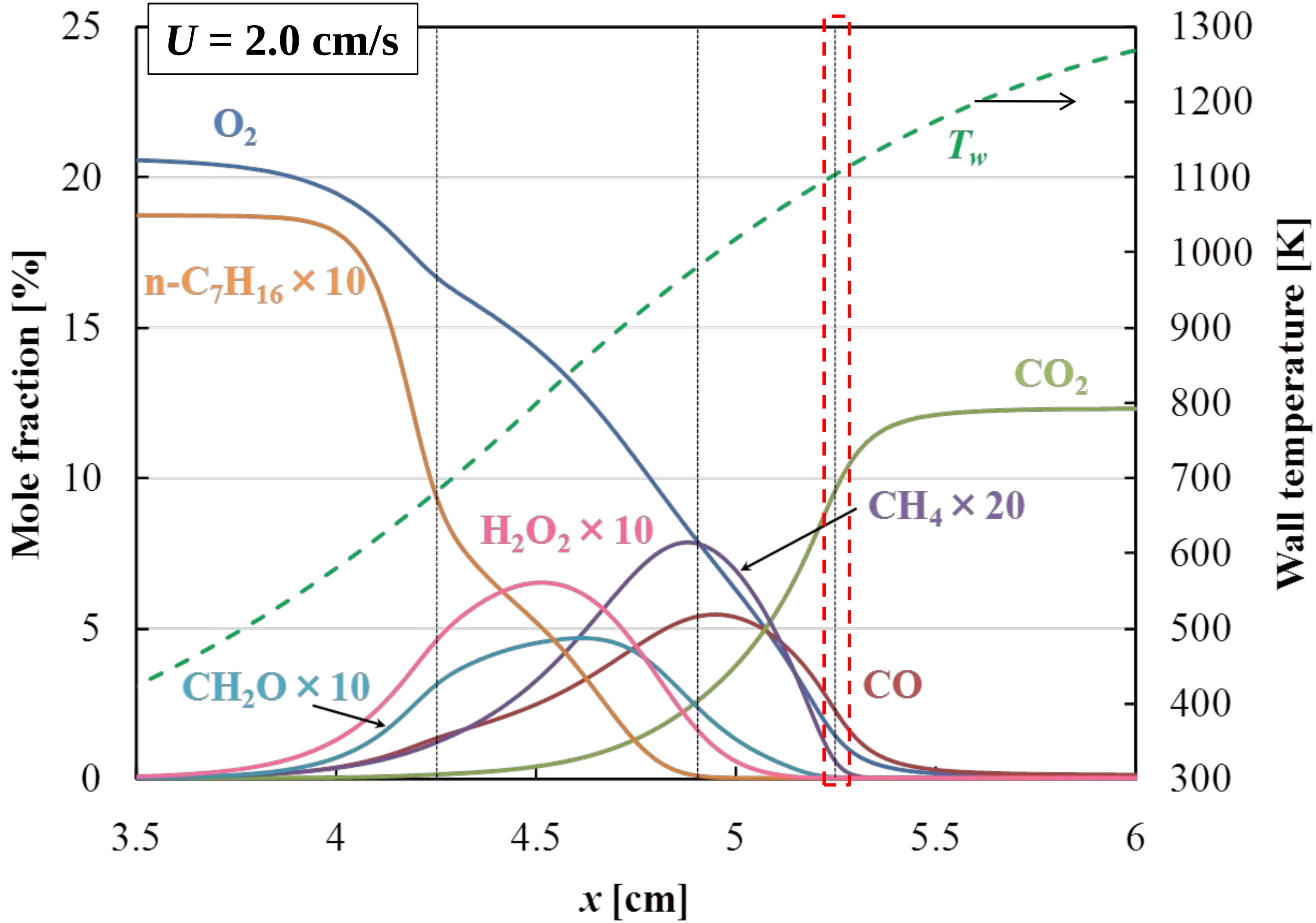
Partial oxidations:

$\mathbf{H_2O_2}$ (+M) $\Rightarrow$ 2OH (+M)

