(5E05)

Characteristics of *n*-heptane and toluene weak flames in a micro flow reactor with a controlled temperature profile

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Background
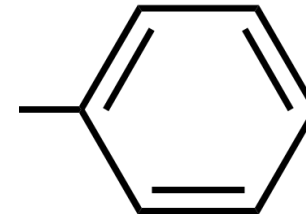
Fundamental ignition characteristics of gasoline surrogate

n–**Heptane** and **toluene** are one of the
major components of gasoline surrogate

n–Heptane	Toluene

- High reactivity (ON = 0)
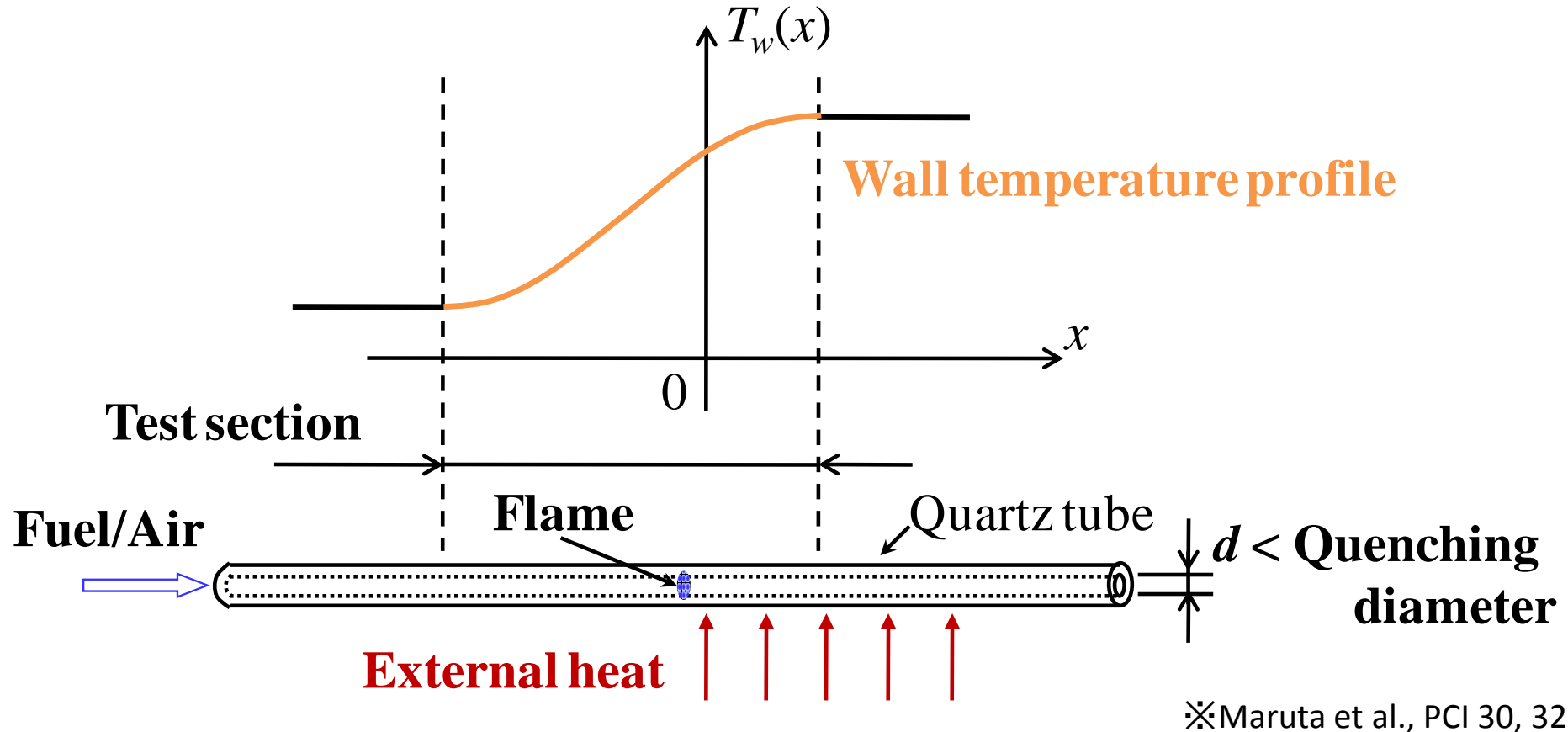- A large number of experiments in a wide range of temperature

- Low reactivity (ON = 120)
- Few experiments especially in low to intermediate temperature

A micro flow reactor with a controlled temperature profile

Micro flow reactor with controlled temperature profile

$T_w(x)$

Wall temperature profile

x

0

Test section

Fuel/Air

Flame

Quartz tube

d < Quenching diameter

External heat

※Maruta et al., PCI 30, 32

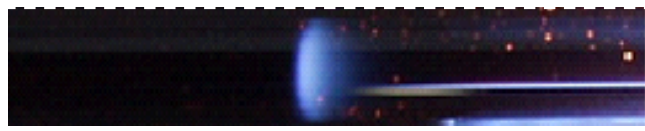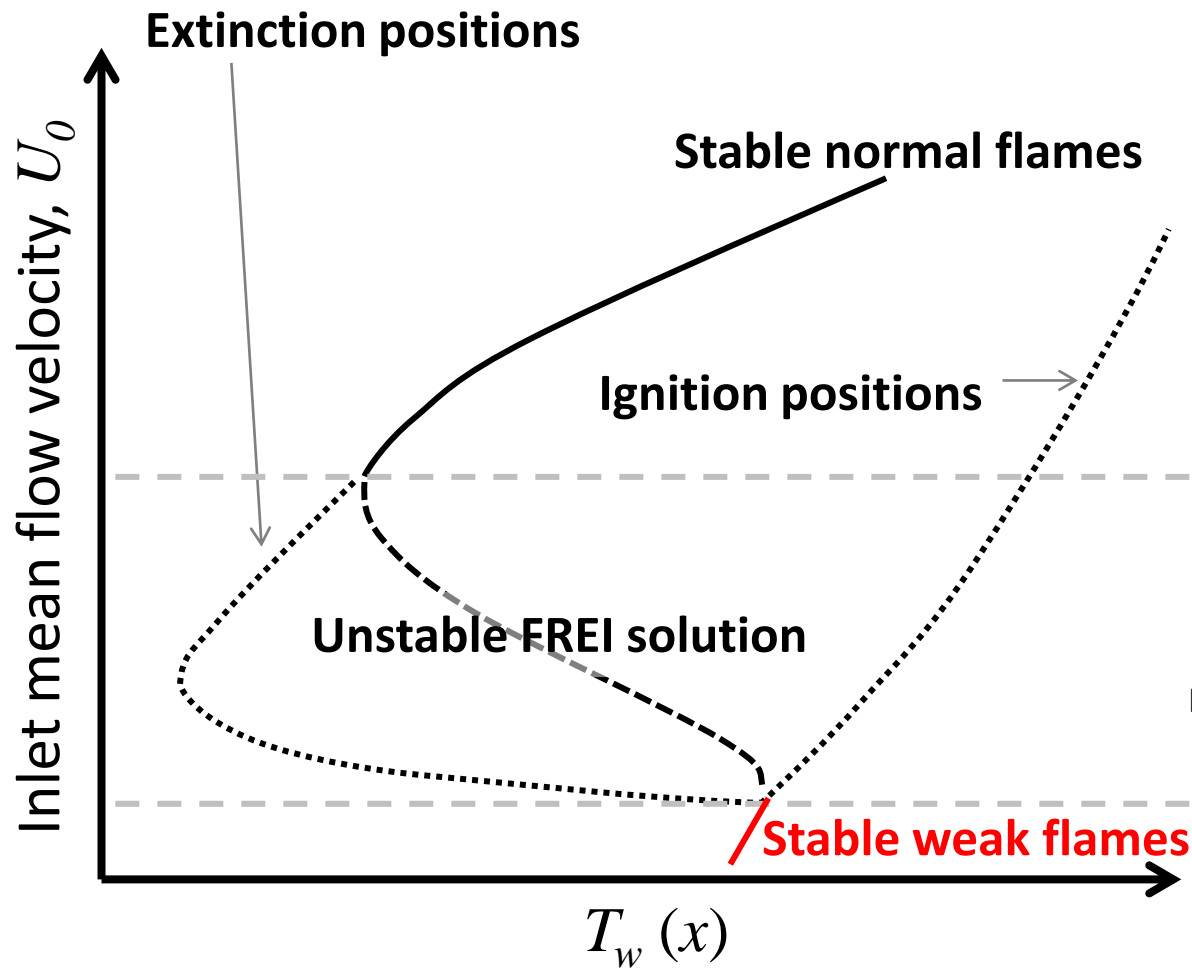- Imposed wall-temperature profile along inner surface of reactor
- Inner diameter of the tube < Quenching diameter
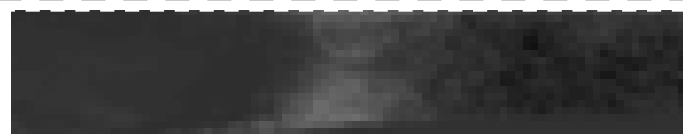- Laminar flow (Re ≈ 1 - 100)
- Constant pressure

