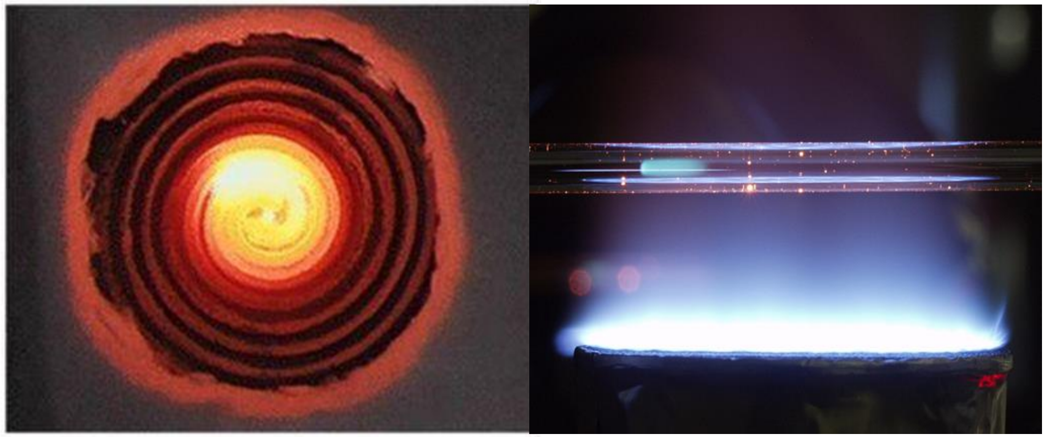
The 1st International Workshop on Near Limit Flames, July 29-30, 2017, Boston, MA, USA



Cool flames in micro channel

Recent progress of weak flames in a micro flow reactor with a controlled temperature profile

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A. Yamamoto, M. Hori, P. Grajetzki, T. Okuno, A.K. Dubey, T. Onda, Y. Kizaki

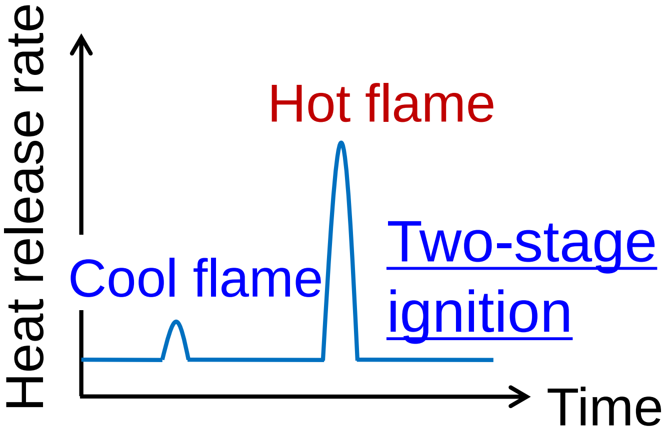
Contents

- Outline of a micro flow reactor with a controlled temperature gradient
- Separated cool flame
- Recent progress of weak flame studies

Background

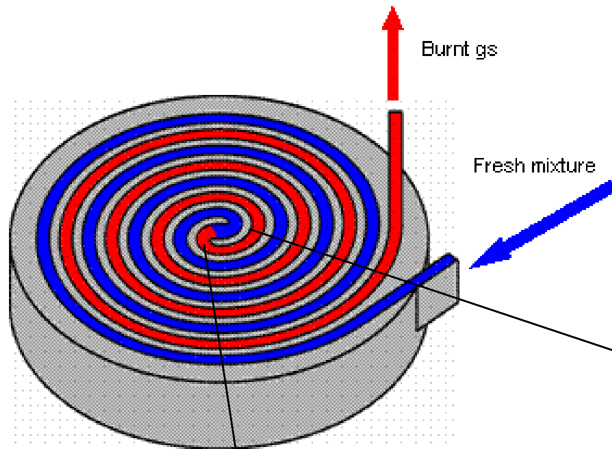
For larger fuel diversity, understandings of ignition and combustion characteristics of various practical fuels are important. Ex. bio-, synthesized-, reformed-fuels, etc.

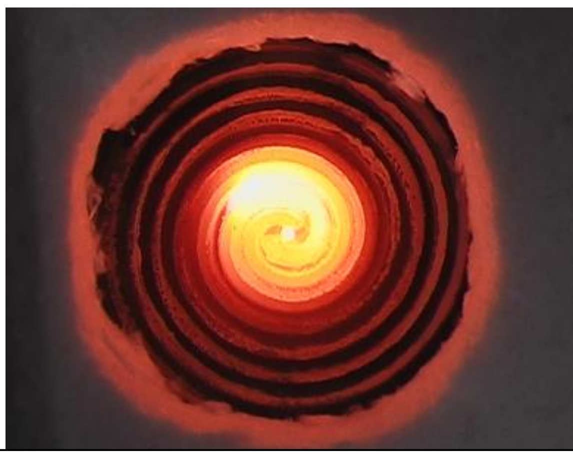
Shock tube, RCM, burners have been extensively used but simple and compact method for examining reaction dynamics is required.



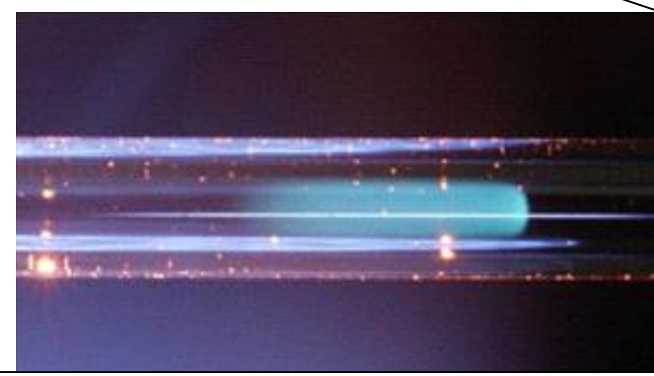
<u>A micro flow reactor with a controlled temperature profile</u>

Microcombustion for fundamental combustion studies



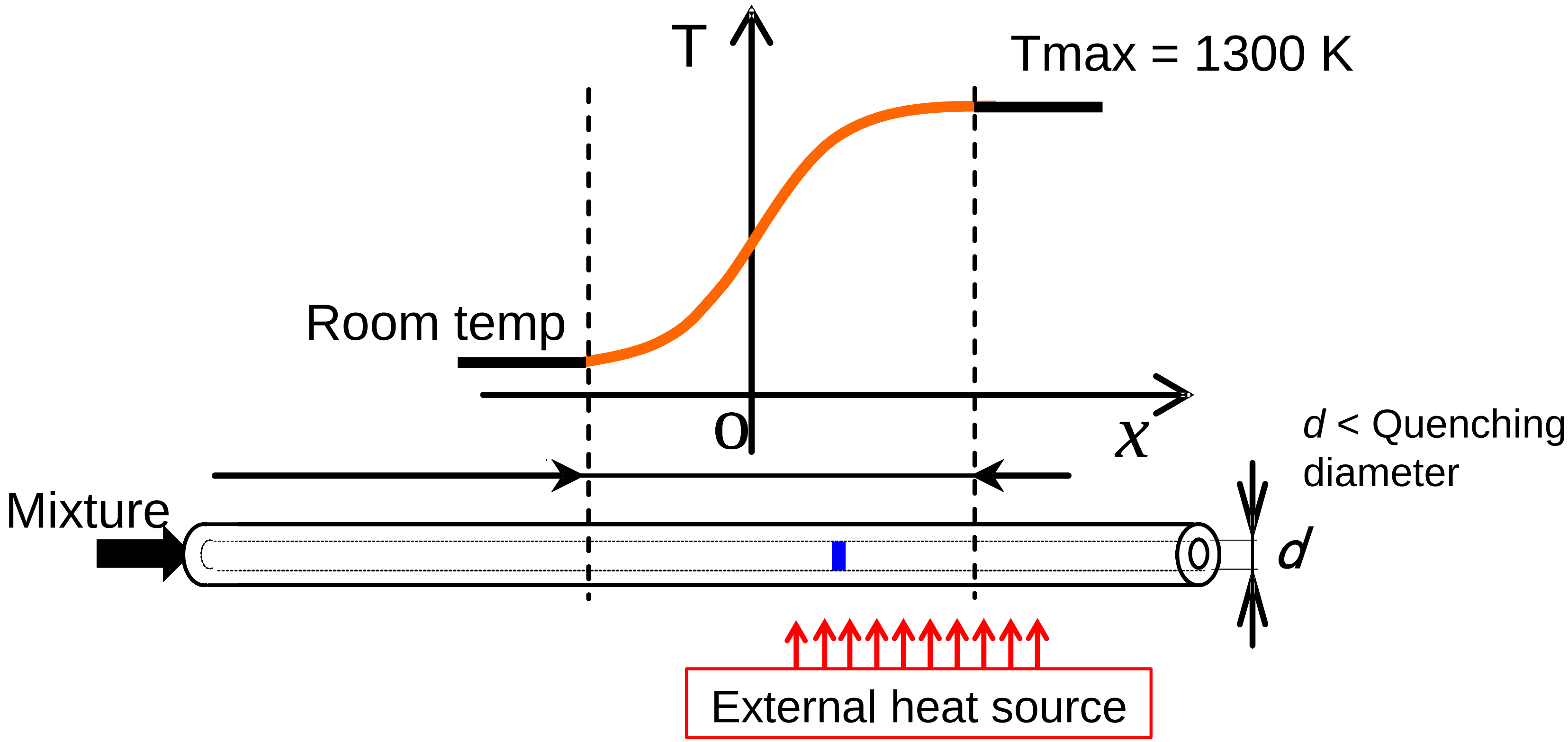


Swiss roll microcombustors for heat sources



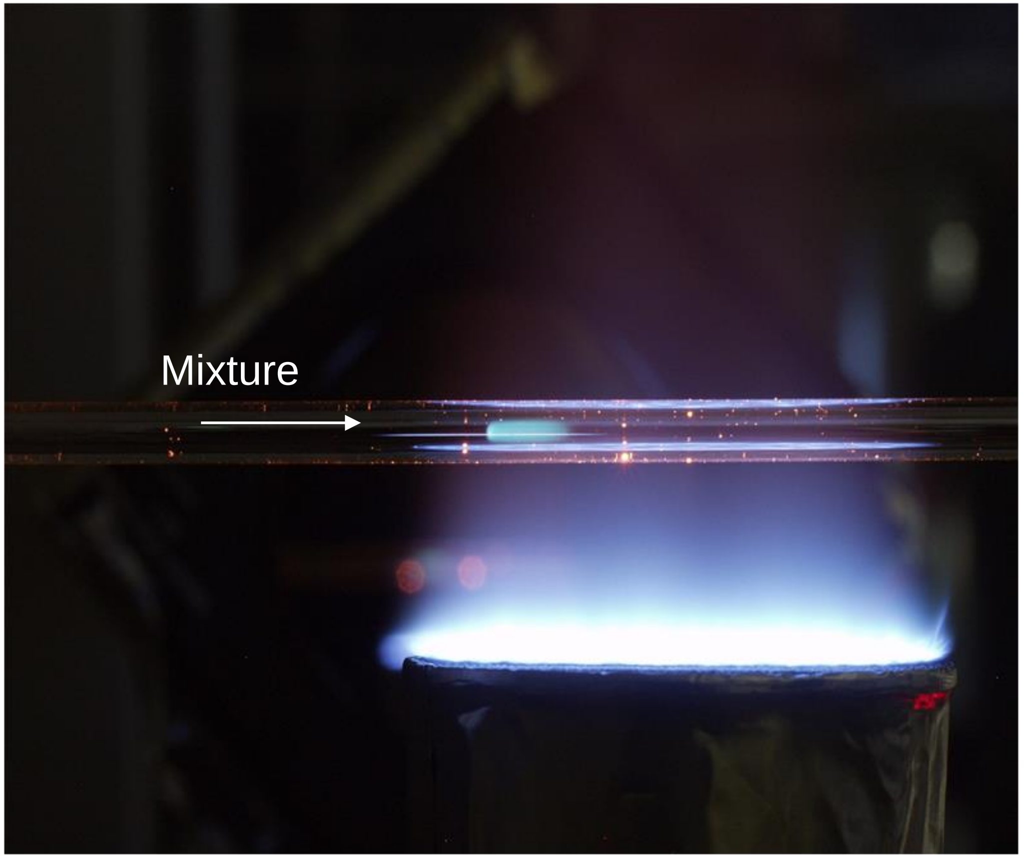
Micro flow reactor with controlled temp. profile

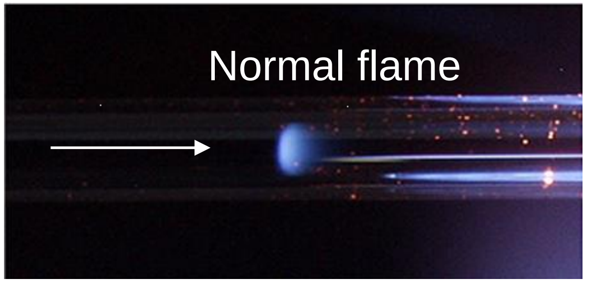
Micro flow reactor with a controlled temperature profile



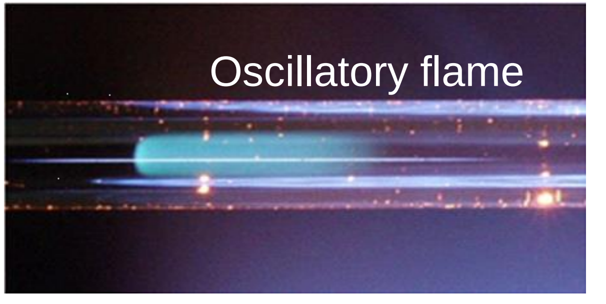
Stationary wall-temperature profile
Diameter of tube < conventional quenching diameter
Gas phase temperature dominated by wall temperature profile
Laminar flow and constant pressure