$\mathbf{CH_2O}$ + OH $\Rightarrow$ $\underline{HCO}$ + H_2O

$\underline{HCO}$ + O_2 $\Rightarrow$ **CO** + HO_2

Computational species profiles -3rd weak flame-



Full oxidations: **CO** + OH ⇒ $\mathbf{CO_2}$ + H

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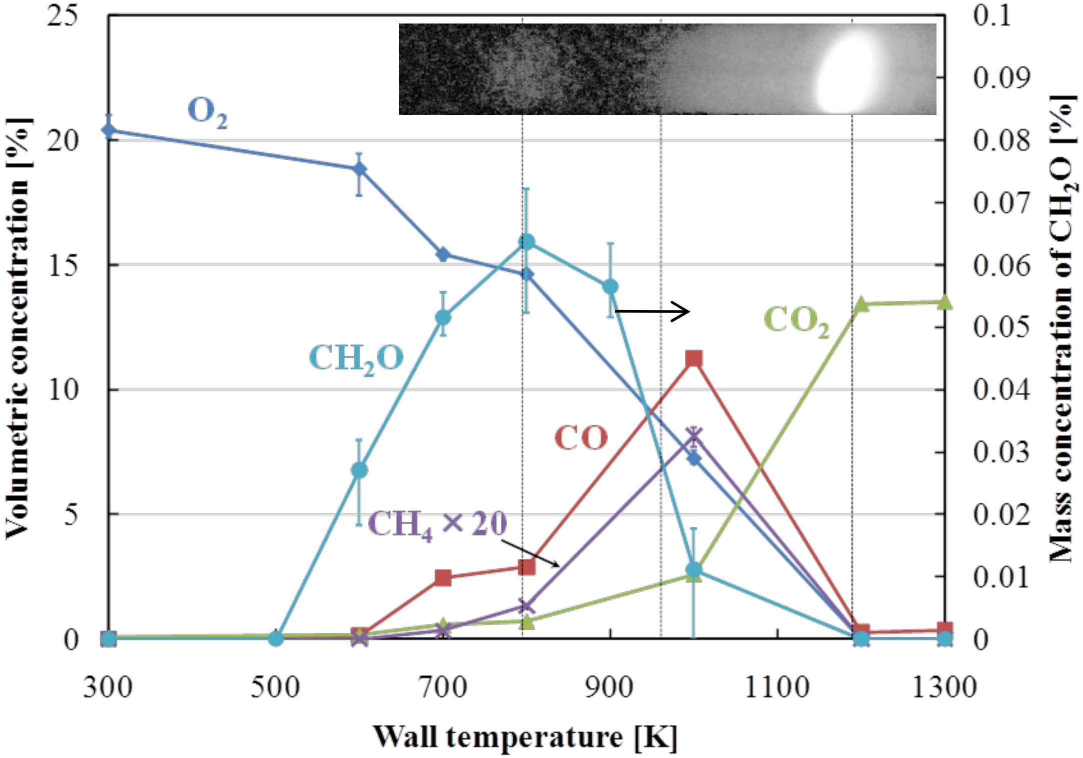
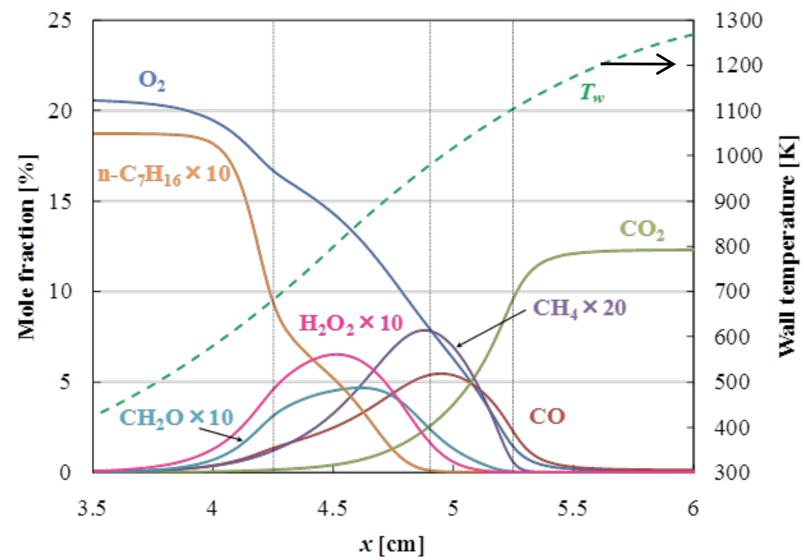
Comparison: measurements and computations