Interpretation of flame behavior in micro reactor

Extinction positions

Stable normal flames

Ignition positions

Unstable FREI solution

Stable weak flames

Inlet mean flow velocity, U_0

$T_w(x)$

* Maruta et al., PCI 30, 32
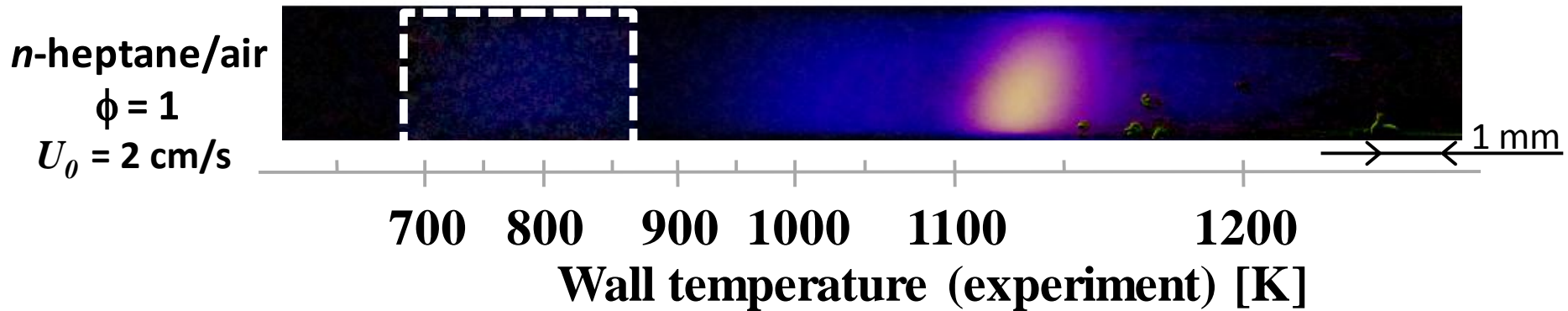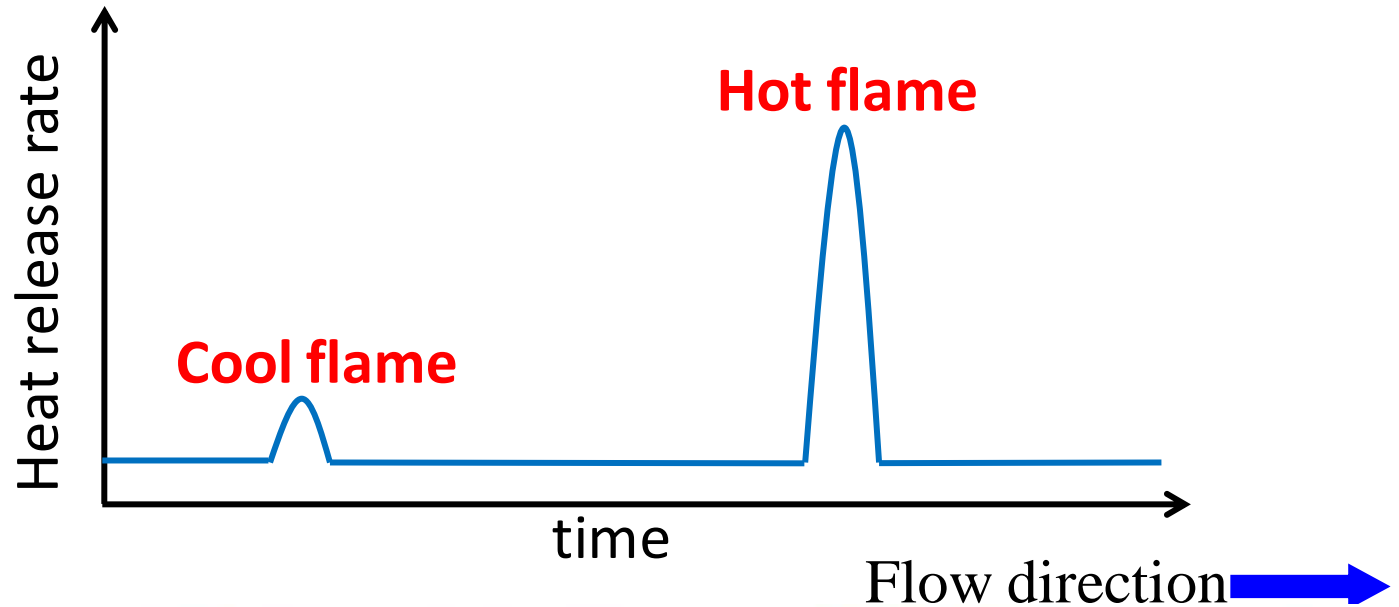* Minaev et al., CTM 11

$\phi = 1$, CH_4/air

Flames with Repetitive Extinction and Ignition

- **Three regimes were observed experimentally, numerically and theoretically**
- **Weak flame branch = ignition branch in Fendell curve**
- **Weak flame temperature ≈ wall temperature**

Reactions in the temperature zone relevant for initiation of ignition

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Separated weak flames and multi-stage ignition

Heat release rate vs. time: Cool flame (small peak), Hot flame (large peak)

n-heptane/air
$\phi = 1$
$U_0 = 2$ cm/s

Flow direction →

Wall temperature (experiment) [K]: 700 800 900 1000 1100 1200

1 mm

* Yamamoto, et al., PCI33

- **Reactions in initiation of ignition can be investigated by steady, spatially-separated weak flames**
- **Spatial separation = identification of onset temperature of reactions**

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Fuel reactivity measurement
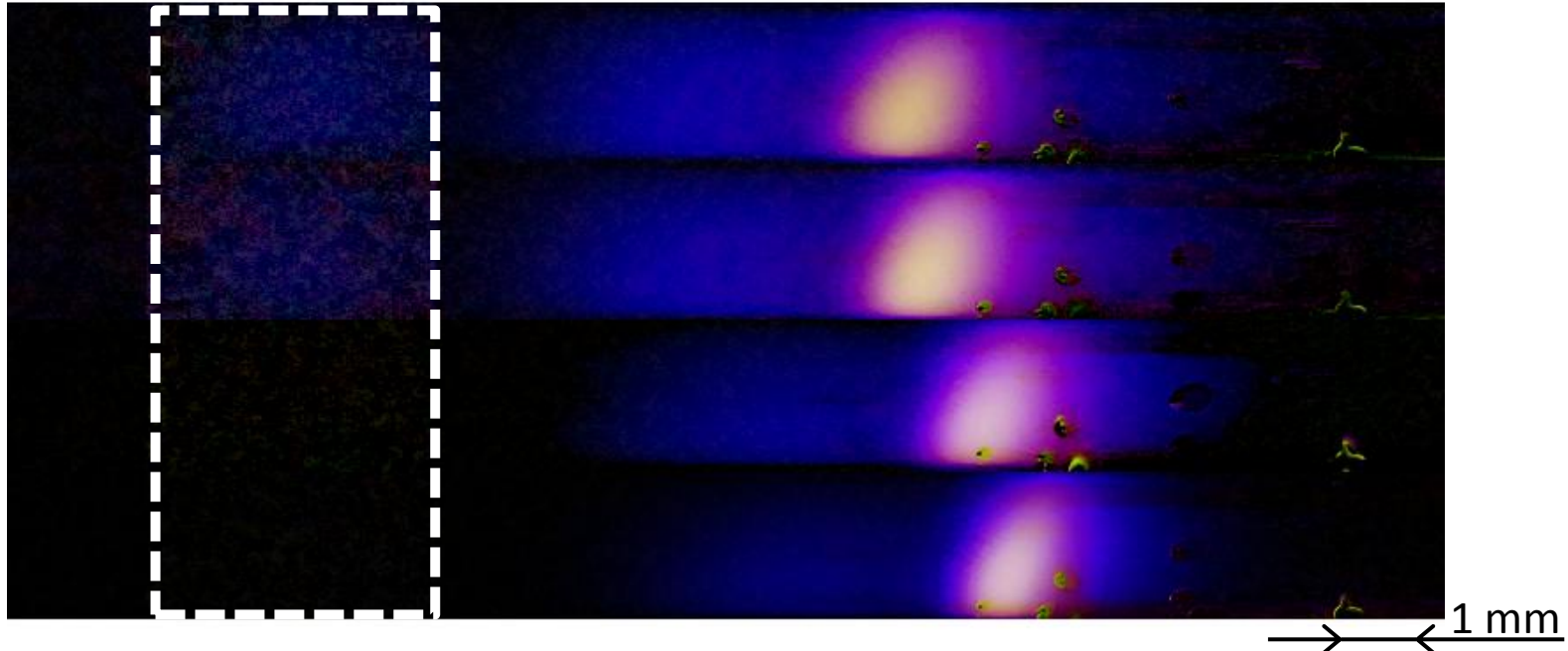
Octane number dependence:

Flow direction ➡

PRF0

PRF20

PRF50

PRF100

1 mm

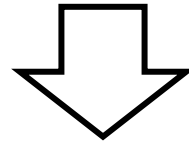$\phi = 1$
$U_0 = 2$ cm/s

700   800   900   1000   1100   1200

Wall temperature (experiment) [K]

**Cetane number dependence:** next presentation (5E06)

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Objective

The methodology of a micro flow reactor with a controlled temperature profile is employed for n–heptane, toluene and their blends
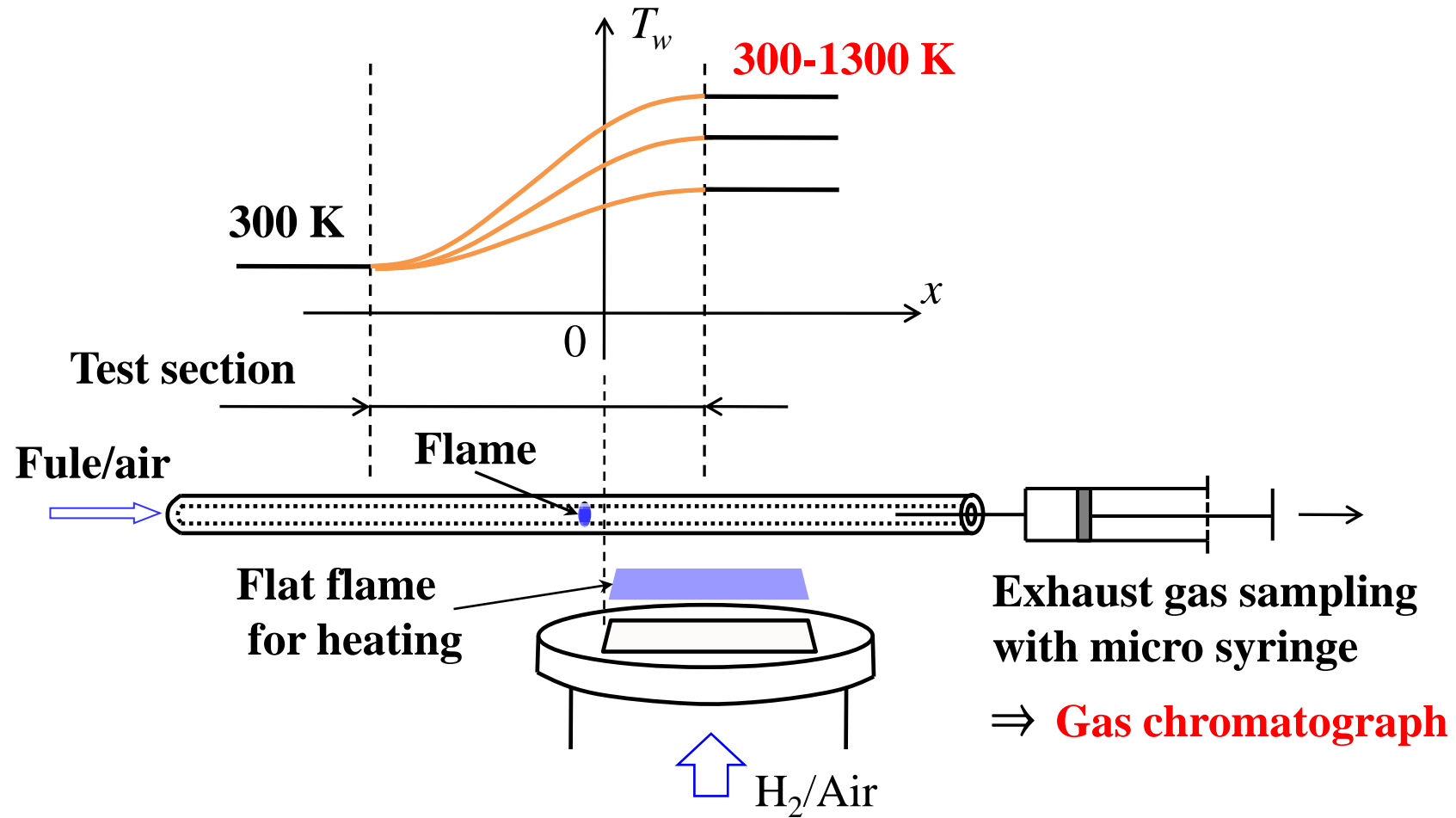
⬇

Investigate n–heptane/air, toluene/air and blends/air weak flames to examine effect of toluene addition to ignition process

Experimental setup

Wall temperature profile

T_w

1300 K

300 K

Test section

O

x

Fuel/Air

Flame

External heat

d = 1 or 2 mm

H_2 / Air
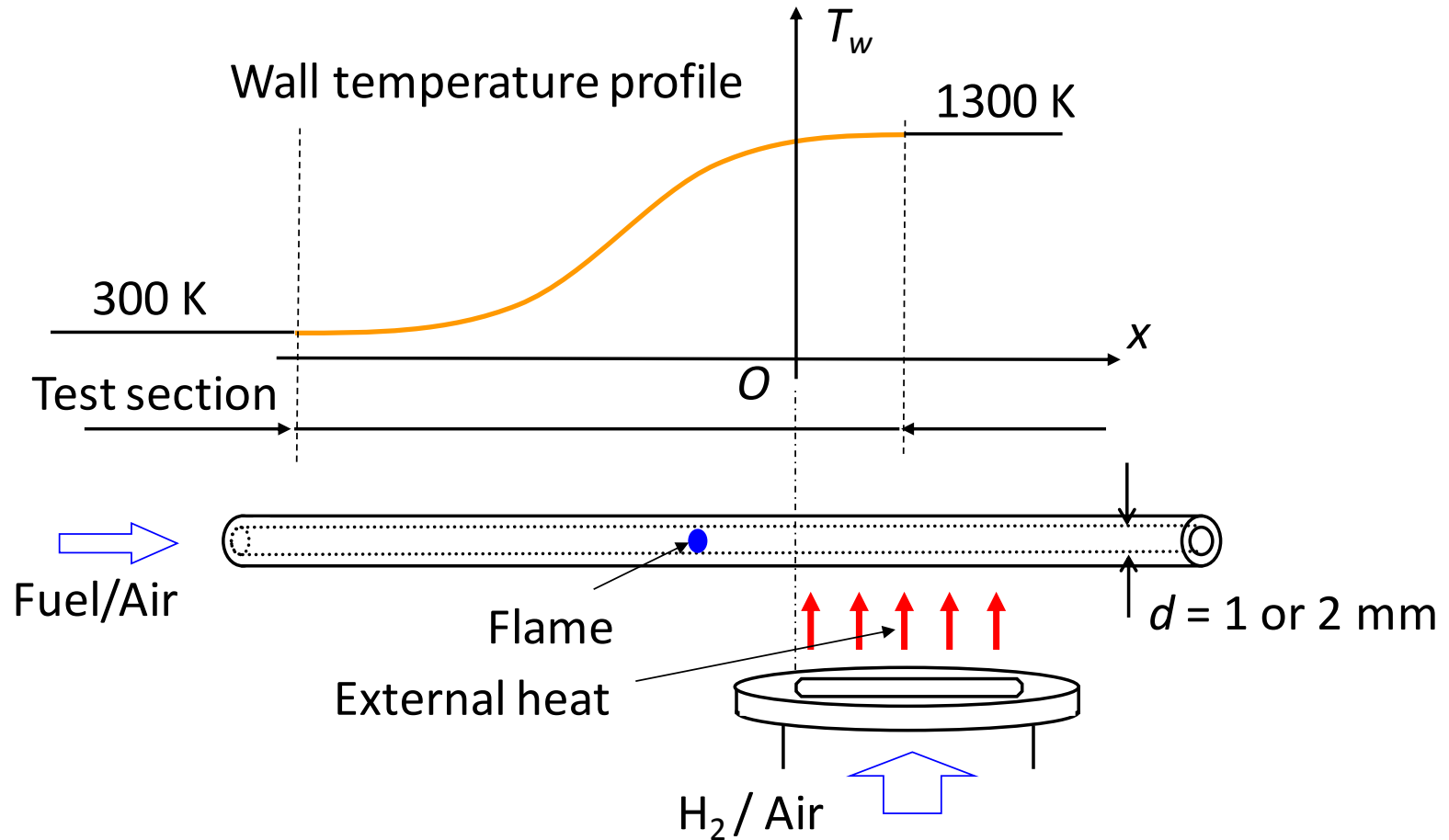
- Stationary temperature profile along inner surface of reactor (300–1300 K for 4 cm)
- U_0 = 2.5 cm/s; P = 1 and 5 atm; d = 1 (P = 5 atm) and 2 mm(P = 1 atm)
- Flame images were taken by CH-filtered camera at 2 min. exposure