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

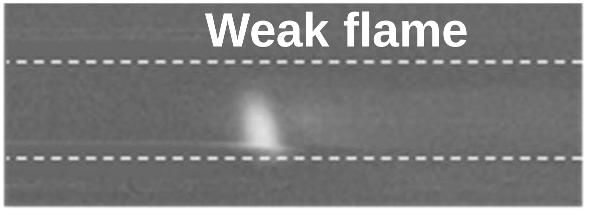




High velocity region



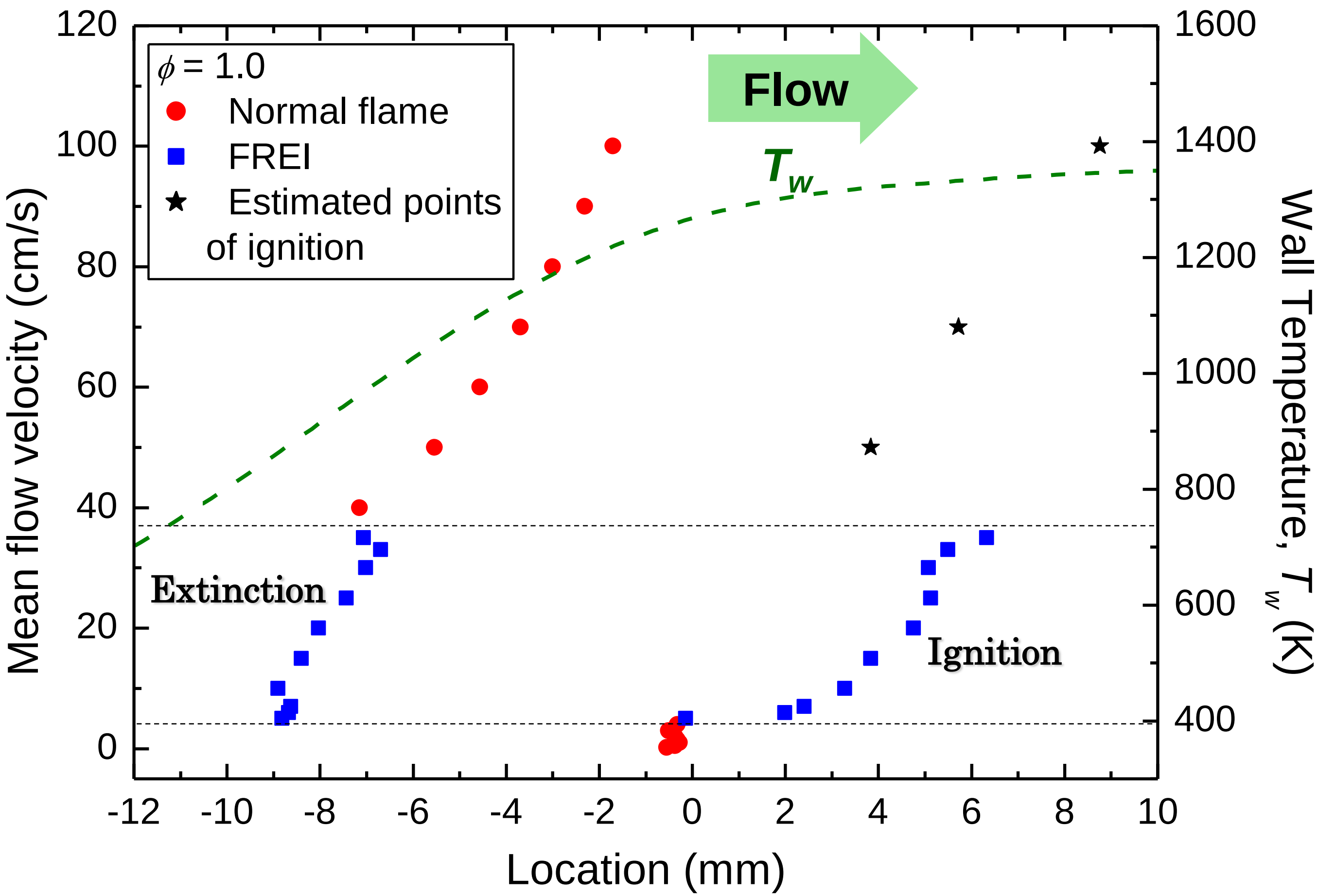
Intermediate velocity region



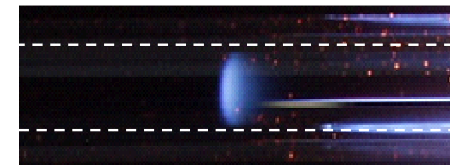
Low velocity region

Three kinds of flame responses

CH_4/air mixture

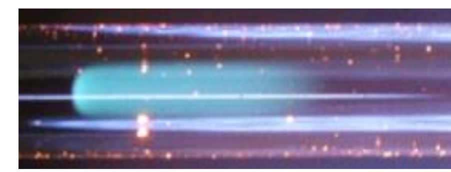


(1) Normal flame



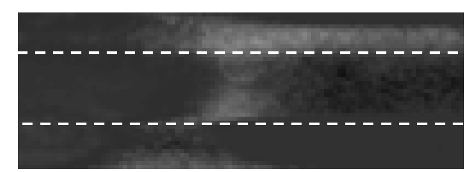
V=50cm/s

(2) Oscillatory flame



V=20cm/s

(3) Weak flame



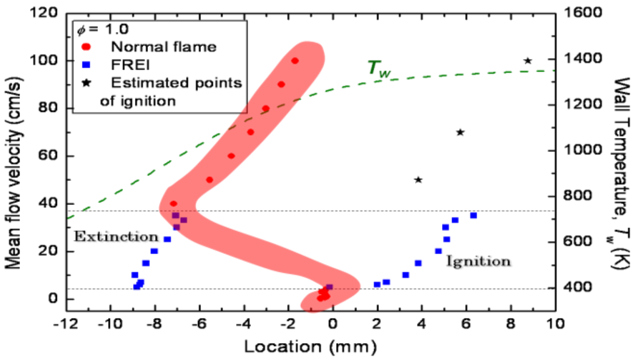
V=0.2cm/s

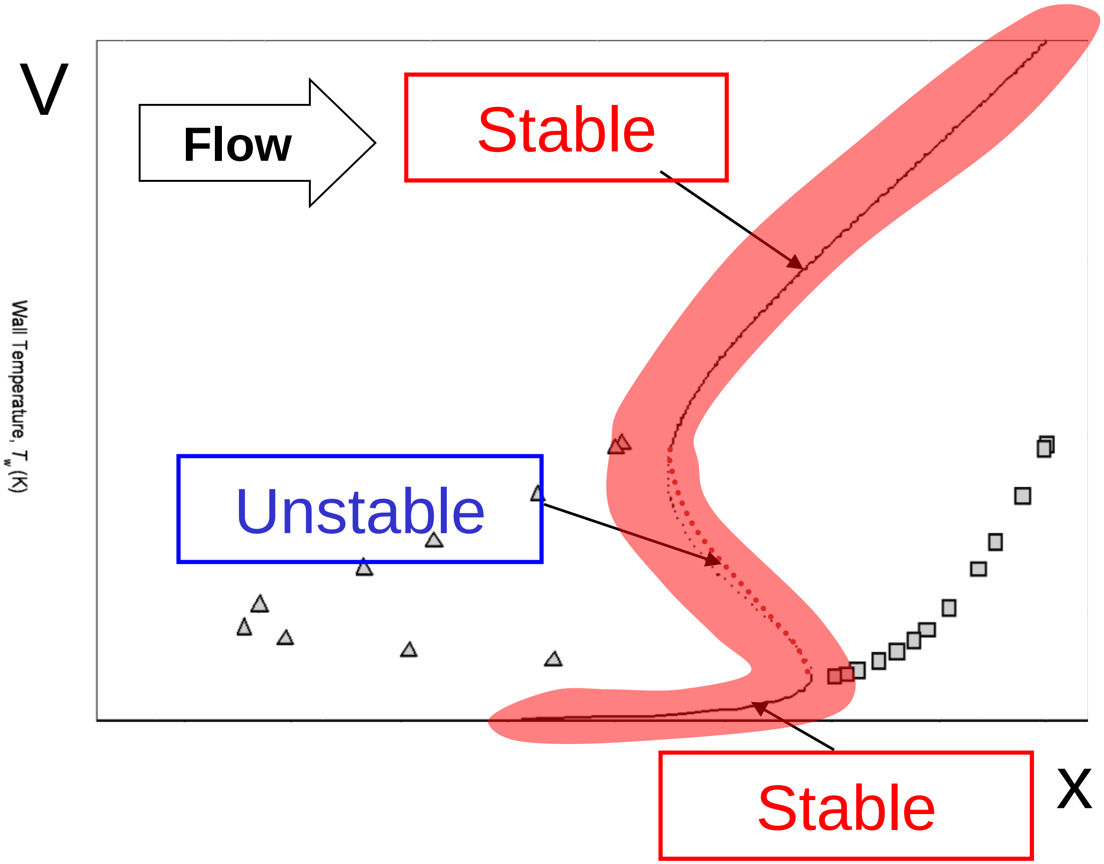
Normal flame, oscillatory flame, weak flame

Maruta et al., PCI 30

Theoretical S-shaped solutions

experiments

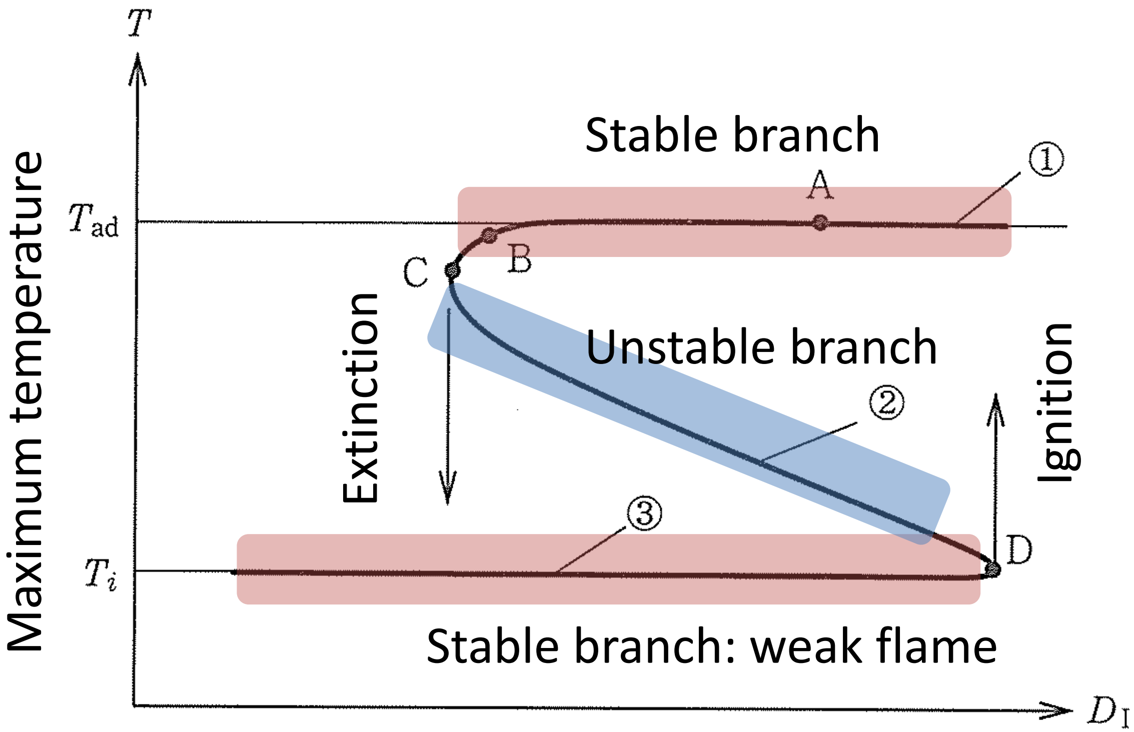




Two stable and one unstable solutions predicted theoretically
Weak flame corresponds to ignition branch of S-curve

Minaev et al., CTM 2007

Analogy between S-curve and conventional Findell-curve



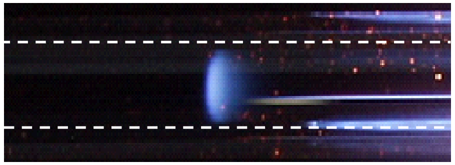
D_a: Damköhler number

$$D_a = \frac{Flow\ residense\ time}{Chemical\ time}$$

- Normal flame: preheated premixed flame
- Oscillatory flame: flames with repetitive extinction and ignition, FREI
- Weak flame: stable weak flame which represent ignition

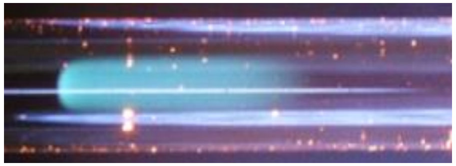
Three flames are utilized for:

(1) Normal flame



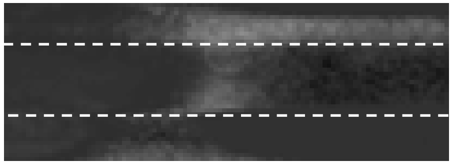
Measurements of laminar burning velocity of highly preheated mixtures

(2) Oscillatory flame



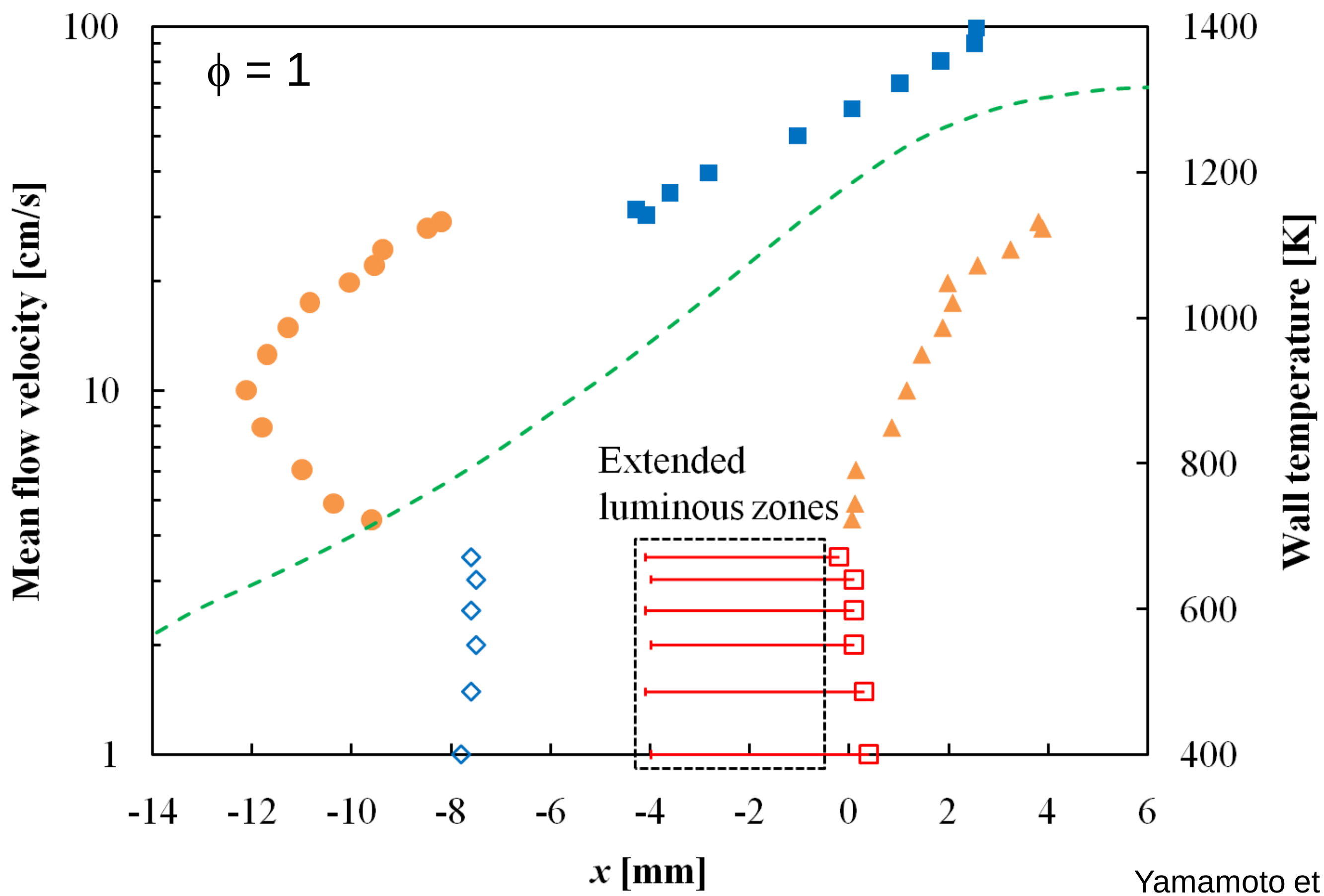
Investigations of non-linear dynamics of given fuels