(U = 2.0 cm/s)

Measurement by GC



Computations



Three-stage oxidation process was experimentally confirmed by gas sampling

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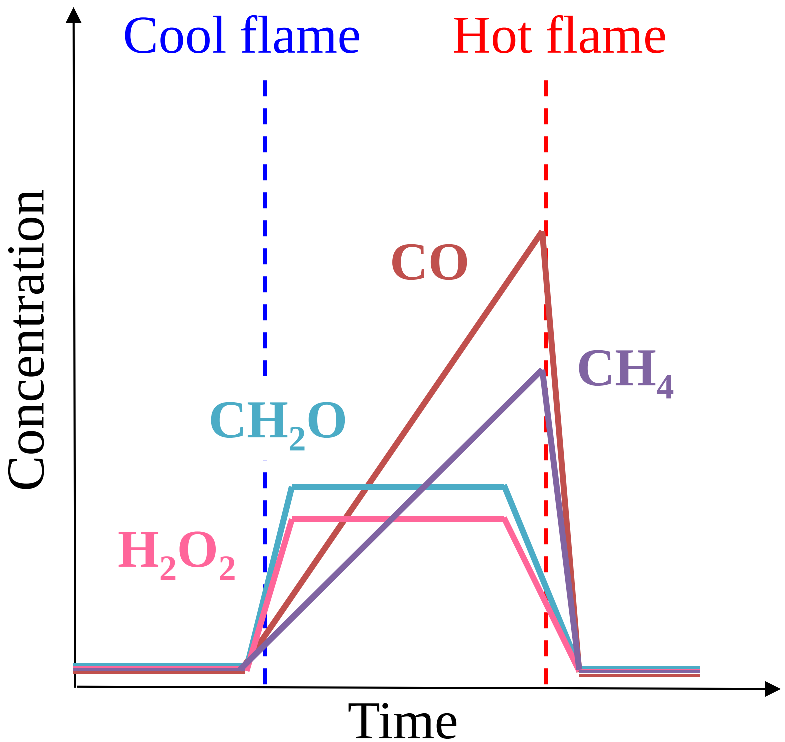
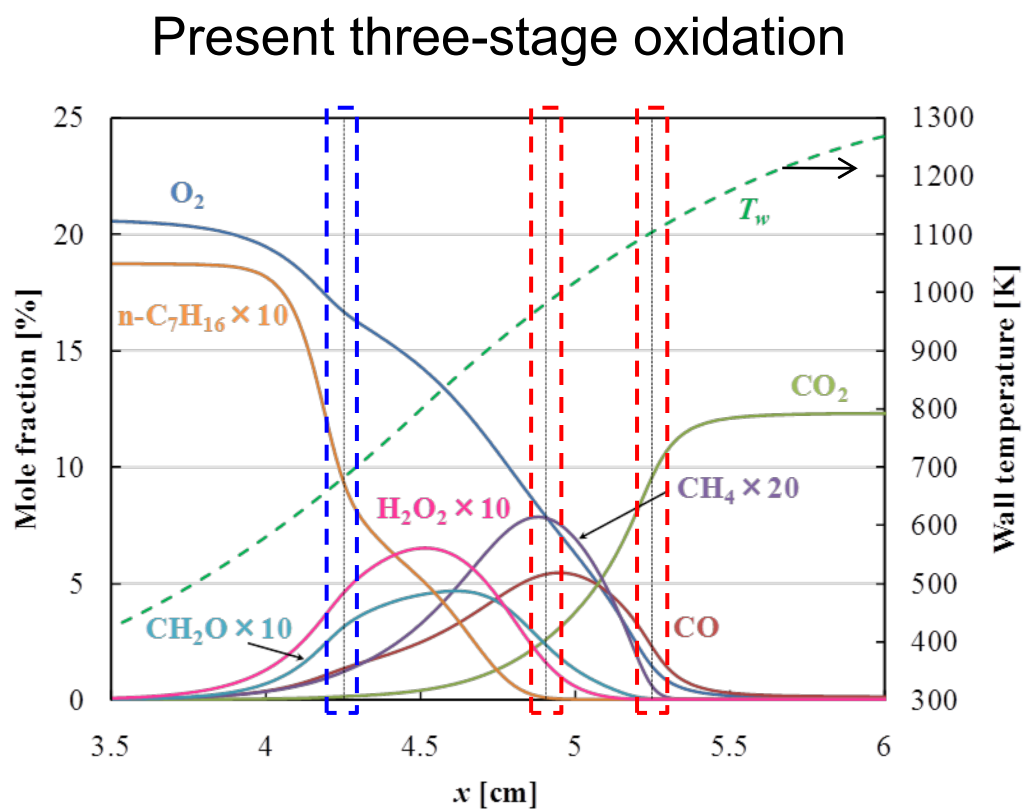
Interpretation of triple weak flames in MFR