Gas sampling

Test section

T_w

300-1300 K

300 K

x

0

Fule/air

Flame

Flat flame for heating

H_2/Air

Exhaust gas sampling with micro syringe

⇒ **Gas chromatograph**

* Yamamoto, et al., PCI33

- **Maximum wall temperature was controlled from 300 to 1300 K**
- **(Partially) burned gas was sampled from the reactor exit**

Mixtures

Case	Label	
Pure n–heptane	100:0	$\phi = 1$, n–heptane/air mixture
N$_2$-diluted n–heptane	50:0	$\phi = 1$, diluted by N$_2$ and the amount of n–heptane is the same as 50:50
n–heptane/toluene blend	50:50	$\phi = 1$, n–heptane:toluene = 50:50, blend/air mixture
Pure toluene	0:100	$\phi = 1$, toluene/air mixture

Computational method

Flame code: PREMIX-based 1-D steady code

Gas-phase energy equation:

Heat transfer with wall

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

Measured wall-temperature profile along
inner surface of reactor was given to T_w

Kinetic models: n–heptane/iso–octane/toluene

Dooley, et al., CNF 157 (2010) 2333-2339.

Conditions:
- d = 2 mm
- U_0 = 2.5 cm/s
- P = 1 atm

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Effect of toluene addition to *n*–heptane at atmospheric pressure
(Flame images)

Pure *n*–heptane

Flow

Luminosity

Second hot flame

2 mm

First hot flame

Cool flame

Wall temperature (K)

700 800 900 1000 1100 1200
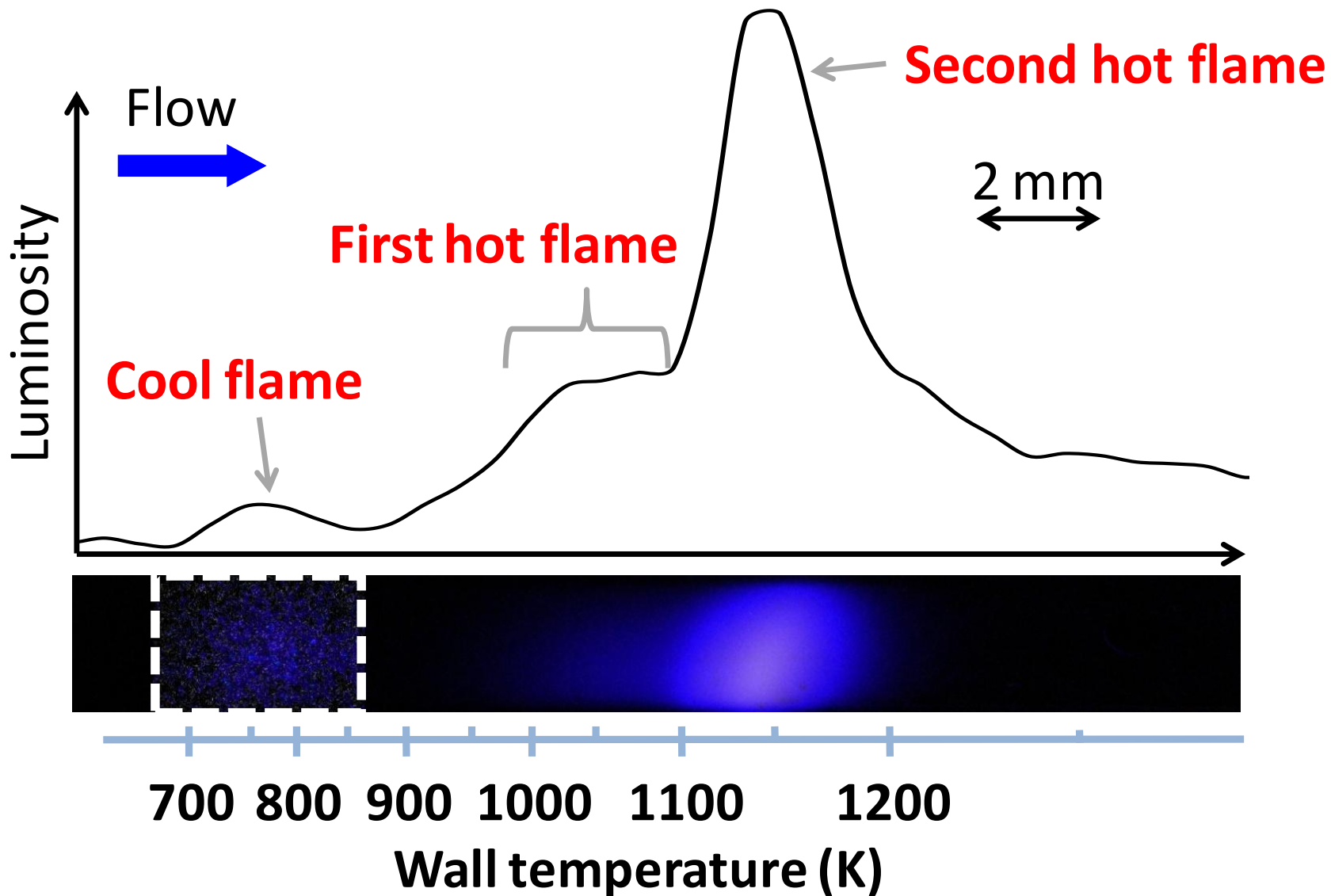
Yamamoto, et al., PCI 33.