(3) Weak flame

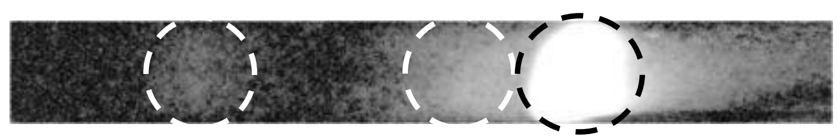


Investigations of ignition relevant properties of various fuels, validation and modifications of kinetics, particularly at low temperature

Triple weak flames, n-heptane



Yamamoto et al., PCI 33



U = 3 cm/s

Triple stationary weak flames observed
Weak flame location insensitive to flow velocity

Computations (one-dimensional)

Code PREMIX-based

Gas-phase energy equation

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

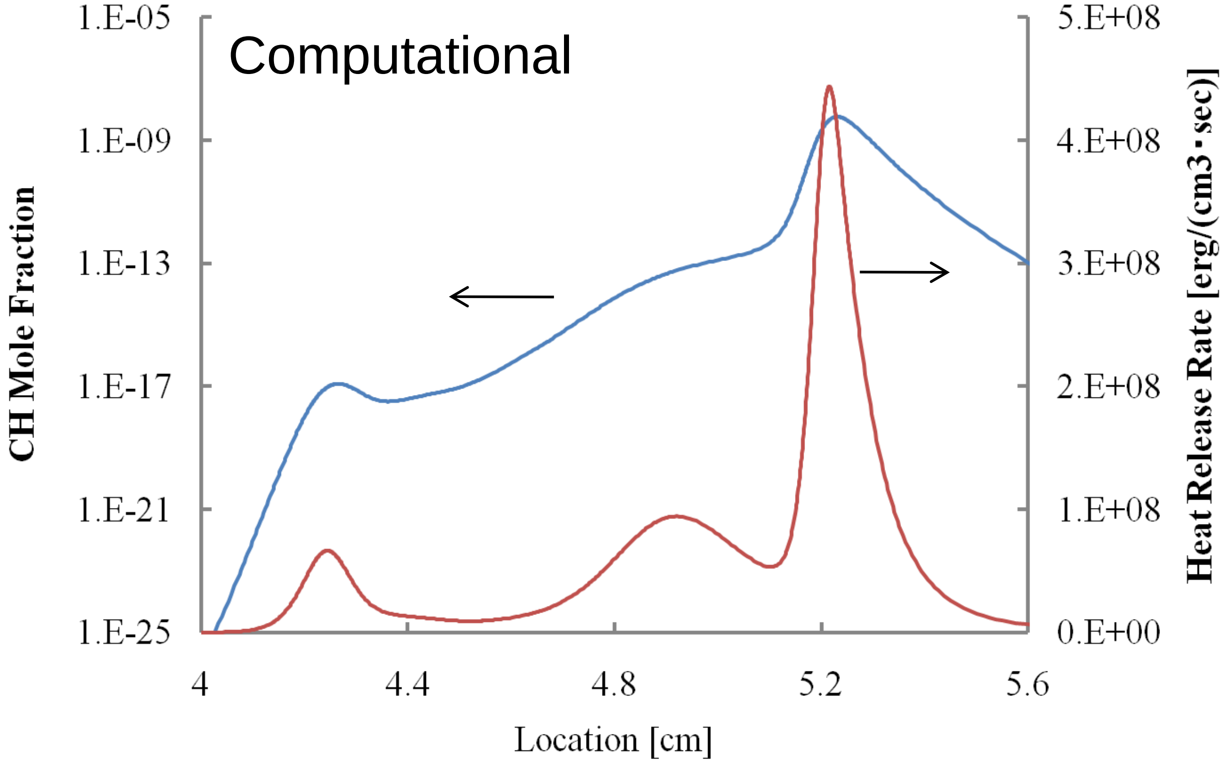
Heat transfer with the wall

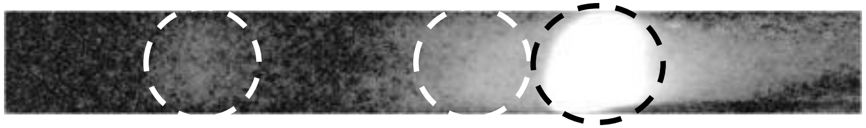
Reaction scheme: *n*-heptane, reduced mechanism from LLNL (159 species, 1540 steps) Seiser et al., PCI 28 (2000)