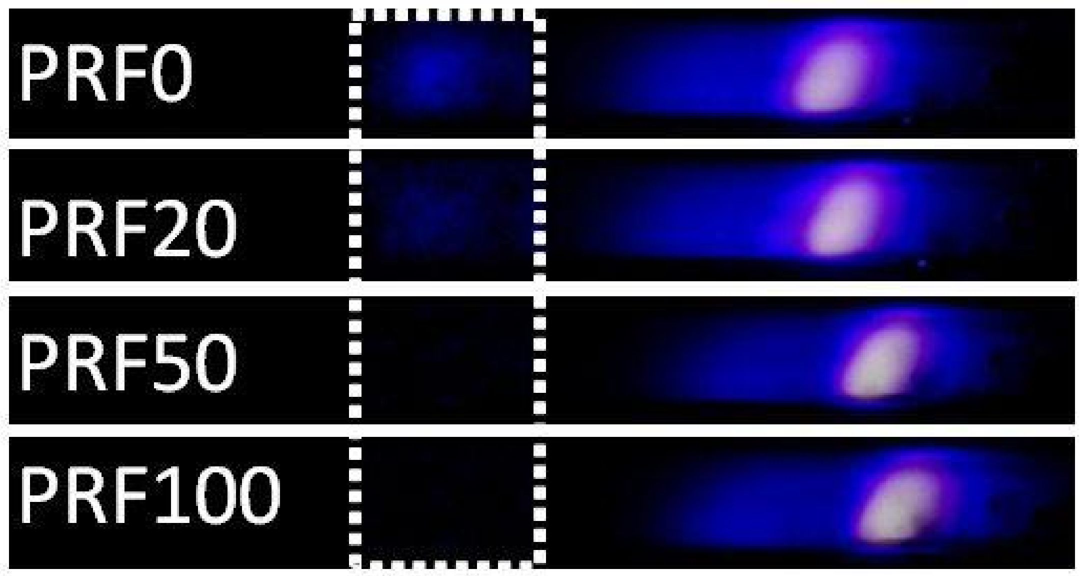


Typical two-stage oxidation: Cool flame + Hot flame

Three-stage oxidation: Cool flame + Separated hot flames (Blue flame & Hot flame)