Pure *n*–heptane (100:0) and pure toluene (0:100)
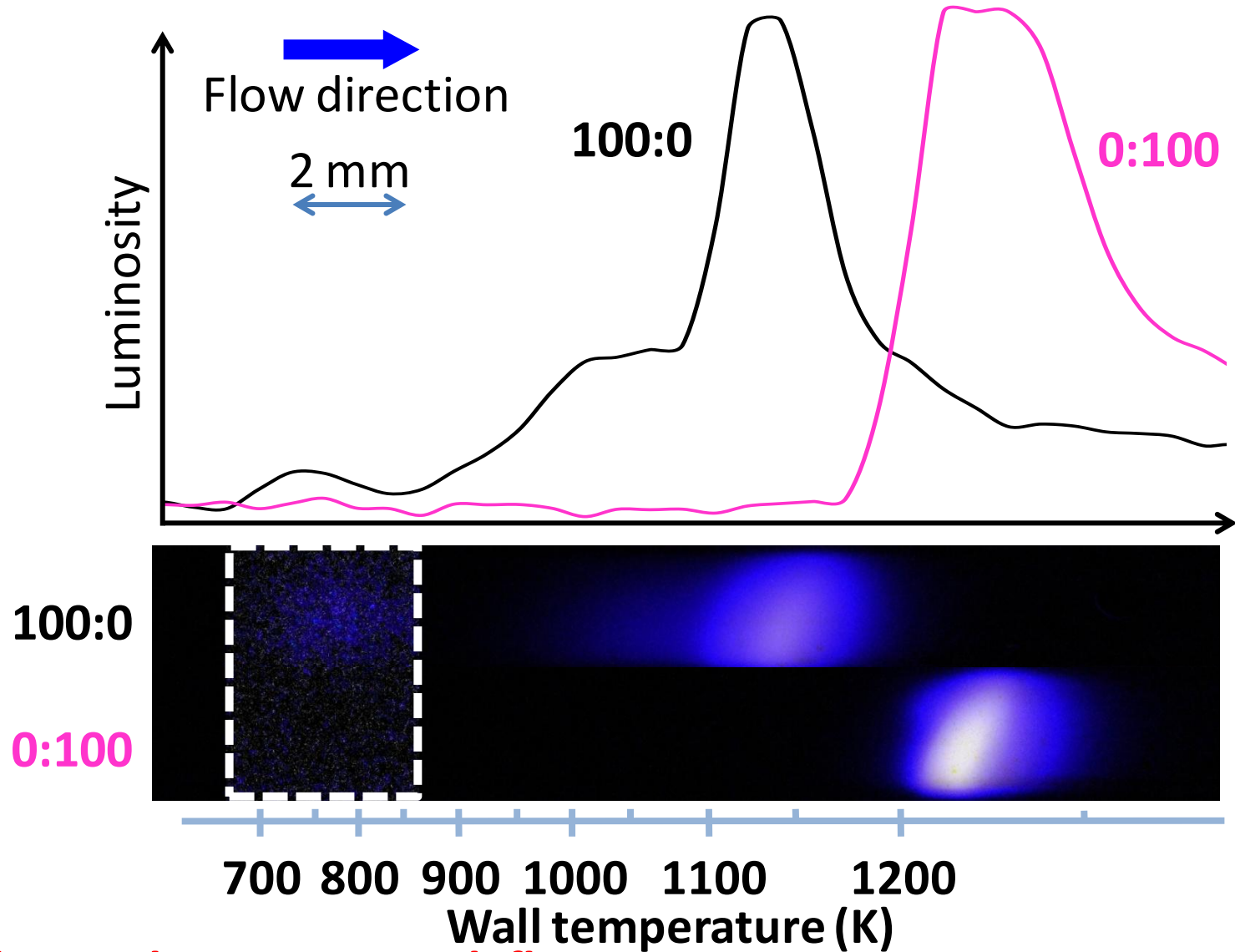
- **Toluene shows one weak flame**
- T_w **at toluene weak flame >** T_w **at 2nd hot flame of** *n*–**heptane**

Pure *n*–heptane (100:0) and blend (50:50)
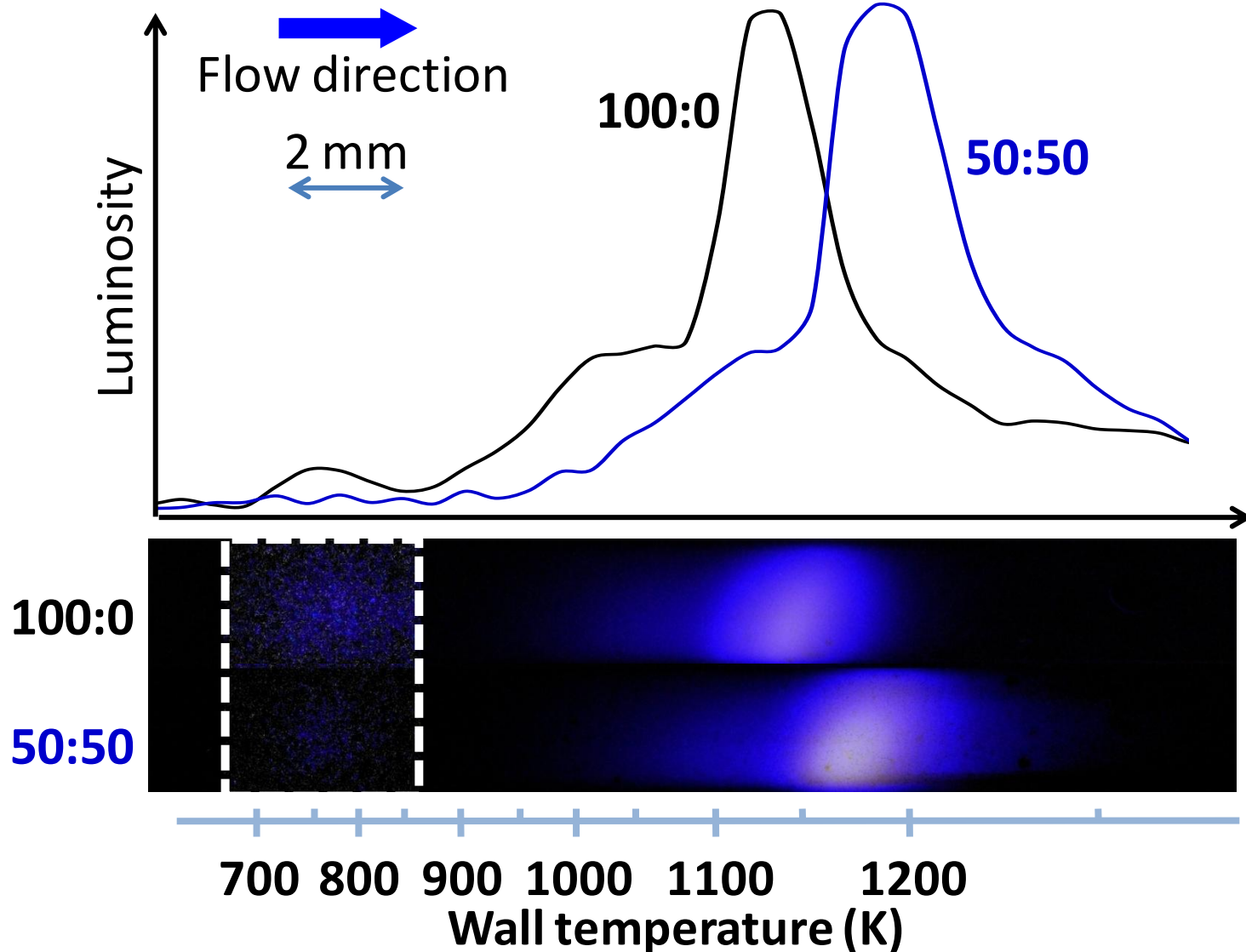
- **Blend shows weaker cool flame than *n*–heptane**
- **1st weak flame of blend is comparable with that of *n*–heptane**
- **T_w at 2nd hot flame of blend is higher than that of *n*–heptane**