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

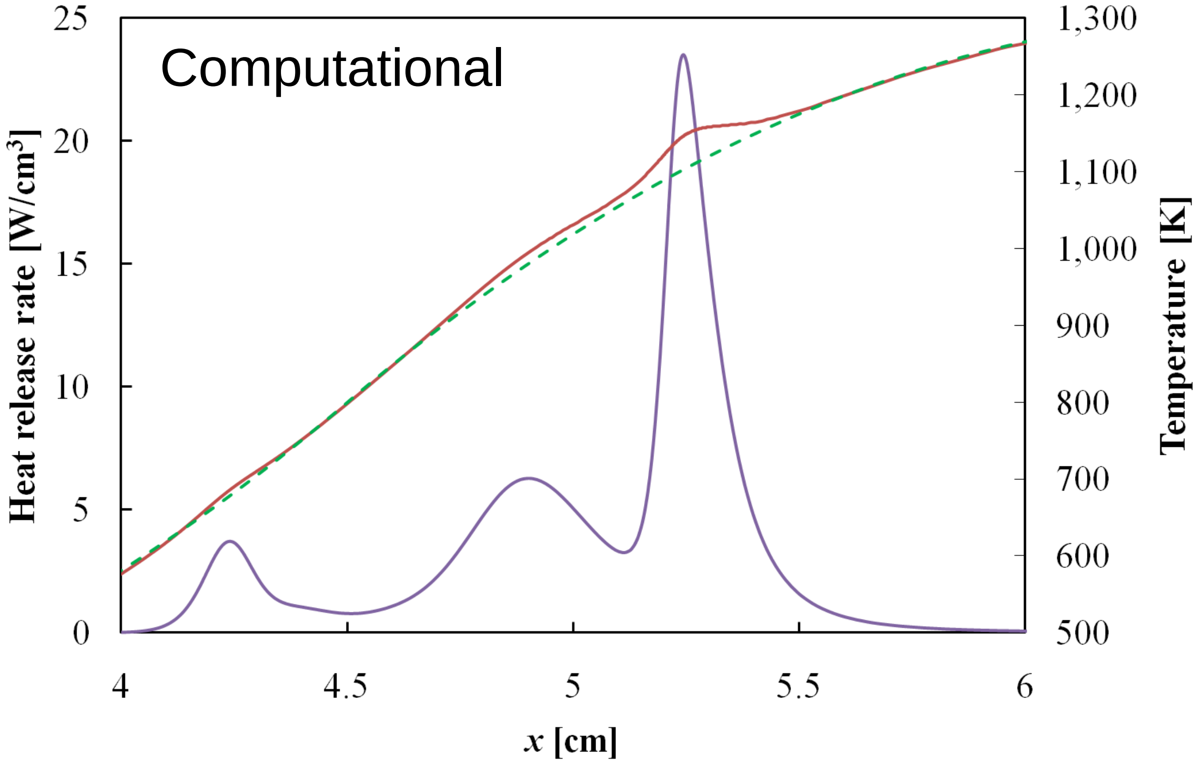


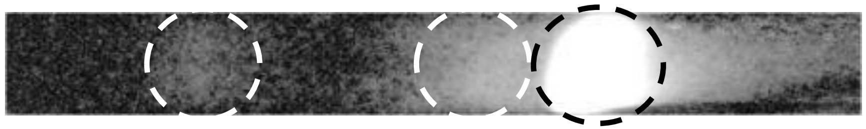


U = 3 cm/s

Three-stage heat releases

Triple weak flames, n-heptane

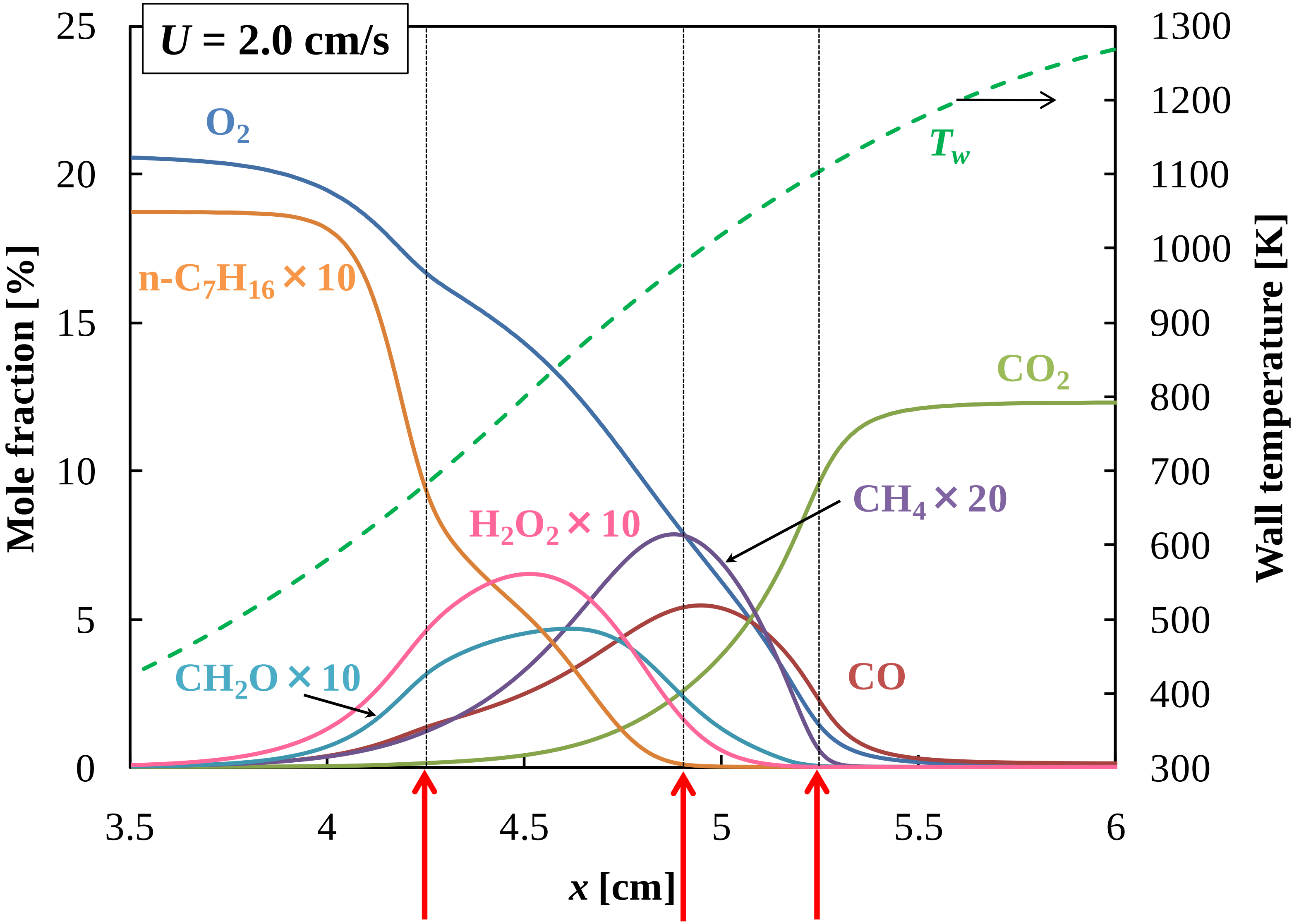




U = 3 cm/s

Three-stage heat releases

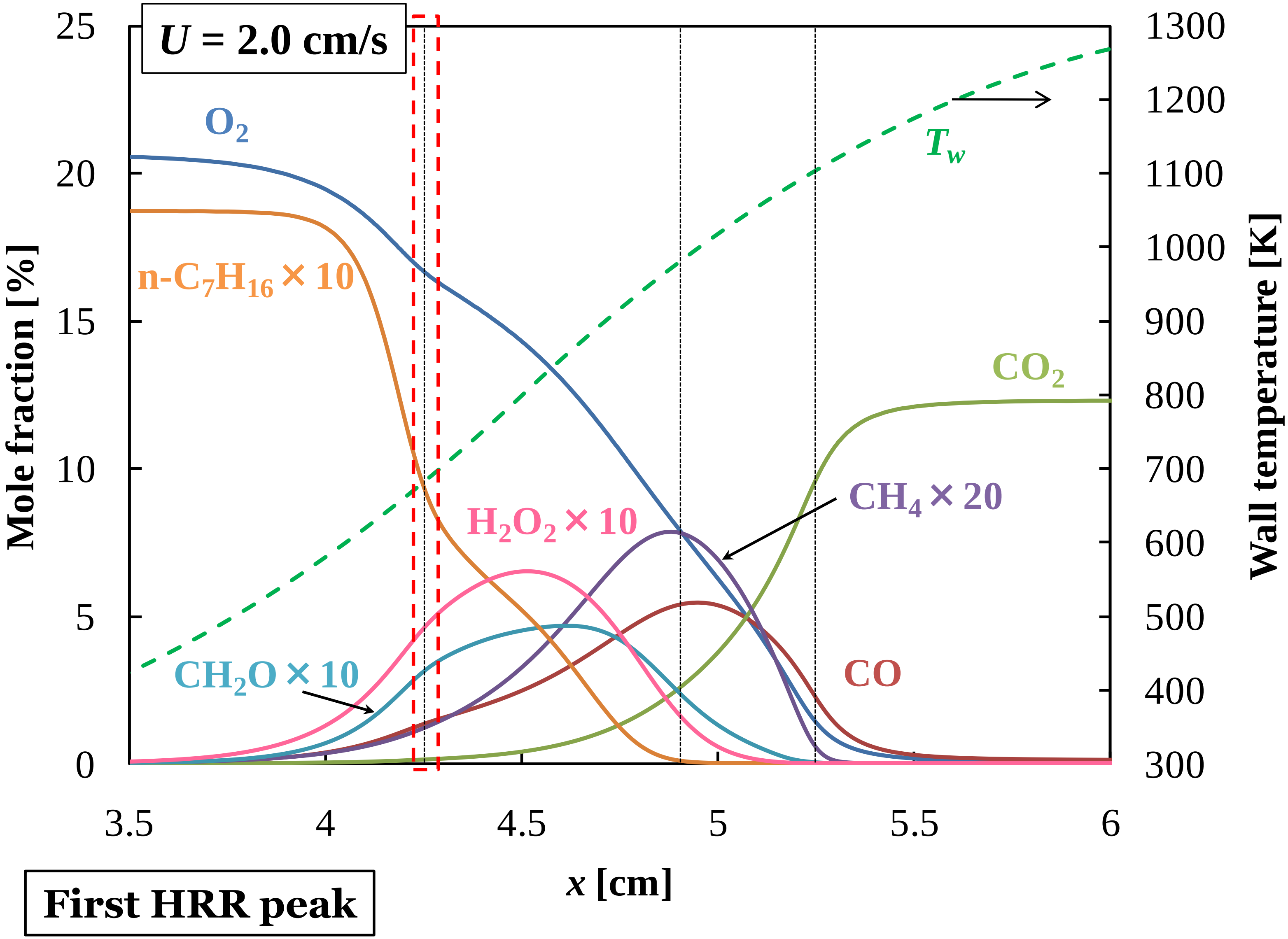
Computational species profiles



Three peaks of heat release rate

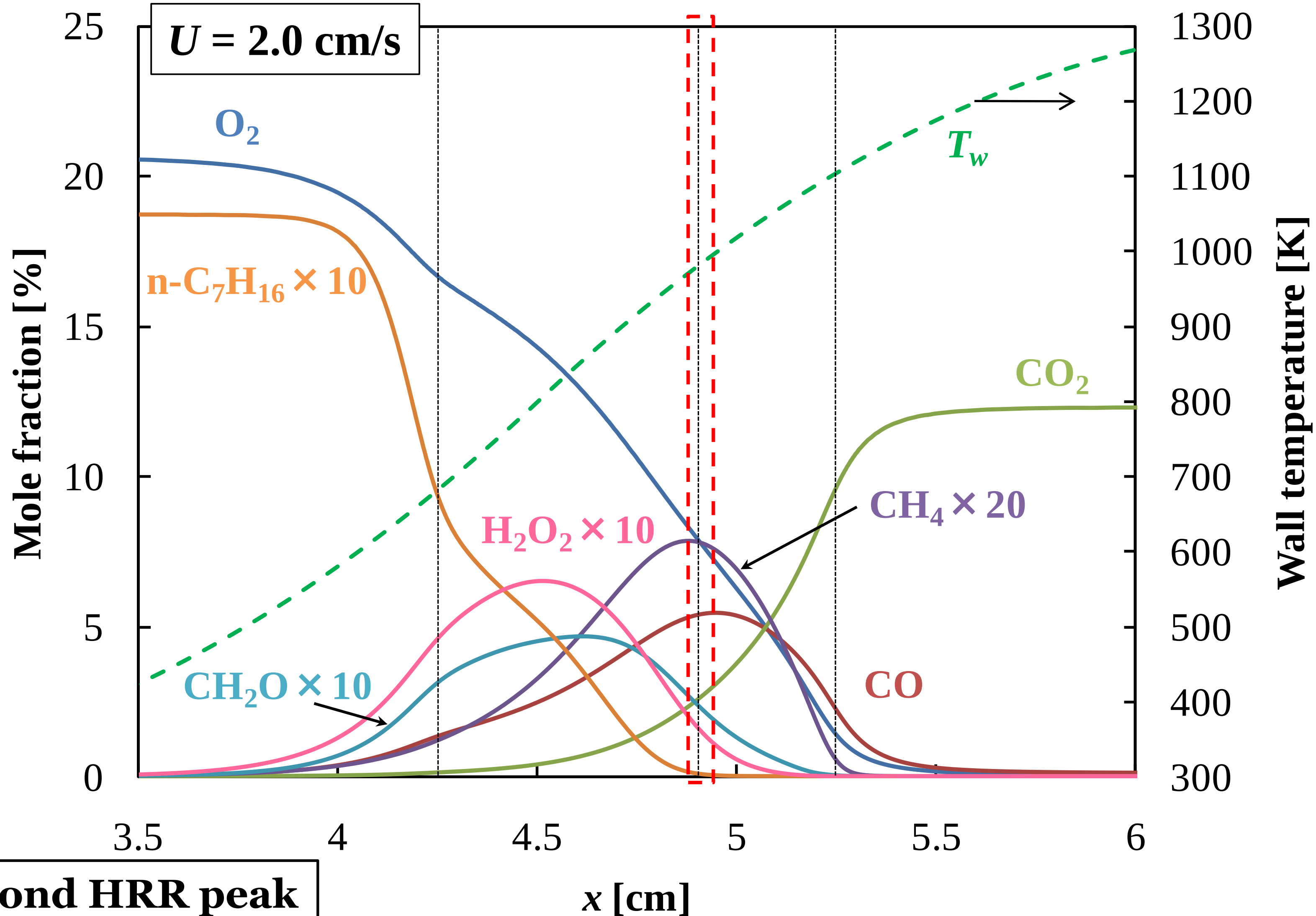
Yamamoto et al., PCI 33

Computational species profiles



LTO: CH_2O, H_2O_2, CO, CH_4 produced

Computational species profiles



Second HRR peak

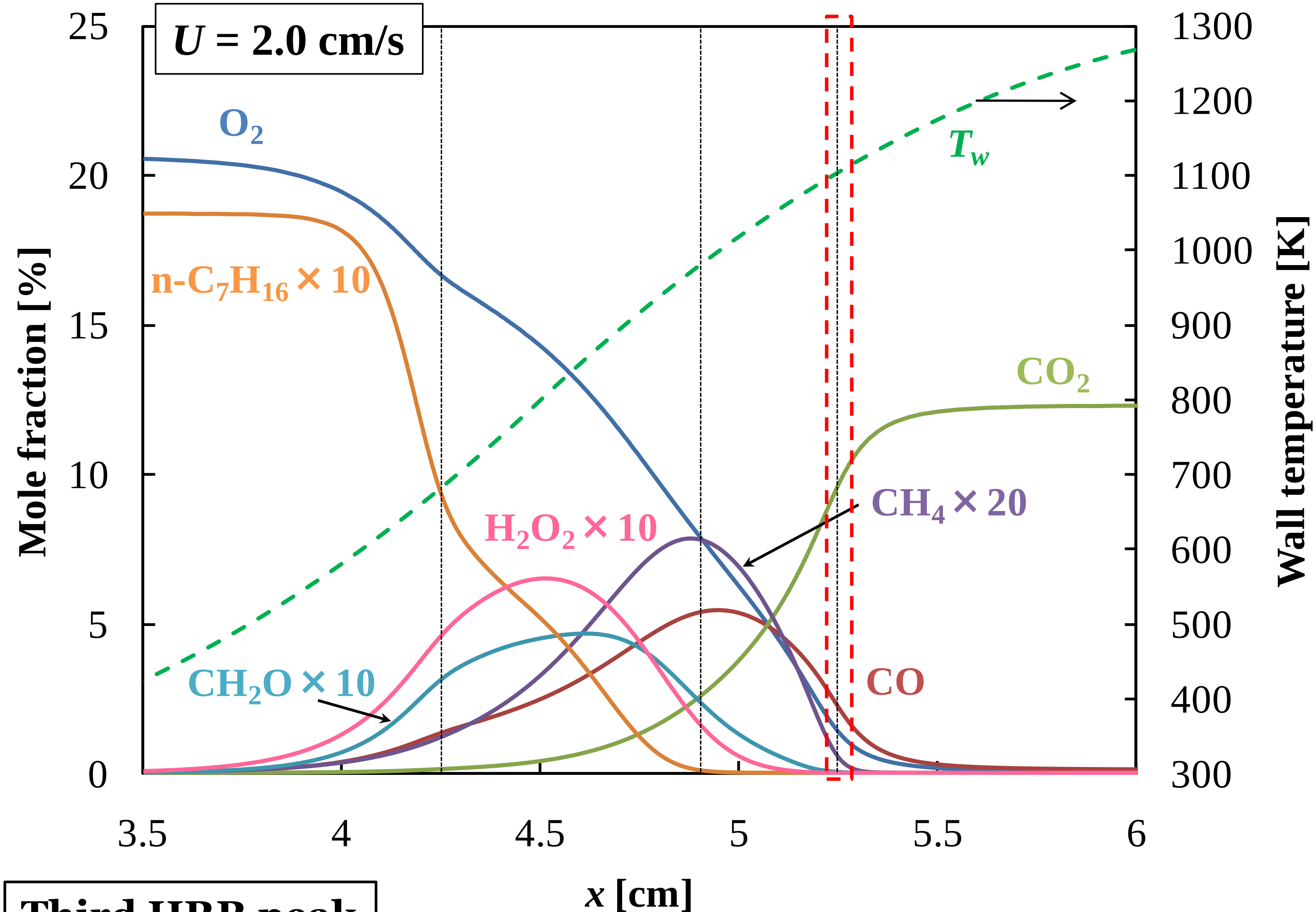
Partial oxidations:

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

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

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

Computational species profiles



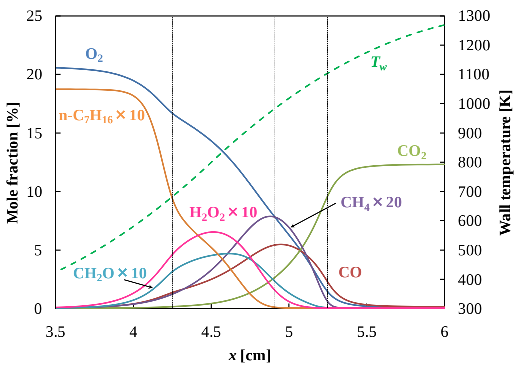
Third HRR peak

Full oxidations: $\mathbf{CO} + \mathrm{OH} \Rightarrow \mathbf{CO_2} + \mathrm{H}$

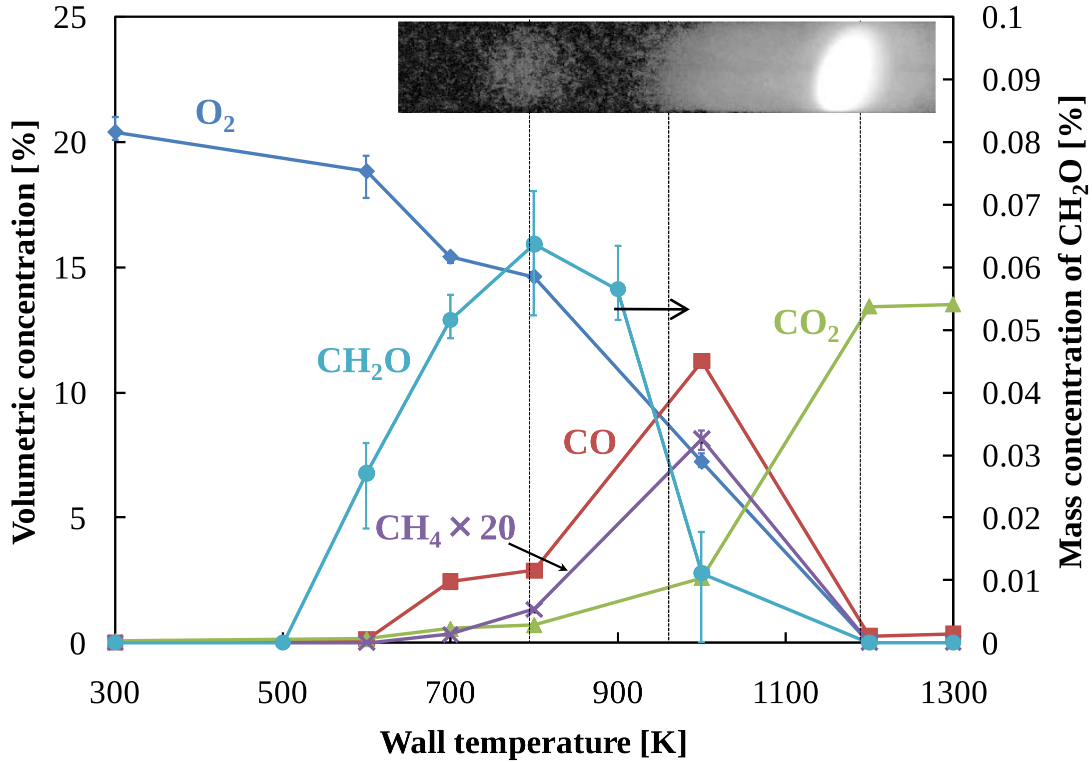
Measurements and computations

(U = 2.0 cm/s)

Computations



Measurement by GC

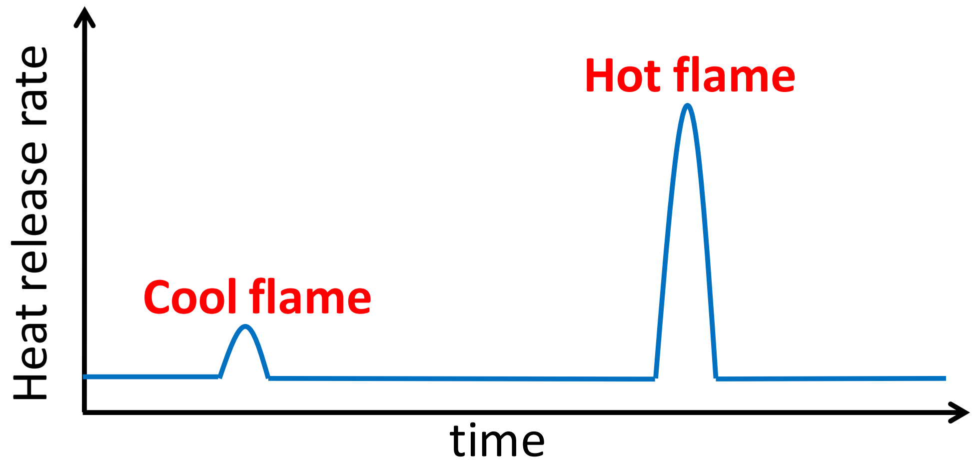


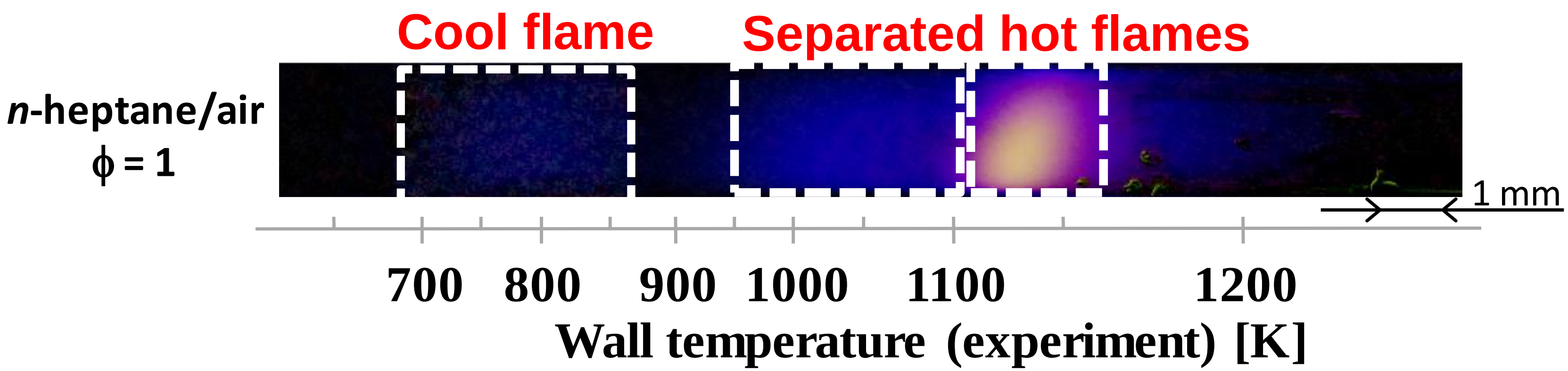
Three-stage oxidation process was confirmed by gas sampling experiment