MFR applied for gasoline PRF

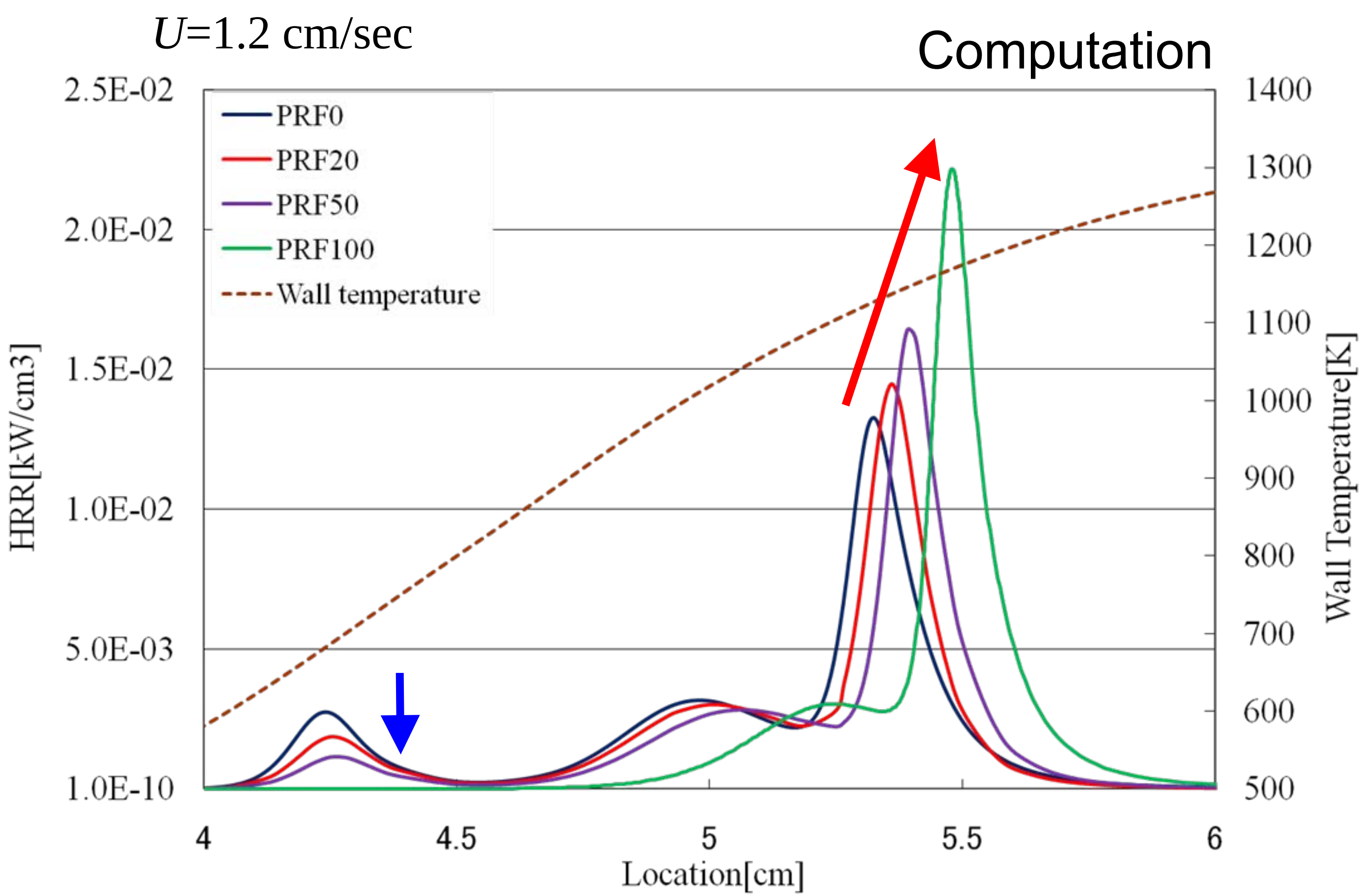
n-heptane + *iso*-octane (PRF)



Appearances of multiple weak flame represent Research Octane Number

Hori et al., CNF159 (2012)