N$_2$-diluted *n*–heptane (50:0) and blend (50:50)
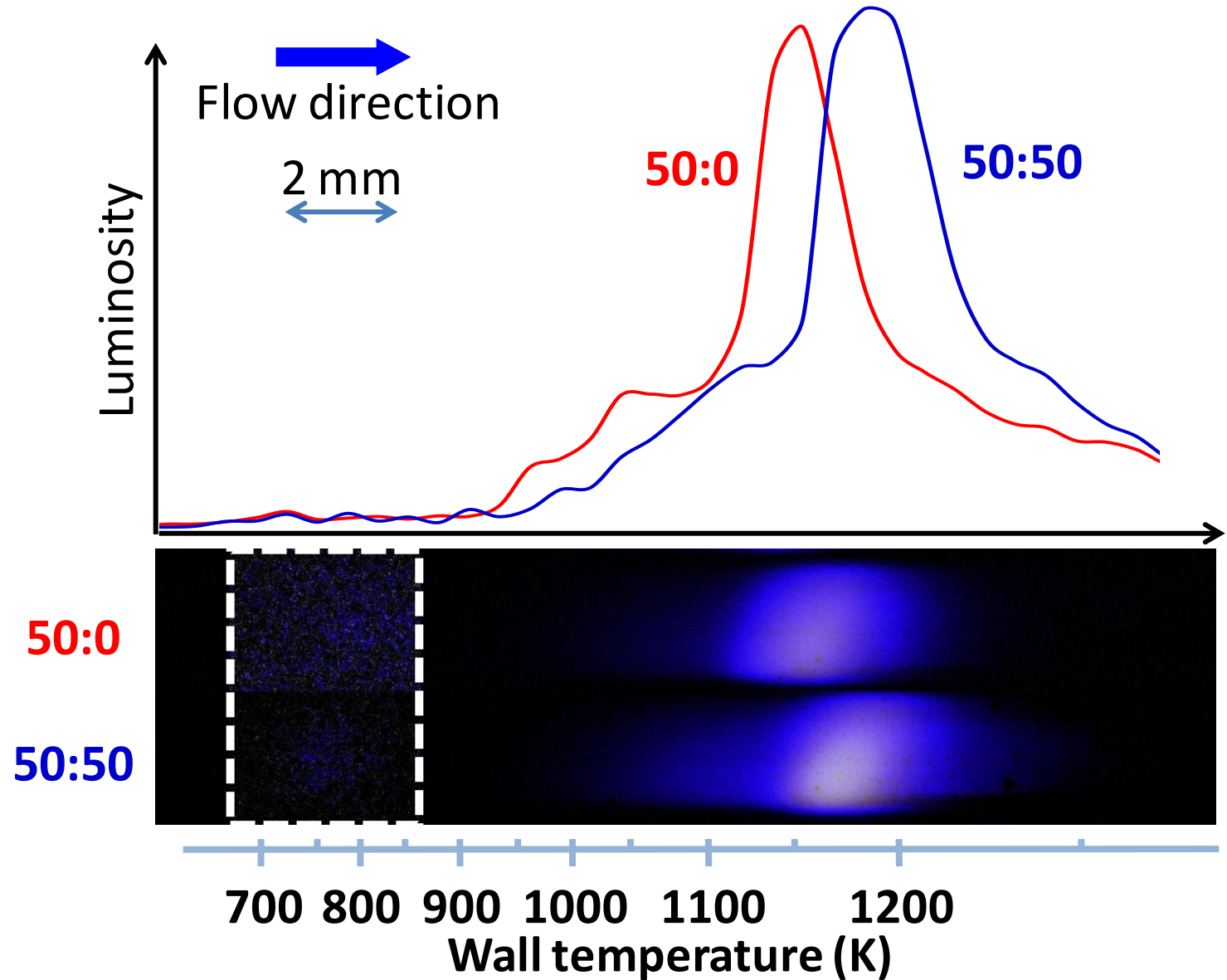
Toluene inhibits ignition of *n*–heptane
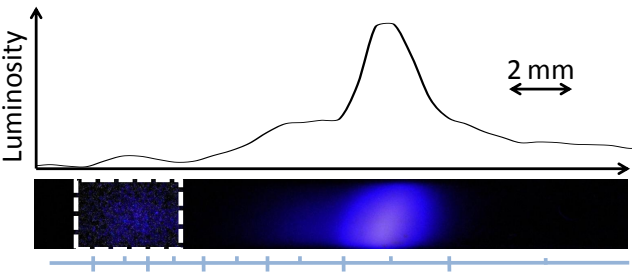
Flame images vs HRR profiles
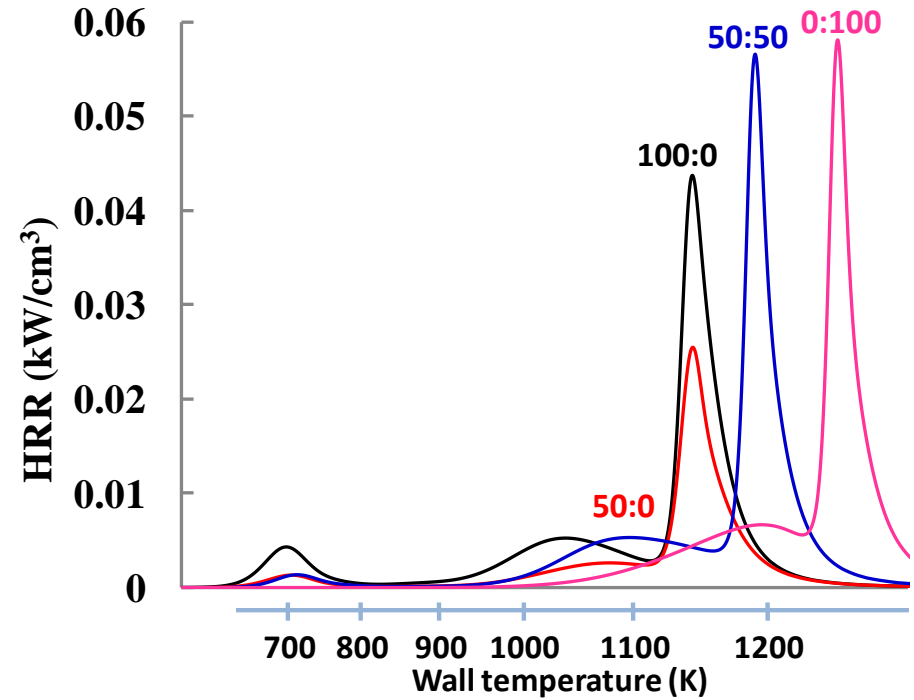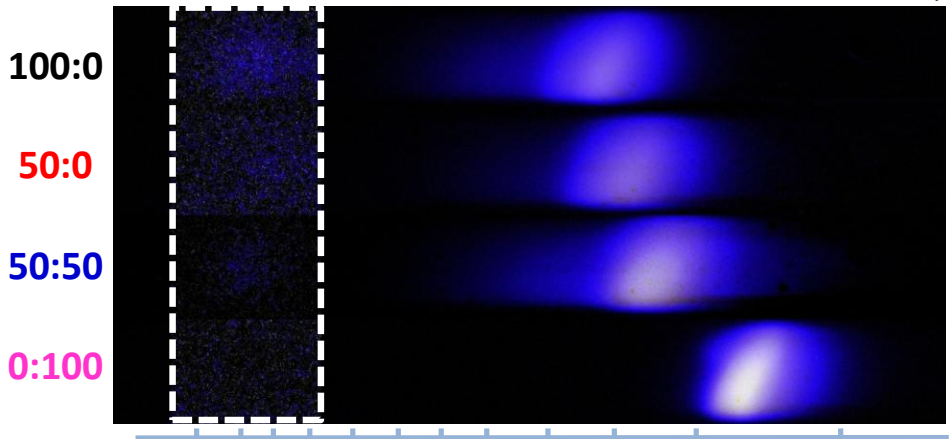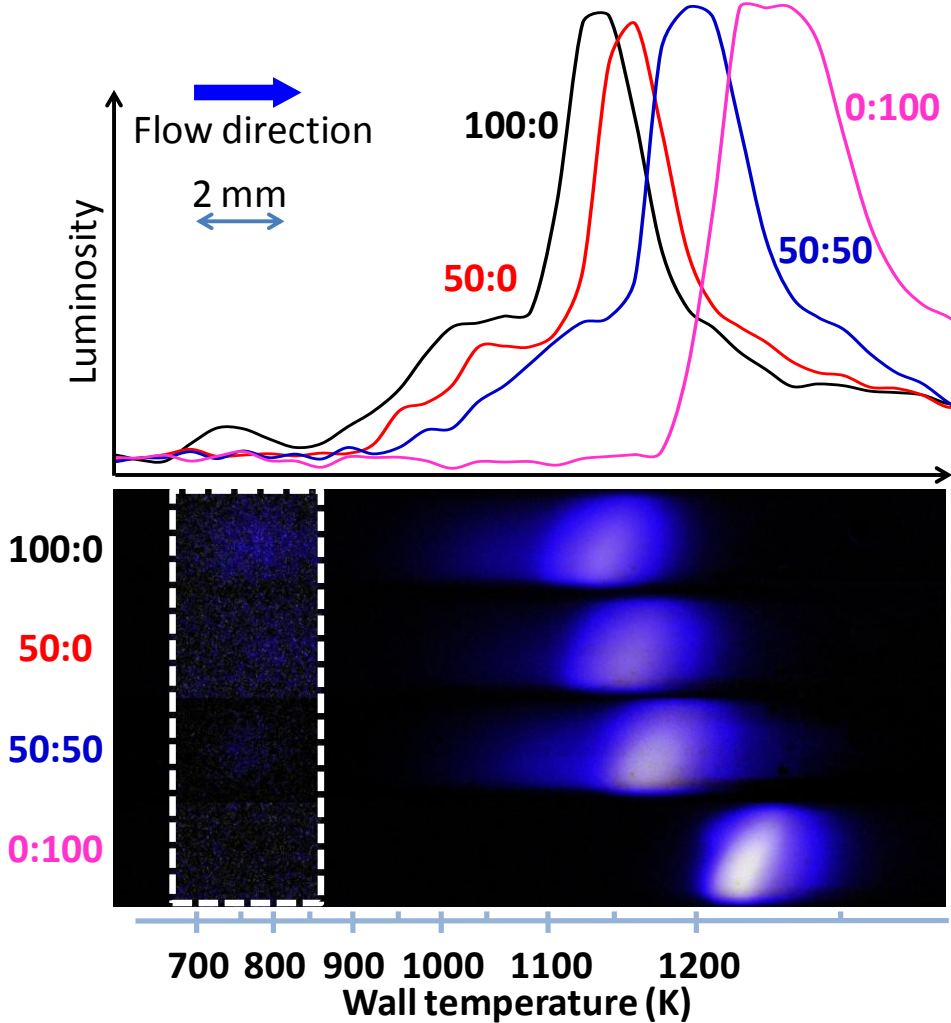
Wall temperature at 2nd weak flame:

pure *n*–heptane < blend (50:50) < pure toluene

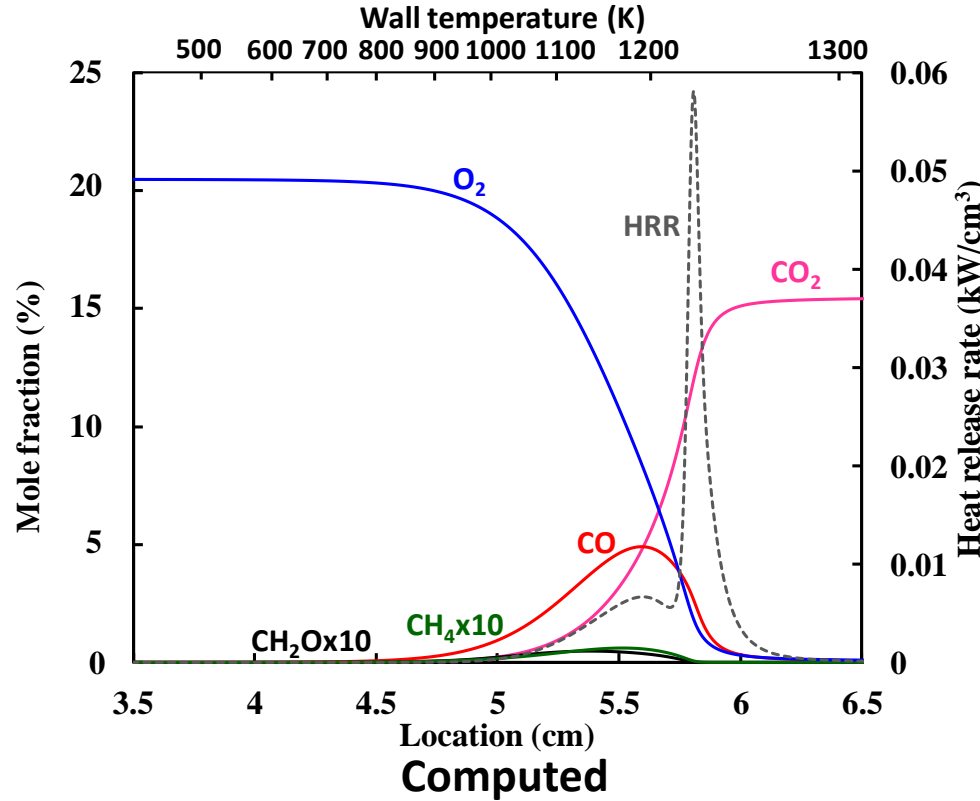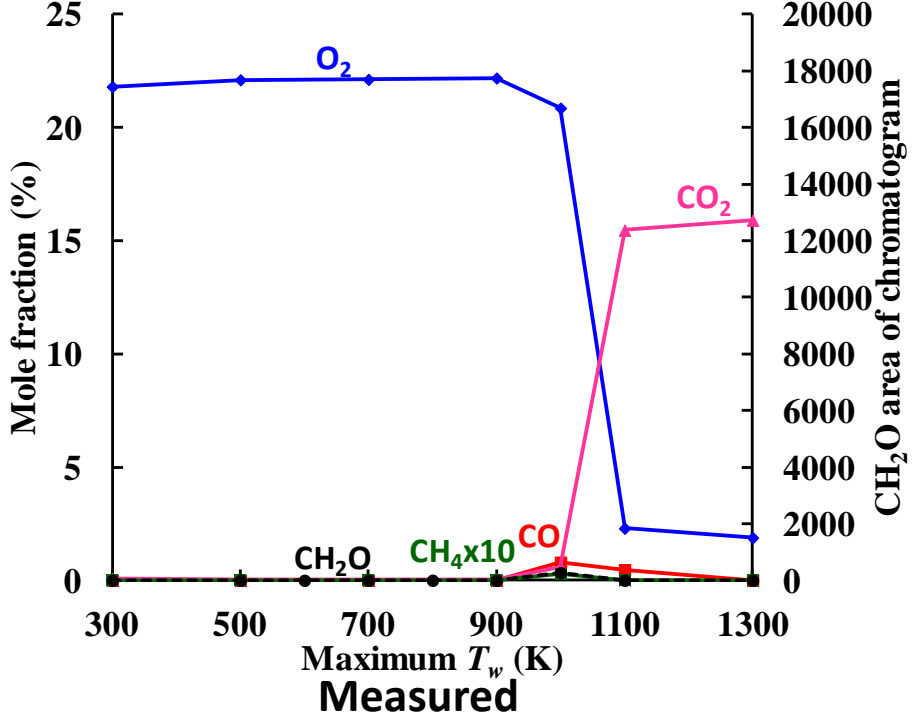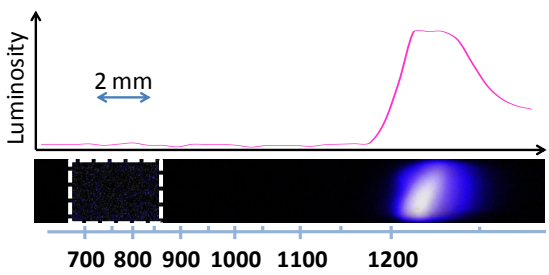# Effect of toluene addition to *n*–heptane at atmospheric pressure
(Species profiles)