Yamamoto et al., PCI 33

Interpretation of triple weak flames

Ignition in
RCM and ST
(**transient**)

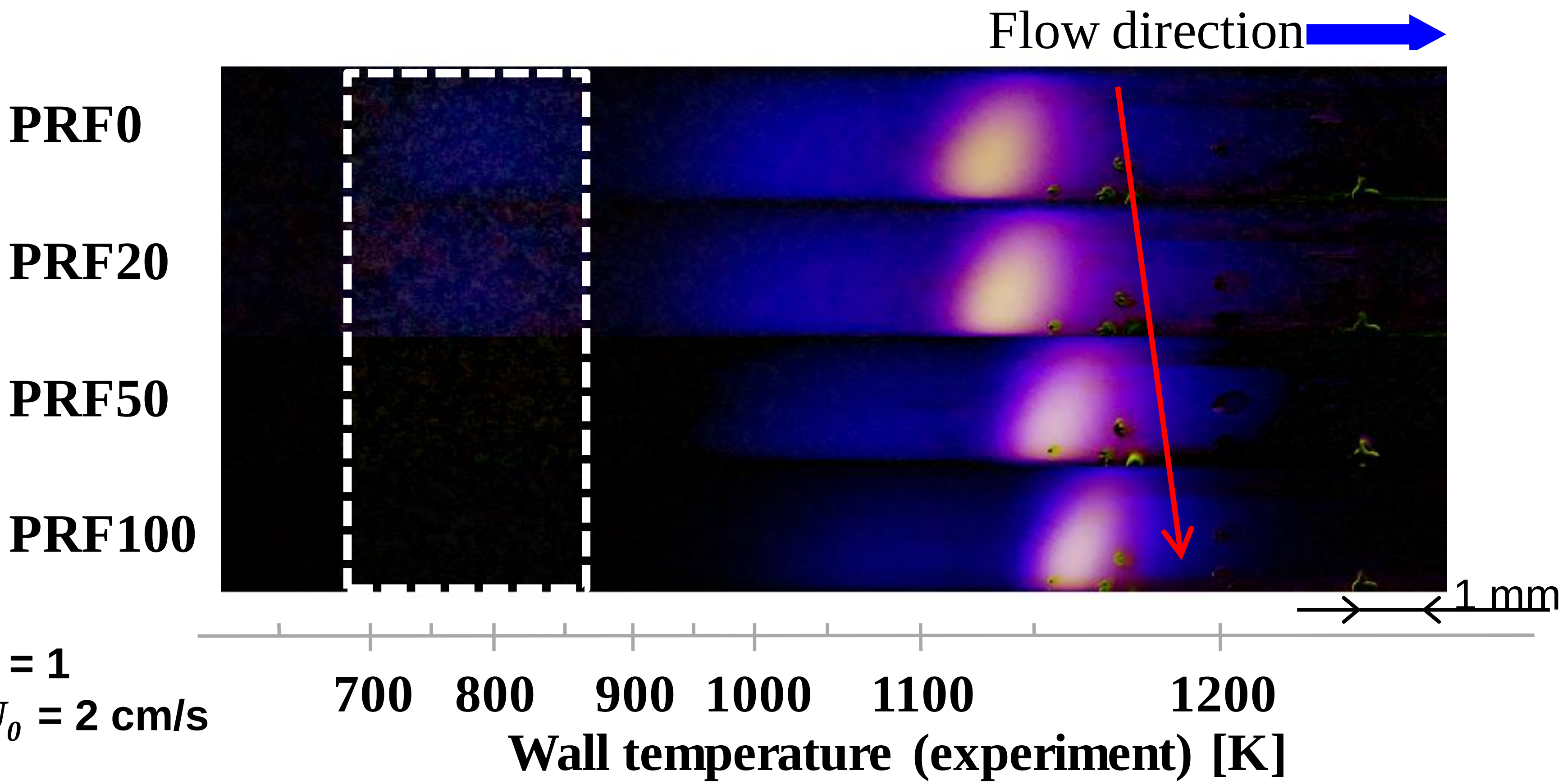




Conventional two-stage ignition converted into steady, three-stage, spatially-separated weak flames in MFR

MFR applied for gasoline PRF

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

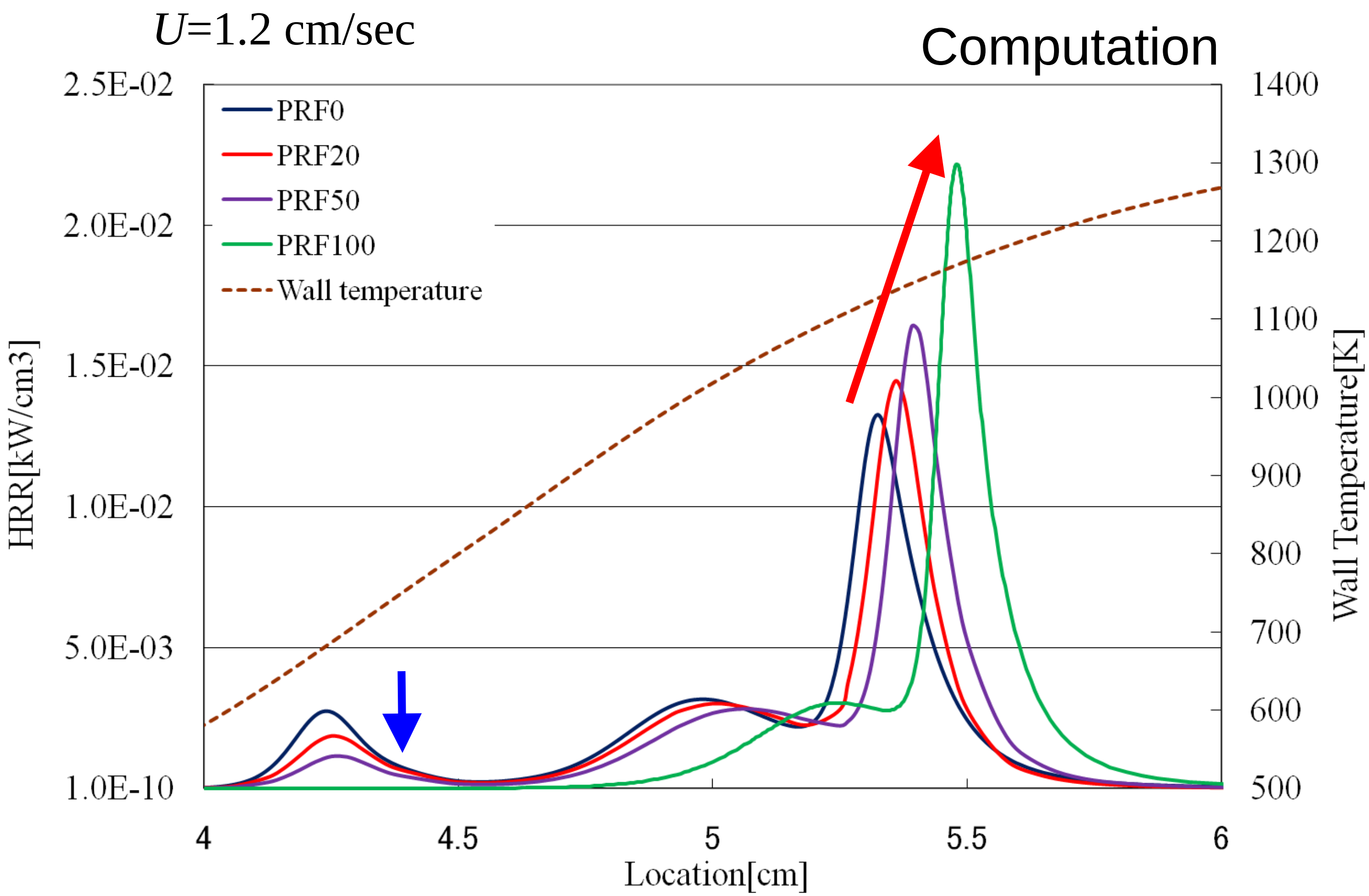


$\phi = 1$
U_0 = 2 cm/s

Appearances of multiple weak flames represent Research Octane Number

* Hori, et al., CNF 2012

Weak flames at different RON

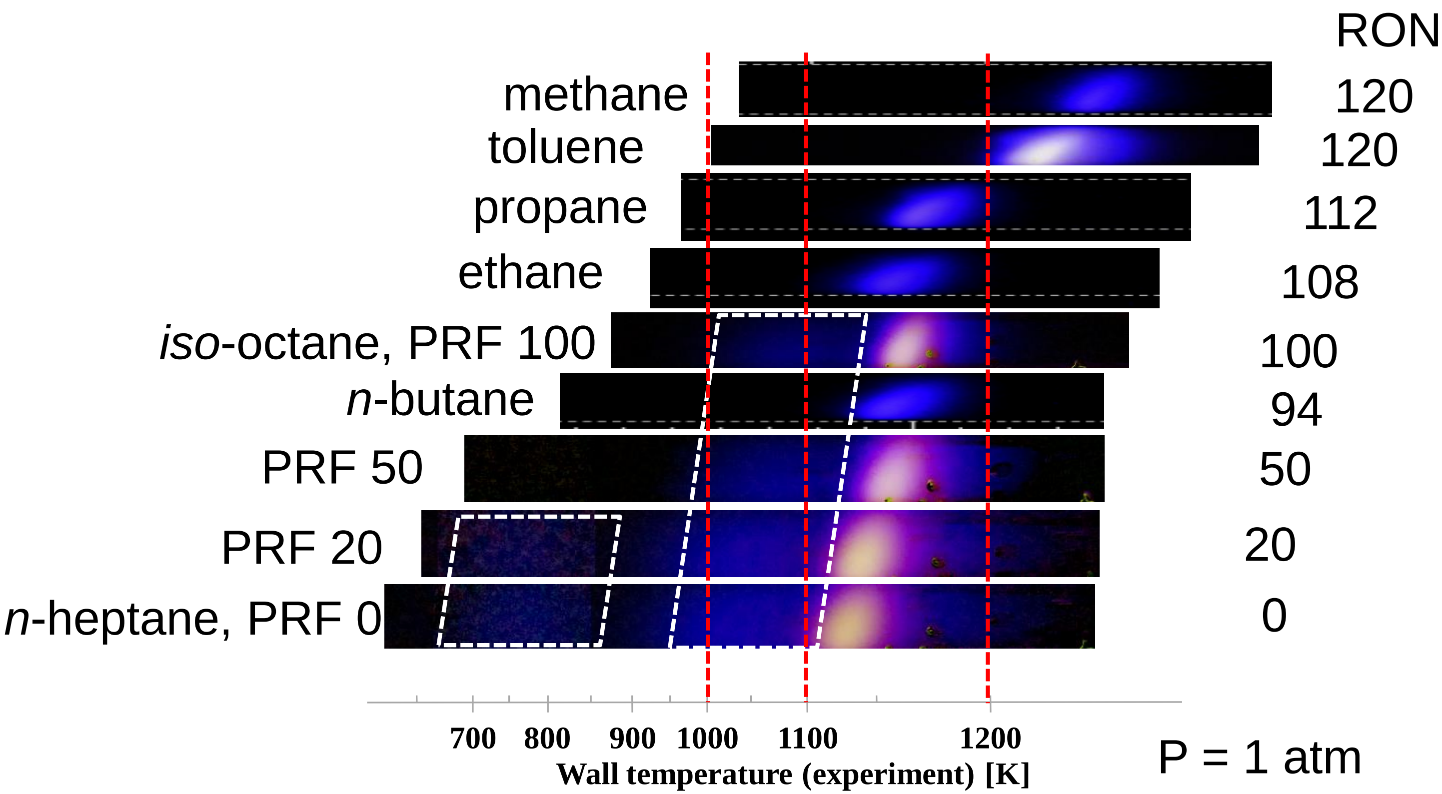


Significant LTO in smaller RON

Weak flame behaviors reproduced

* Hori, et al., CNF 2012

Weak flame appearances for various RON

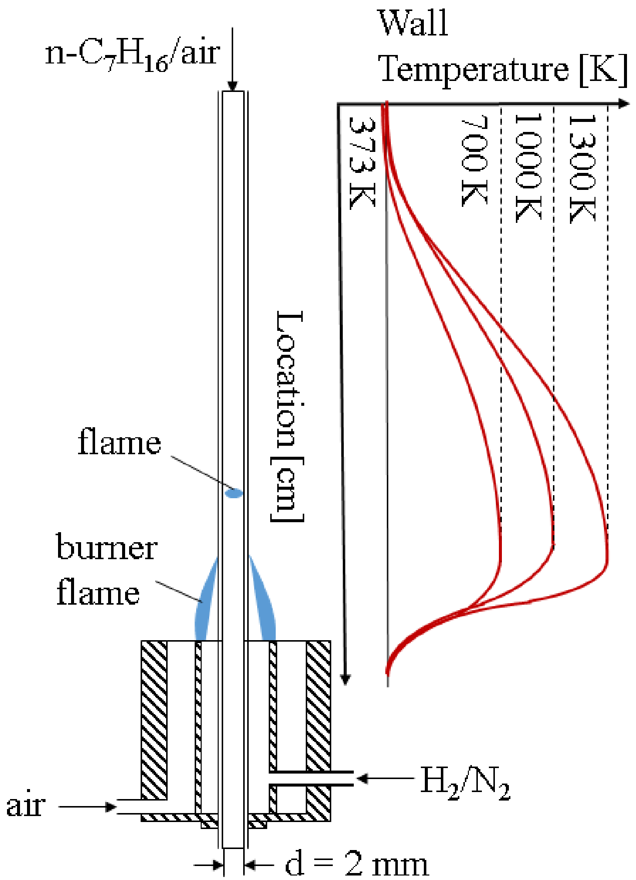


Weak flame locations: monotonic function of RON

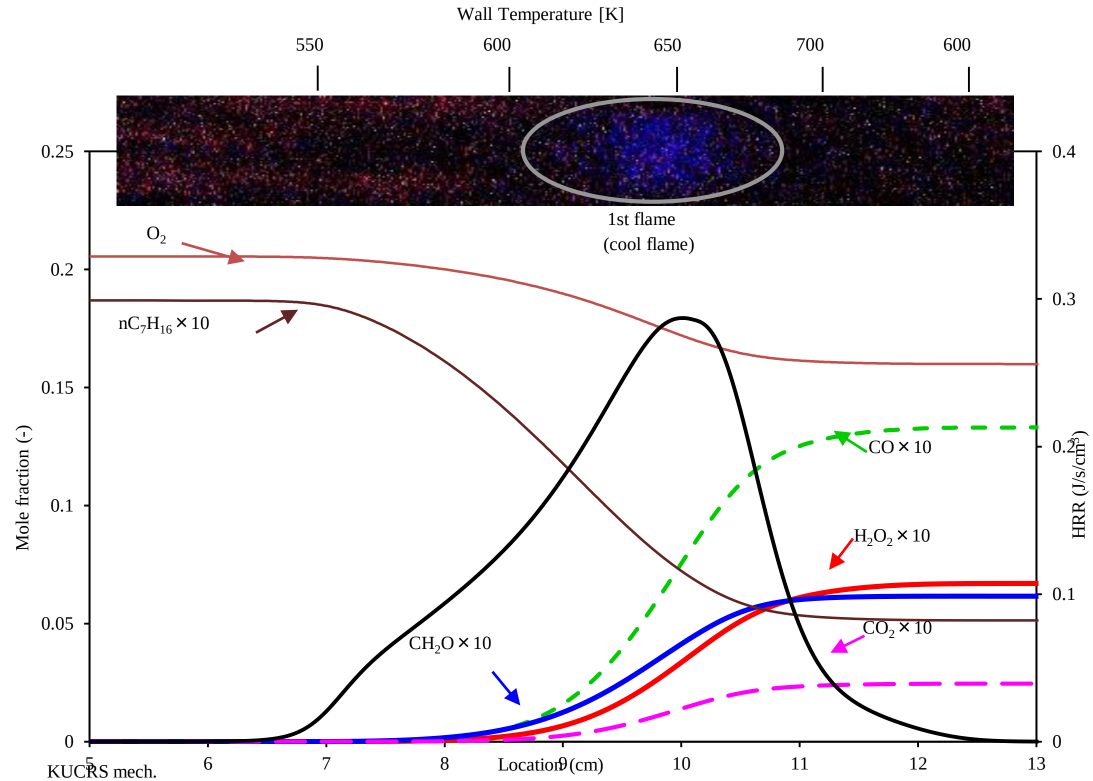
Second weak flame: visible when RON < 100

First weak flame: visible when RON < 20

Structure of a separated cool flame in MFR



KUCRS mech.