Weak flames at different RON



Significant LTO in smaller RON
Weak flame behaviors reproduced

Weak flames at elevated pressures

PRF0 / air, *U*=2.0 cm/sec

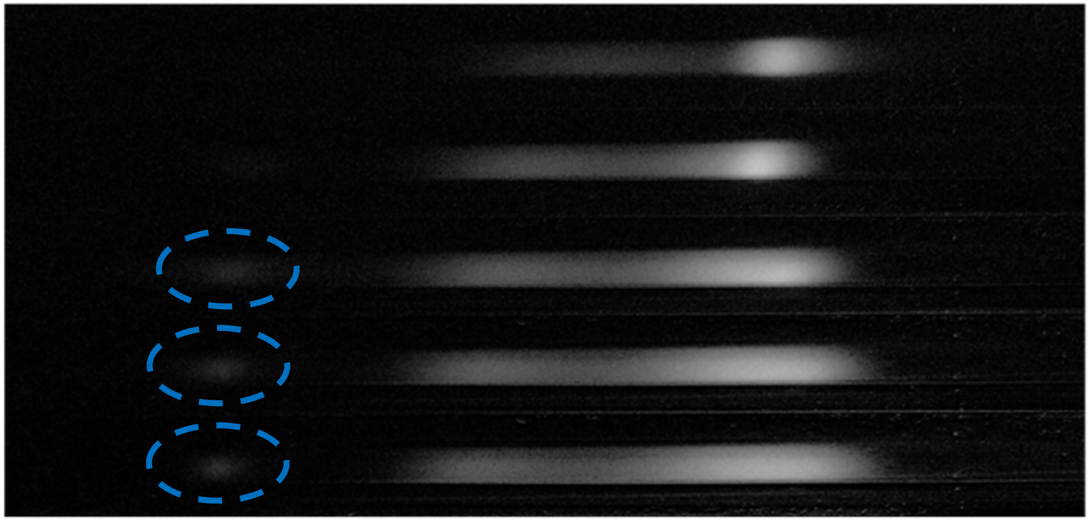
1 atm

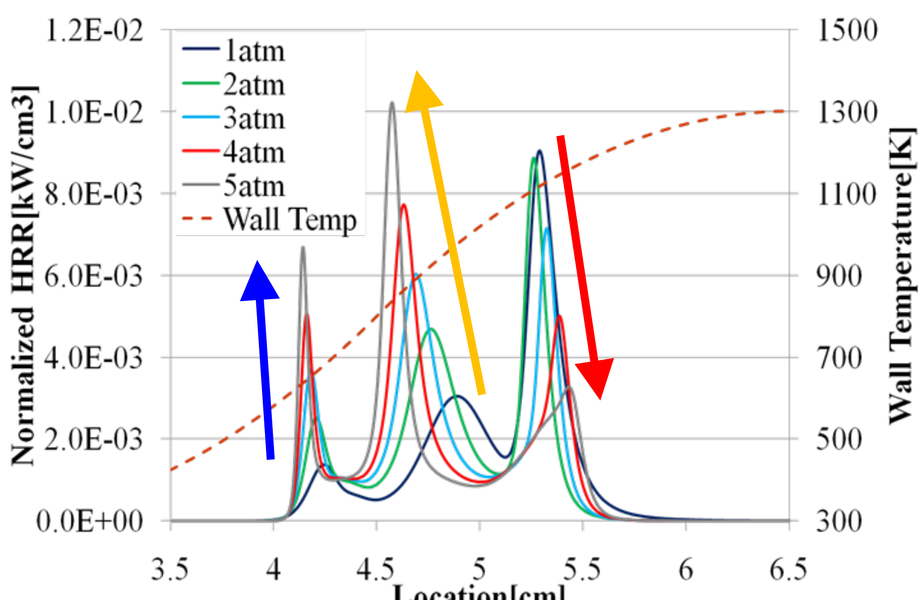
2 atm

3 atm

4 atm

5 atm





PRF20, 50, 100 similar Tendencies but weaker LTO

Hori et al., CNF159 (2012)

Fuels addressed

methane (CH_4)

↓

DME (CH_3OCH_3)

↓

n-heptane (C_7H_{16})

iso-octane (C_8H_{16})

toluene (C_7H_8 or $C_6H_5CH_3$)

↓

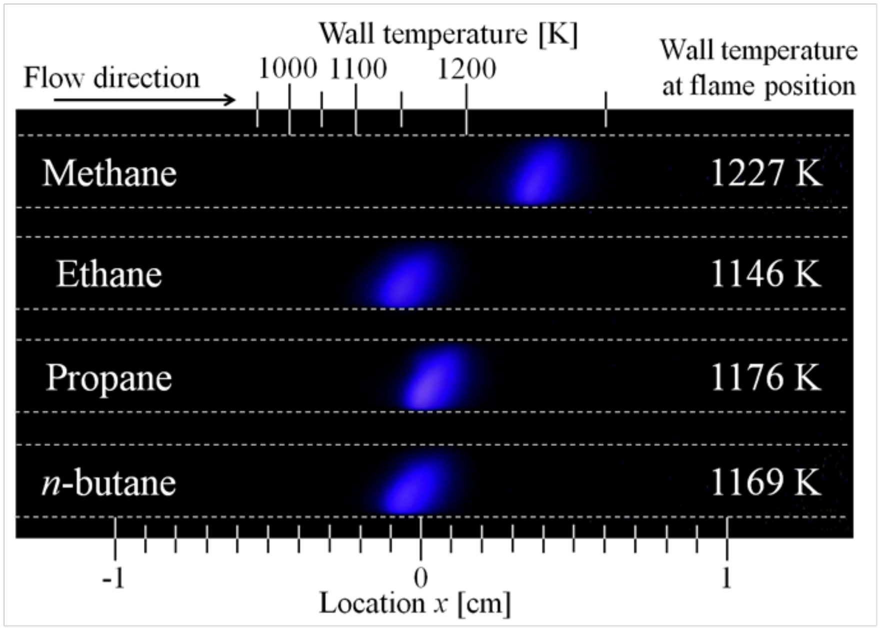
methane (CH_4)

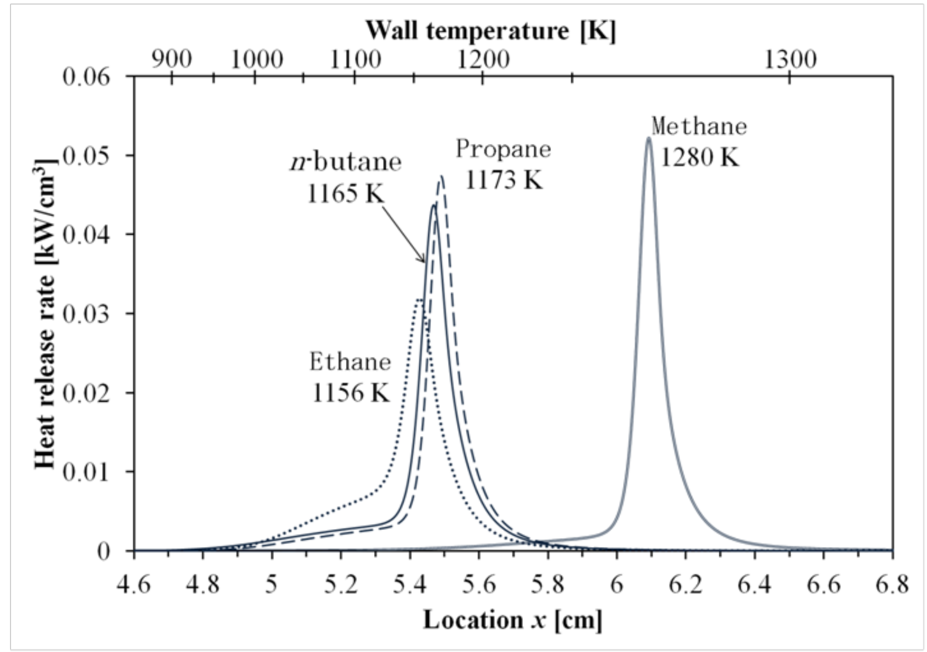
ethane (C_2H_6)

propane (C_3H_8)

n-butane, *iso*-butane (C_4H_{10}) → (Kamada et al., WIPP)

Natural gas components
(Kamada et al., WIPP)