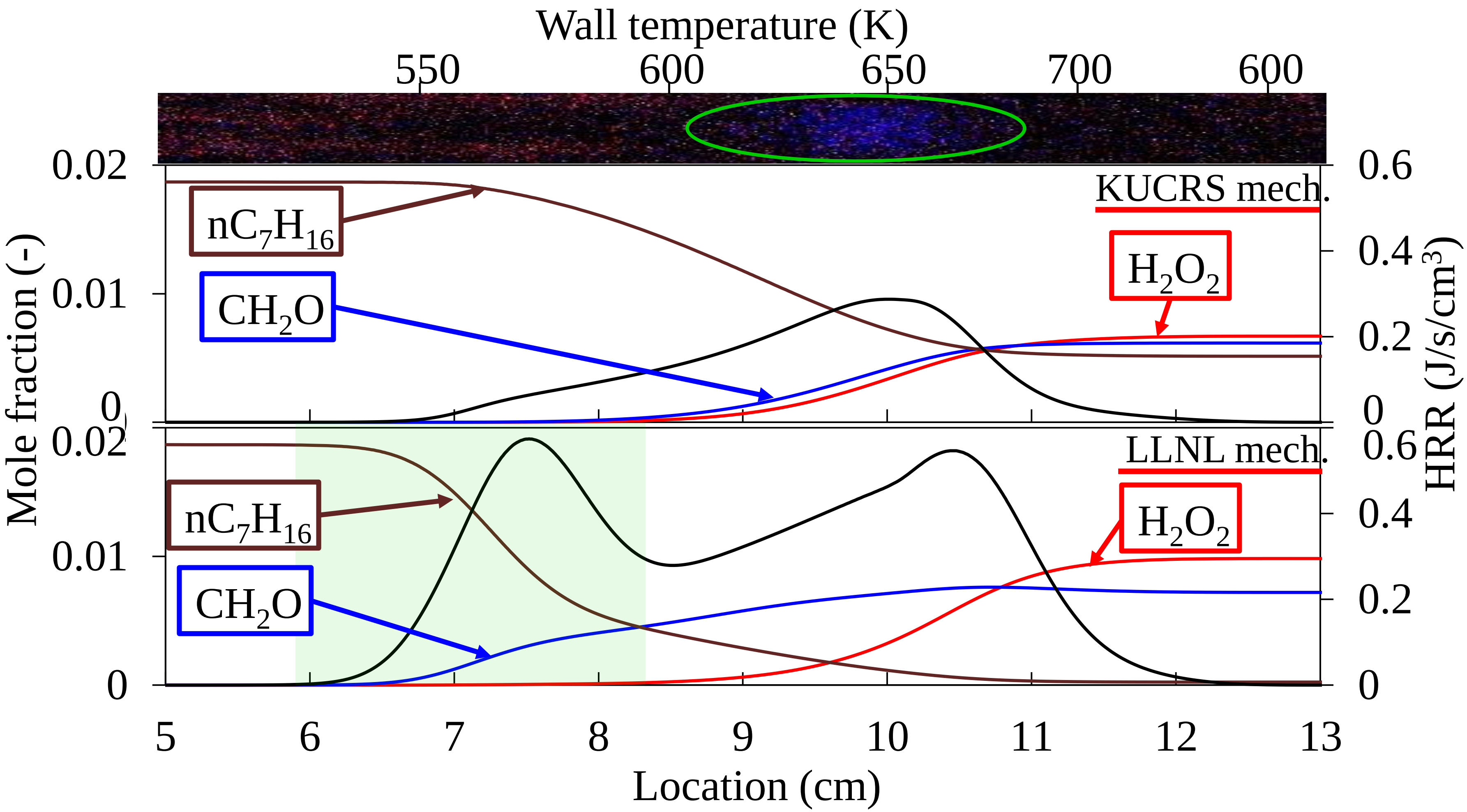


Vertical MFR
Small temp. grad.
Sym. & Higher res.

Tatsumi et al., Heat Transfer Symposium 2017.
Also, will be presented at ICDERS 2017.

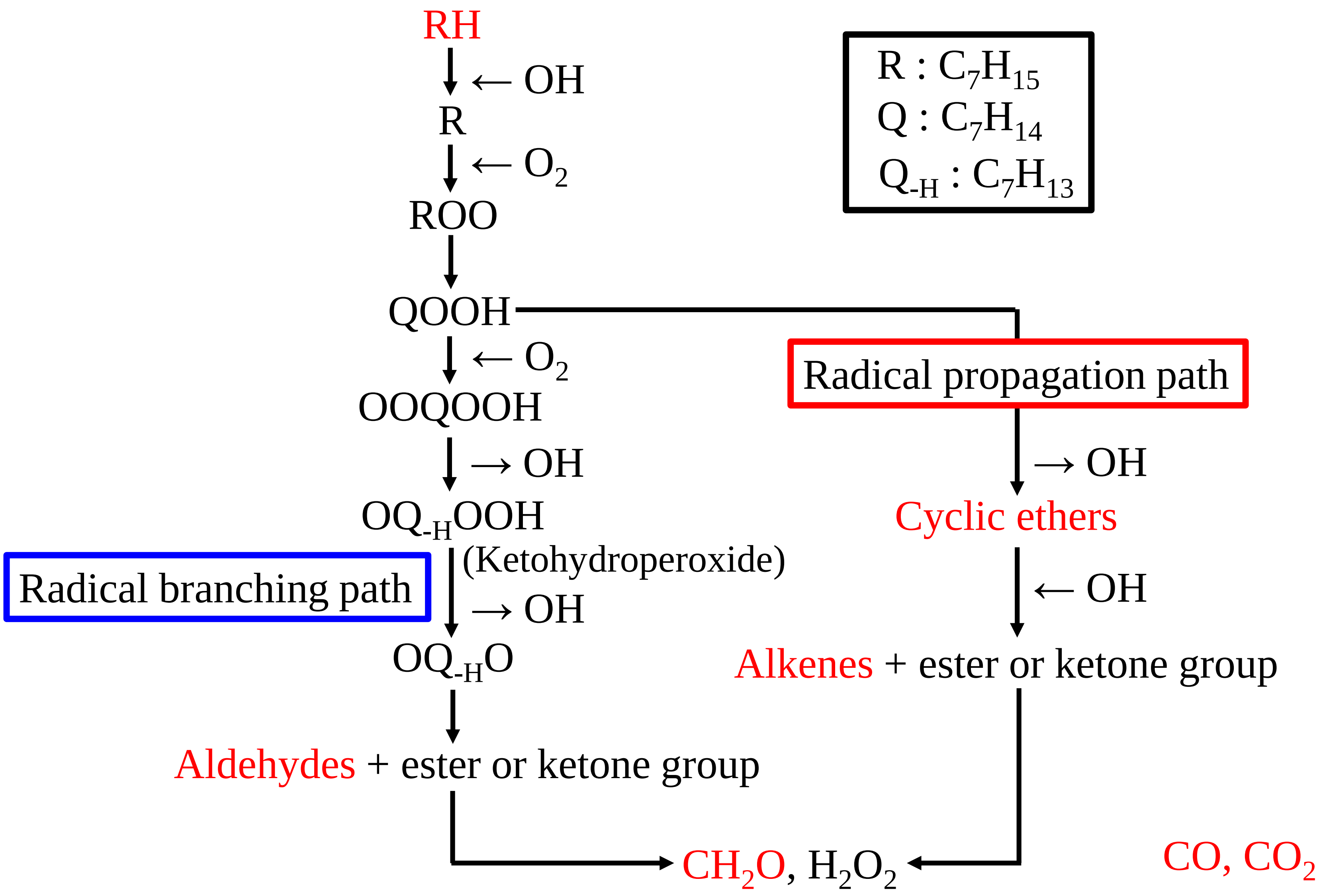
Structure of a cool flame, computation

Conditions : nC_7H_{16}/air, $\phi = 1$, $P = 1$ (atm), $V = 2$ (cm/s), Exposure time 30 (minutes)



Tatsumi et al., Heat Transfer Symposium 2017.
Also, will be presented at ICDERS 2017.

Reaction paths in a cool flame



Reactions in radical branching path

Conditions : nC_7H_{16}/air, $\phi = 1$, $P = 1$ (atm), $V = 2$ (cm/s), $T_{w,max} = 700$ (K)   KUCRS mech.

QOOH ($C_7H_{14}OOH$)

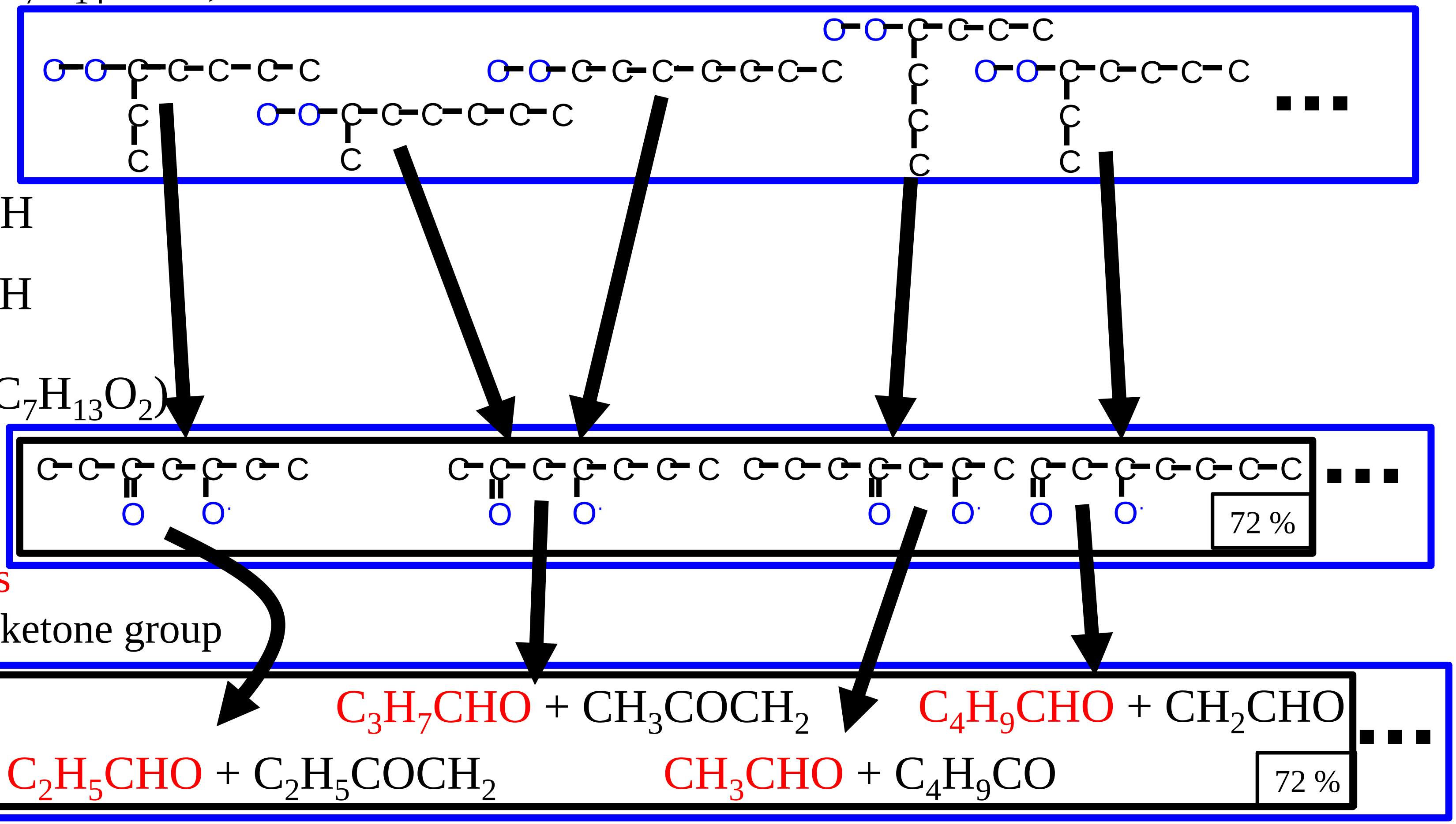
OOQOOH

$OQ_{-H}OOH$

$OQ_{-H}O$ ($C_7H_{13}O_2$)