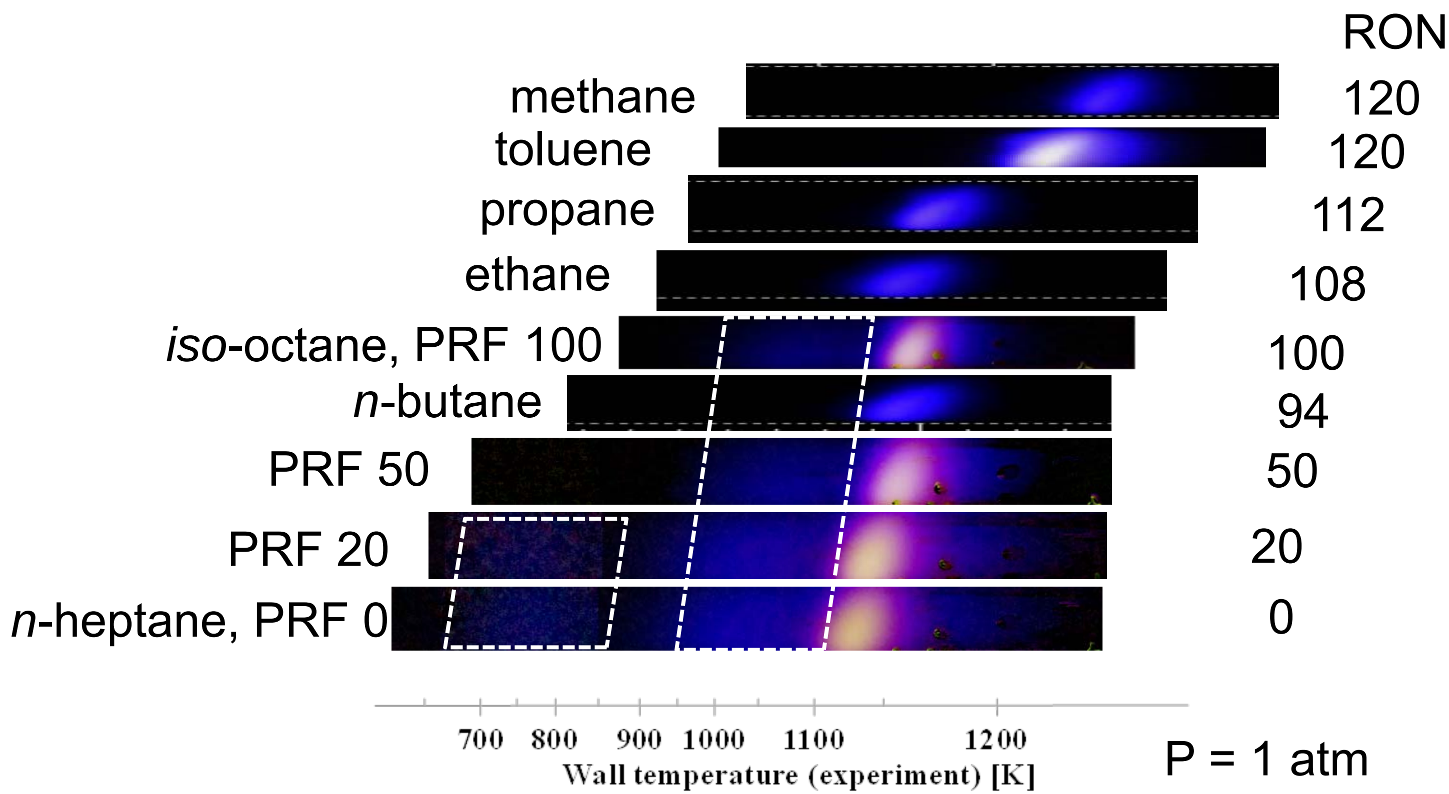




Similar single weak flame (hot flame) observed for each fuel
Different flame locations
Computations reproduced experimental observation

Weak flames at various RON

Data collected at slightly different conditions,
i.e., flow velocity, exposure time, temperature profile



3rd weak flame (main flame) location (temp.) monotonic function of RON
2nd weak flame (blue flame) observable when RON < 100
1st weak flame (cool flame) observable when RON < 20

Conclusions and future, 1 of 2

Micro flow reactor with prescribed temperature profile was introduced

-Three kinds of flame response (S-shaped)

-Weak flame corresponds to ignition branch

-Multiple weak flame utilized for fuel characterization

-Multiple weak flames at elevated pressures

-Appearances of weak flame correlated with RON

Conclusions and future, 2 of 2

Diesel fuels and Cetane numbers

n-cetane (hexadecane, $C_{16}H_{34}$)
iso-cetane (2,2,4,4,6,8,8-heptamethylnonane, $C_{16}H_{34}$)
n-decane ($C_{10}H_{22}$)
α-methylnaphthalene ($C_{11}H_{10}$) → (Suzuki et al., 5E06)

Ethanol → (Nakamura et al., 1E02)
Syngas
Oxyfuel combustion → (Li et al., WIPP)
Effect of surface reaction → (Kizaki et al, WIPP)
PAH and soot

Optical diagnosis

LIF, CRDS for precise species profile measurements

Higher pressures

High pressure chamber (up to 20 bar) fabricated

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Acknowledgements

IHI, IIC, HONDA R&D, JAXA, NEDO, HITACHI, TG, MEXT

Micro flow reactor now commercially available