Aldehydes

+ ester or ketone group



Reactions in radical propagation path

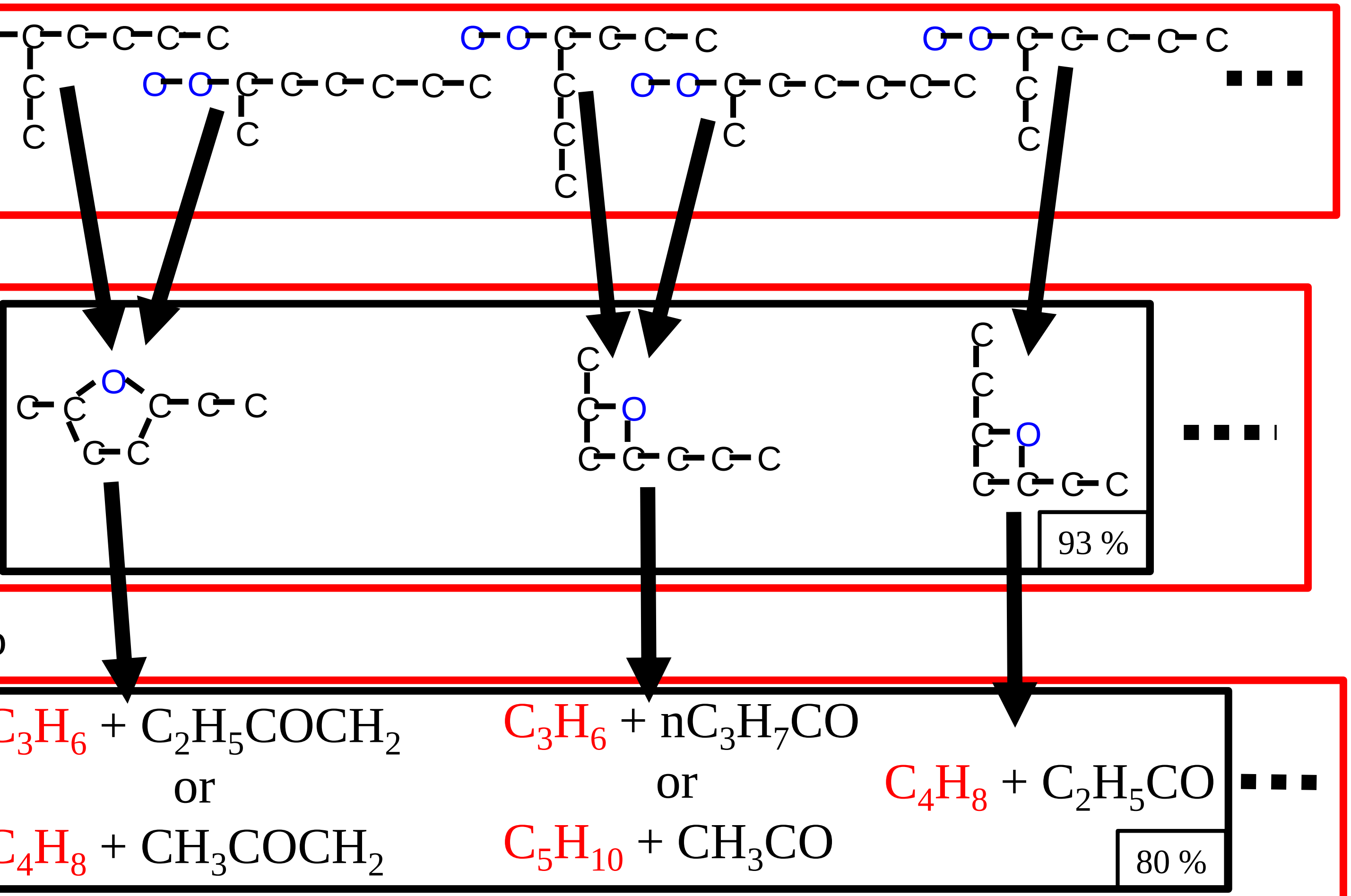
Conditions : nC_7H_{16}/air, $\phi = 1$, $P = 1$ (atm), $V = 2$ (cm/s), $T_{w,max} = 700$ (K)   KUCRS mech.

QOOH ($C_7H_{14}OOH$)

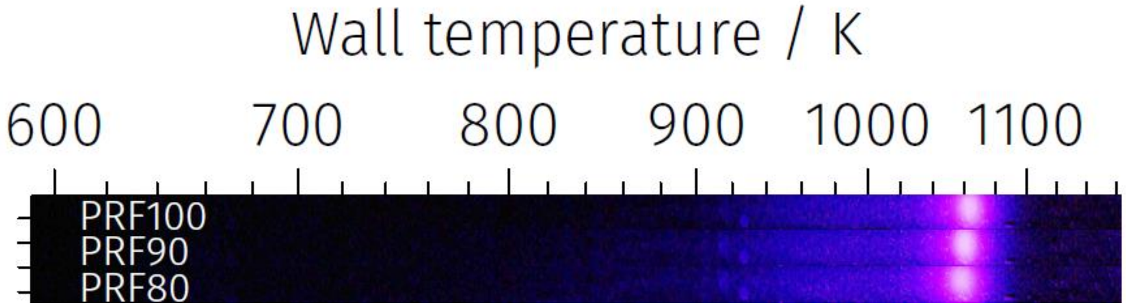
Cyclic ethers

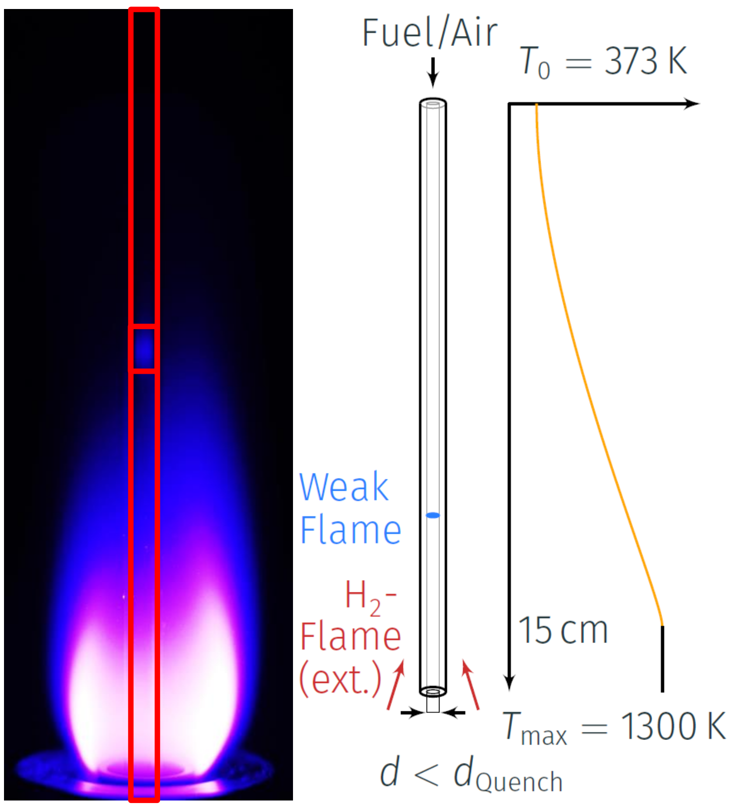
Alkene

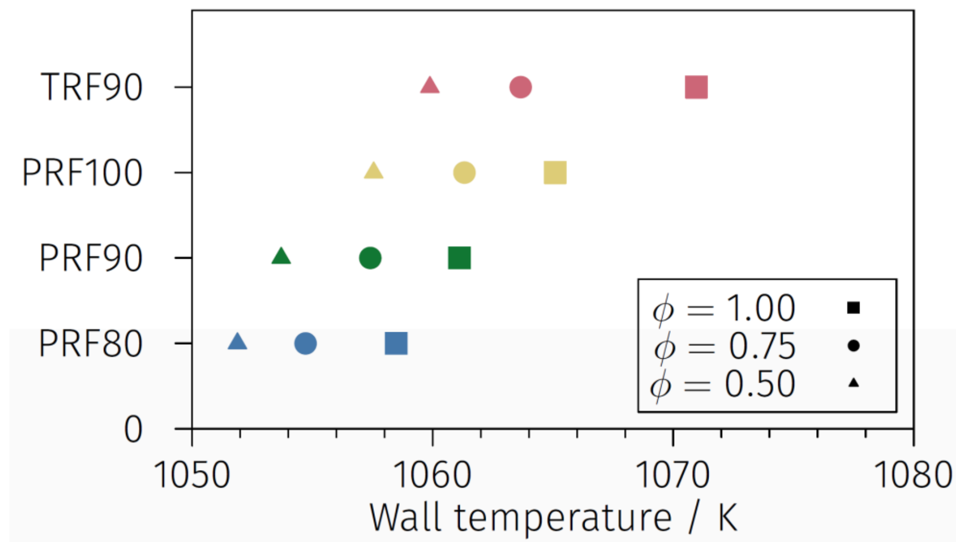
+ ester or ketone group



PRFs, ultra lean, higher resolution







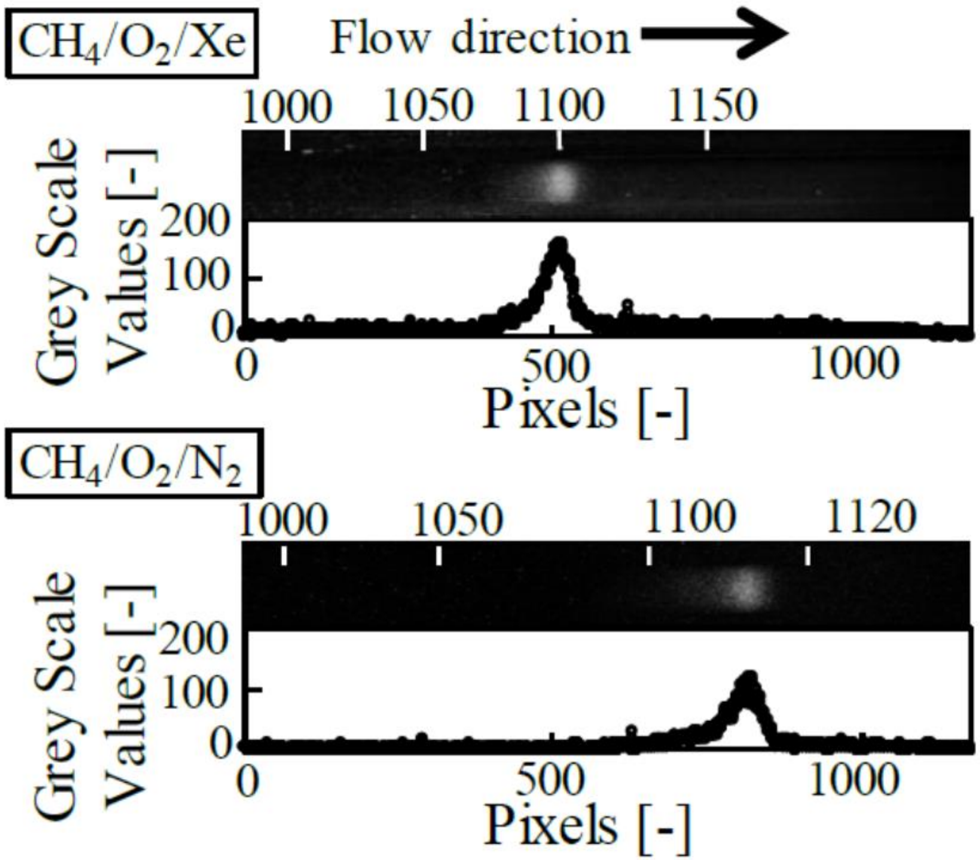
Vertical-type reactor

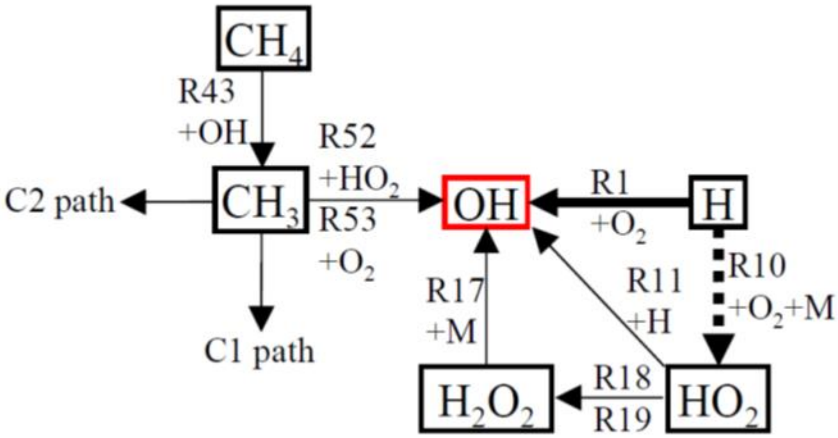
Grajetzki, et al., 36 Symp, WIP.

CH_4, ultra lean and Xe dilution

Fuel: CH_4; O_2/Inert = 0.141; ϕ = 0.3

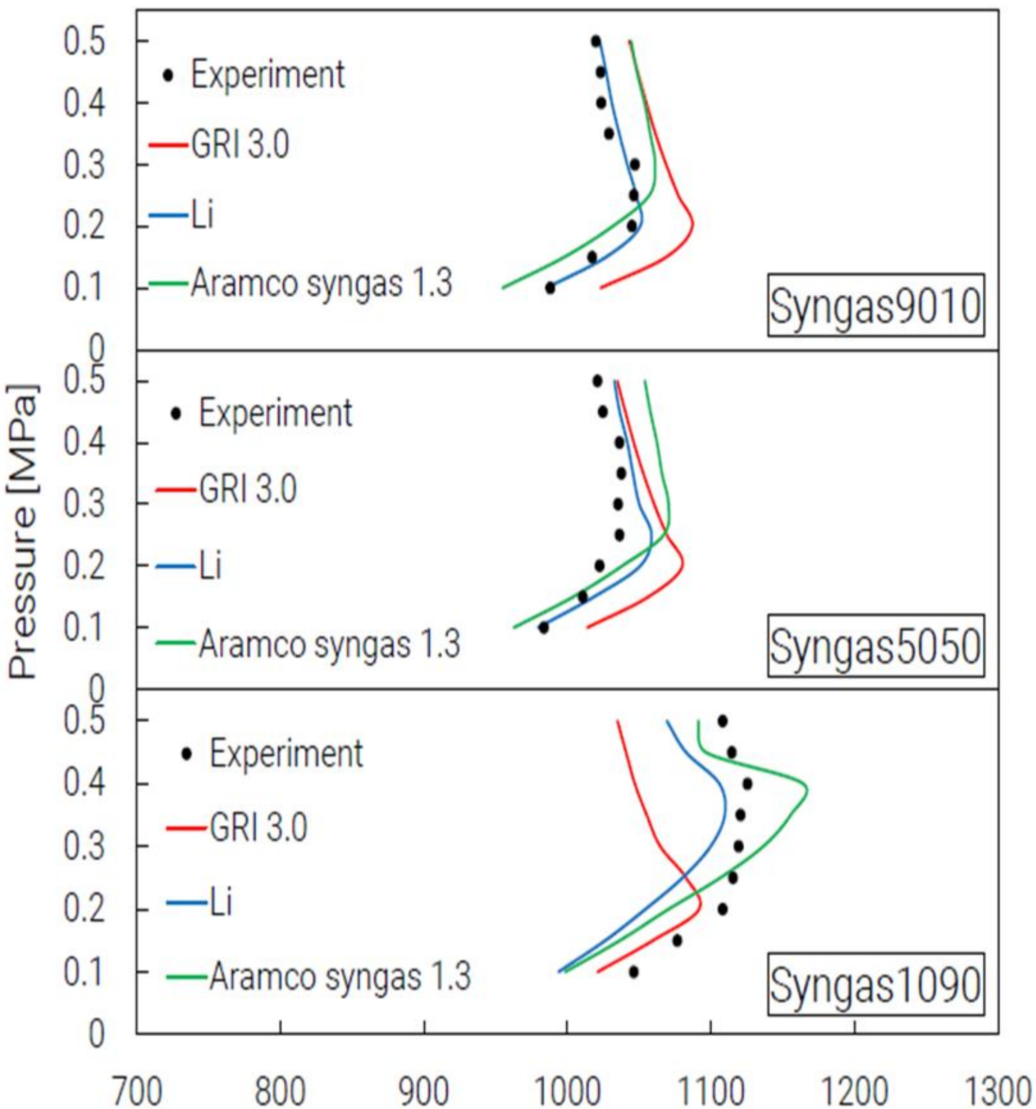
Conducted for analyzing microgravity experiments on interaction between flameball and counterflow flames

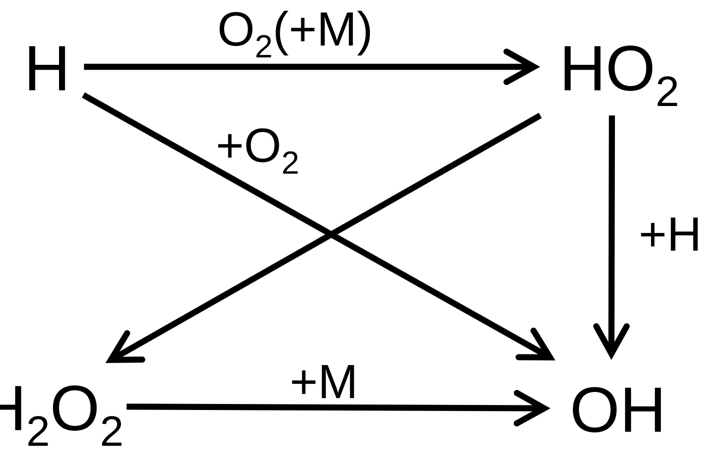




Okuno et al., PCI 36.

Syngas, elevated pressures

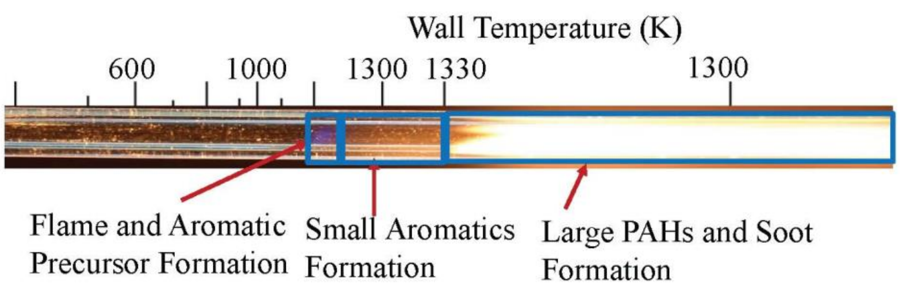


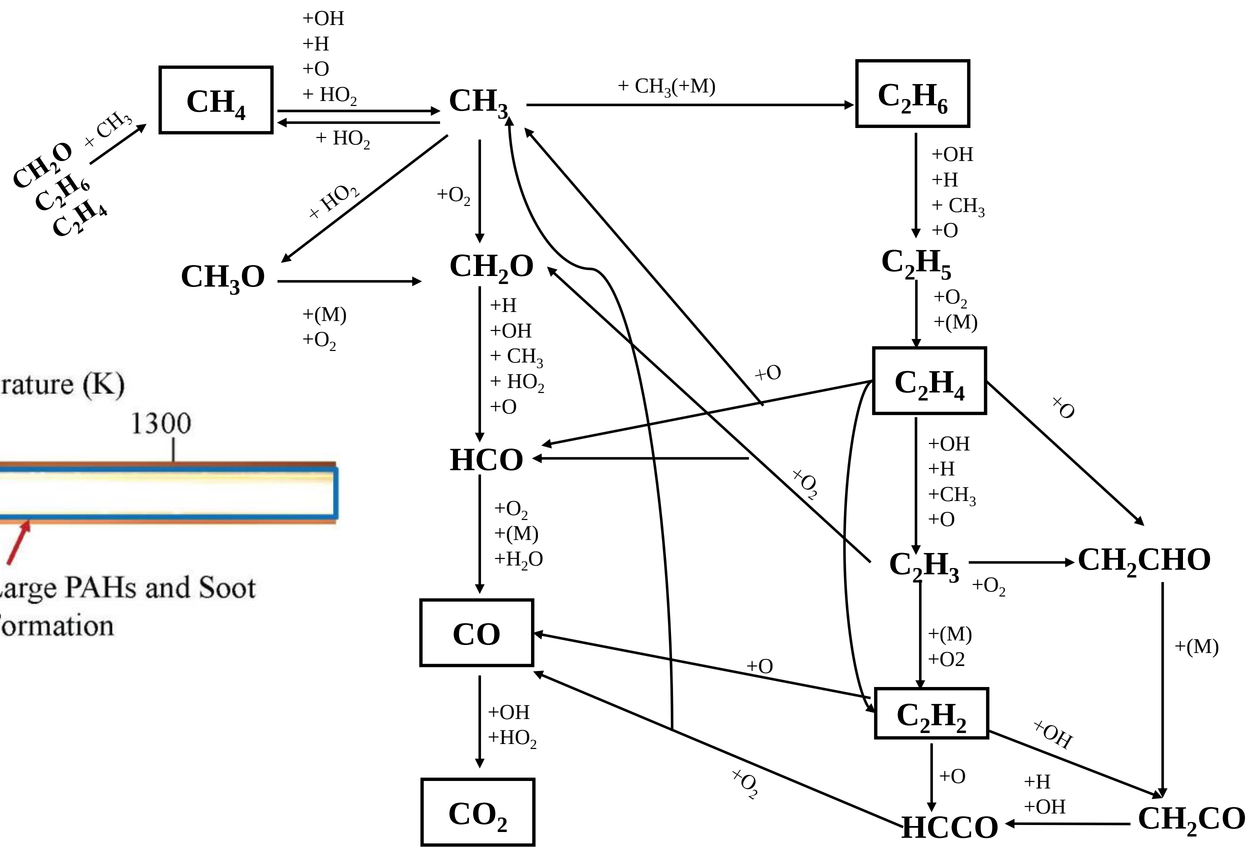


Relevant to H_2-O_2 explosion peninsula

Tanaka et al., 36symp. WIPP.

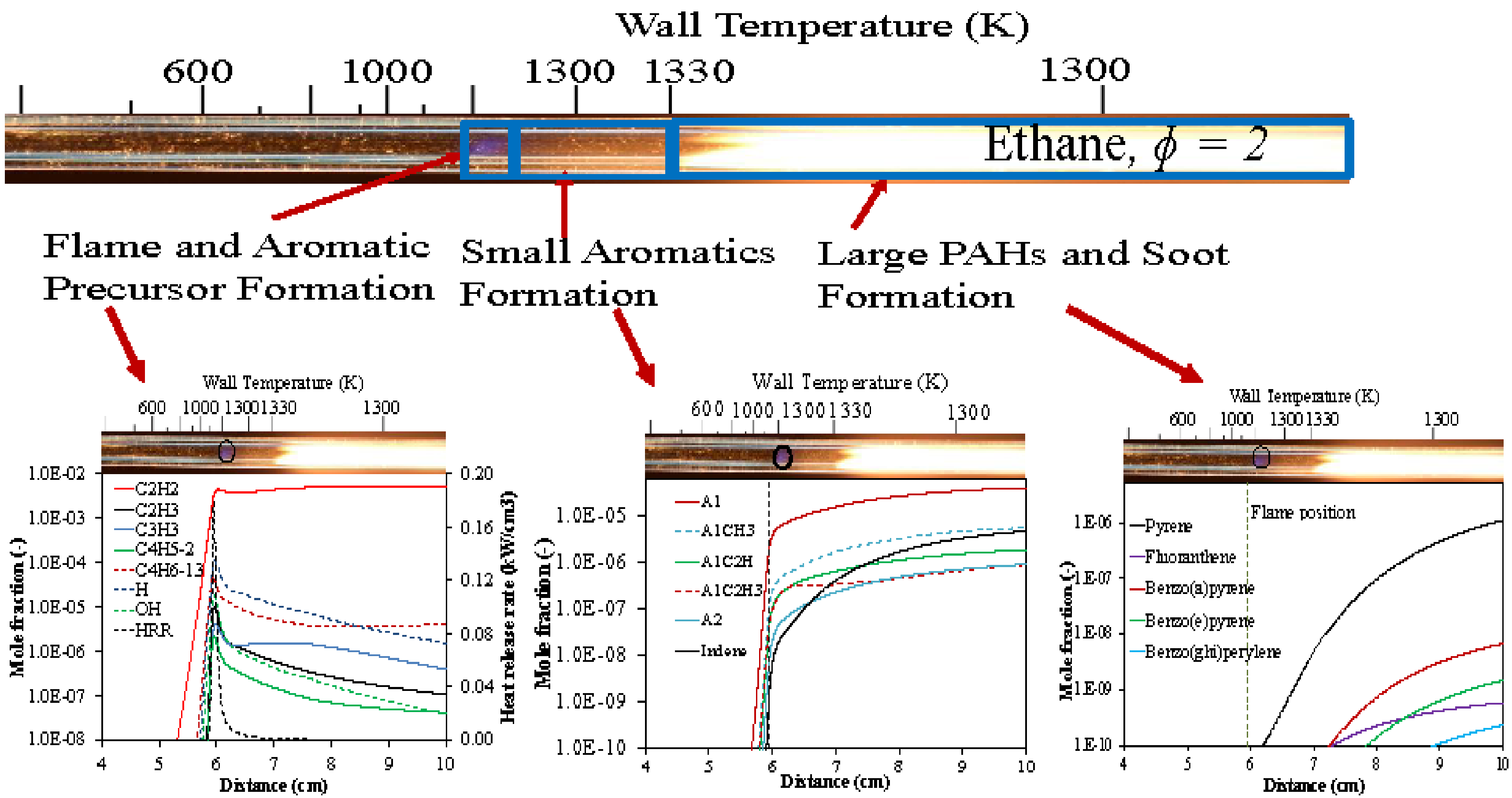
Soot and PAH formations at temperature below 1400 K





* Dubey et al., CNF 2017.

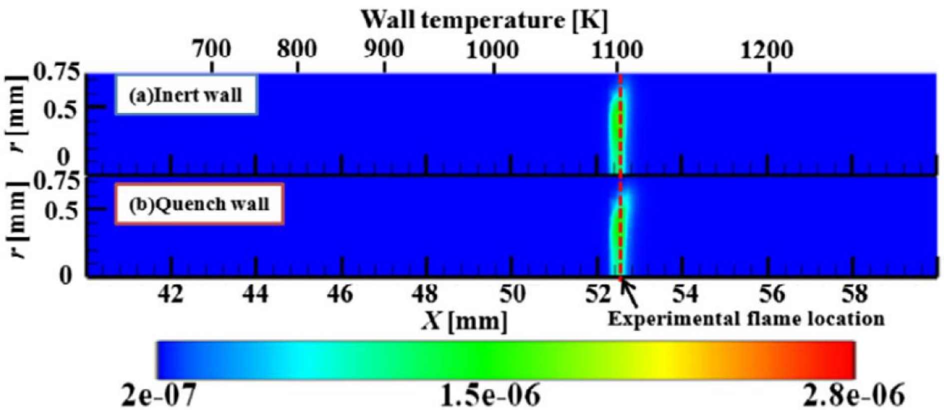
Soot and PAH formations at temperature below 1400 K

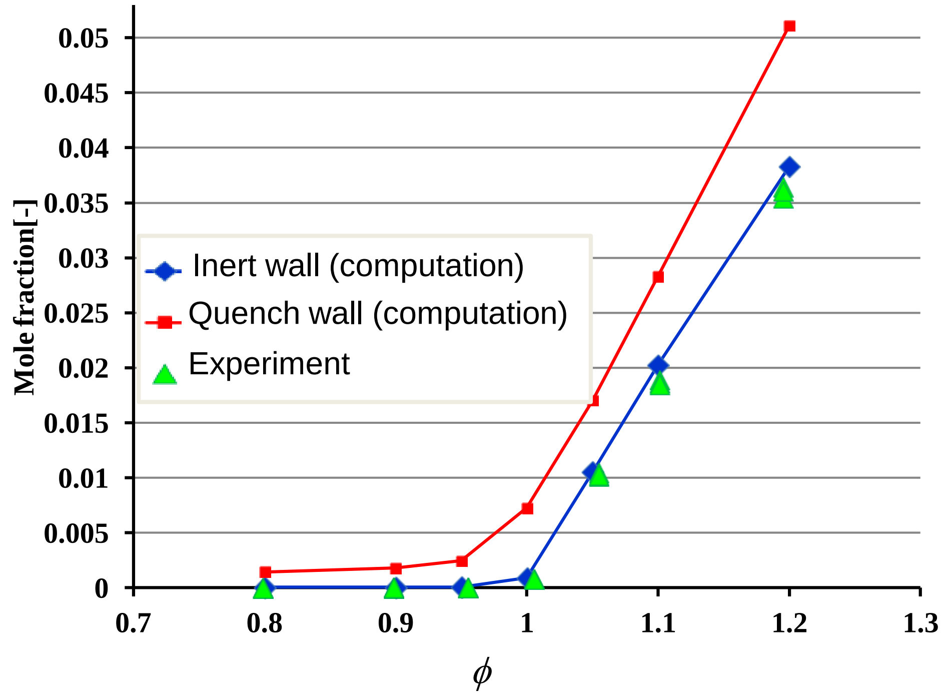


* Dubey et al., CNF 2017.

Effect of radical quenching at wall

CH$_4$/air; $\phi = 1$; d = 1.5 mm, 1 atm





Inert: GRI3.0
Quench: GRI 3.0 + Raimondeau

- CO mole fraction of burned gas:
  Quench case > Inert case
- Experimental results agree with Inert case

→ radical quenching effect negligible

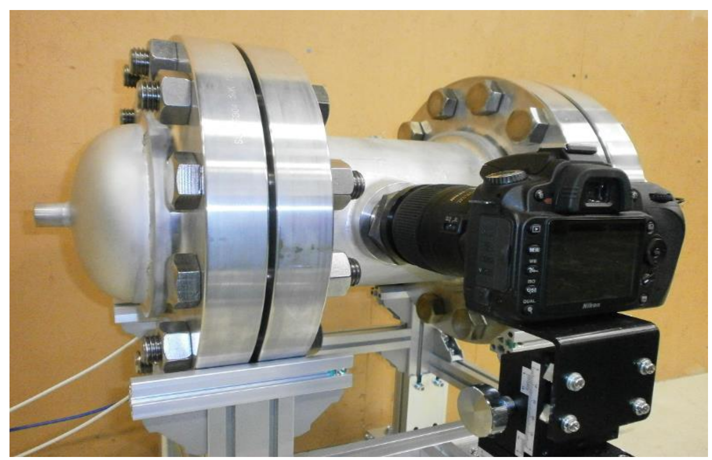
Kizaki, et al., PCI35 (2015)

Conclusions

Micro flow reactor with prescribed temperature profile can be a new platform for study on chemical kinetics particularly for low temperature conditions

Acknowledgements

IHI, NEDO, HITACHI, TOKYO GAS, JSPS, JST



IHI, IIC, HONDA R&D, MAZDA