Comparison of species profiles: pure *n*–heptane
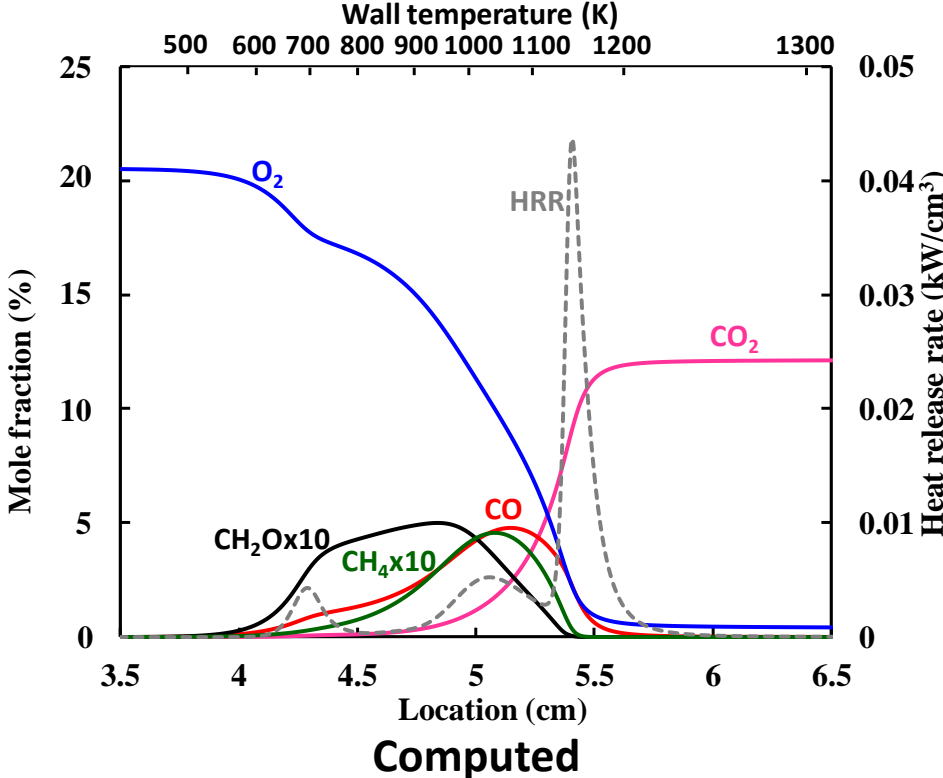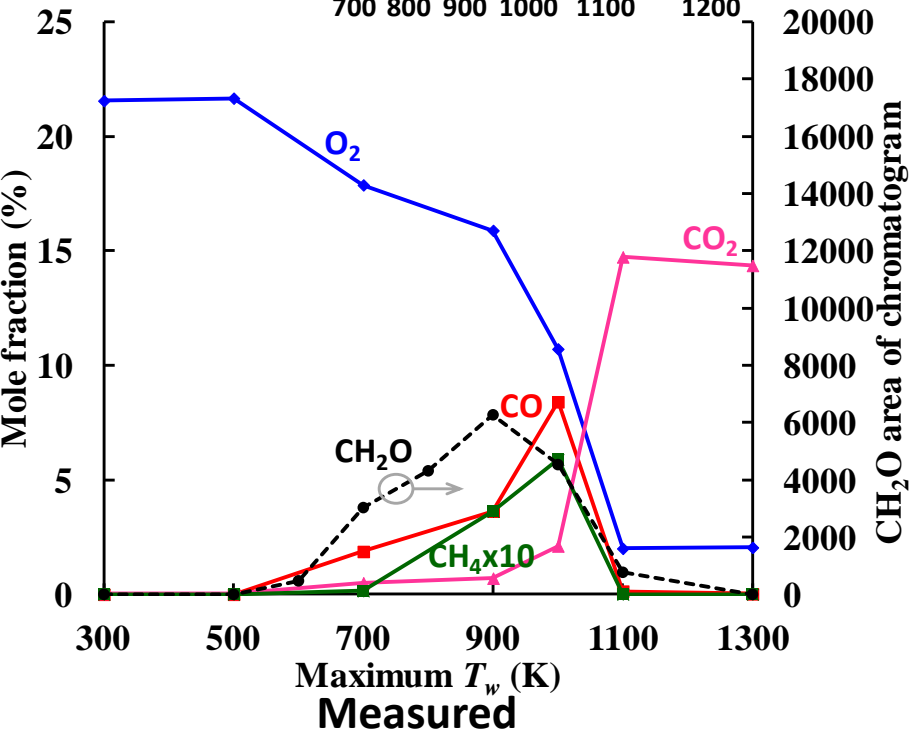
Measured

Computed

Cool flame: CH_2O is produced
1st hot flame: CH_2O is oxidized; CO and CH_4 are produced
2nd hot flame: CO and CH_4 are oxidized

Comparison of species profiles: pure toluene

Measured

Computed

- **Experiment: one weak flame; Computation: two HRR peaks**
- **Computed CO > measured CO**

The mechanism would overestimate reactivity at 1st hot flame

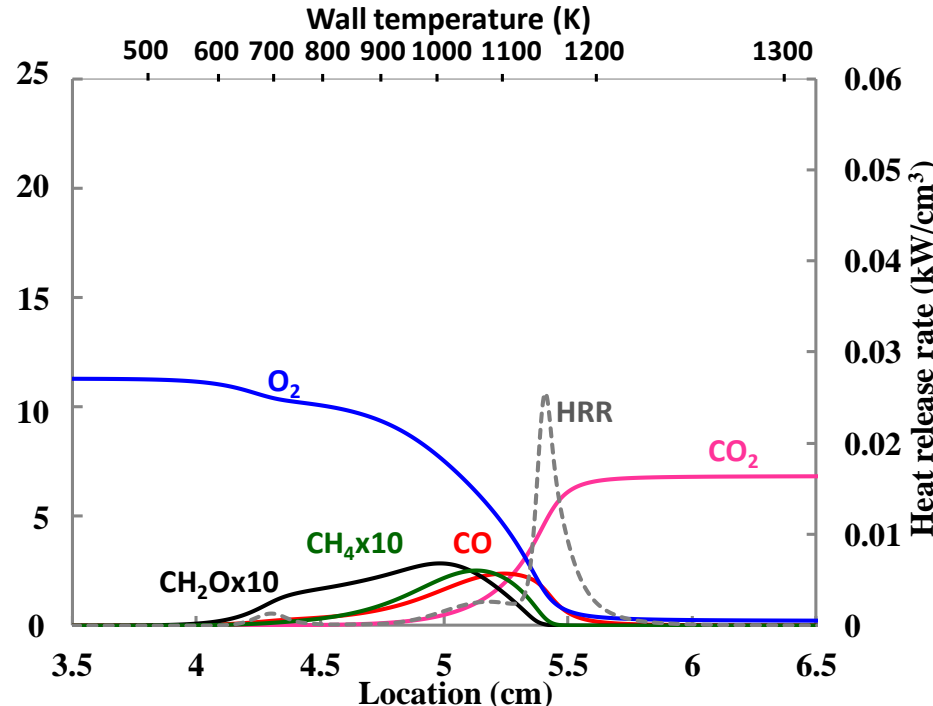# Comparison of species profiles: blend (50:50)
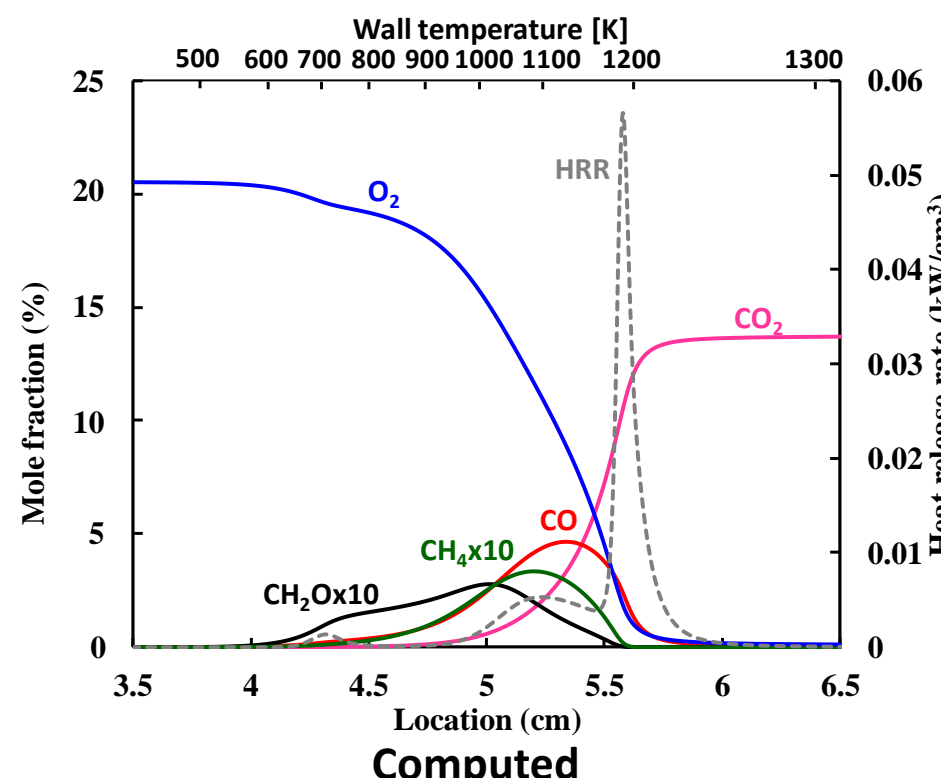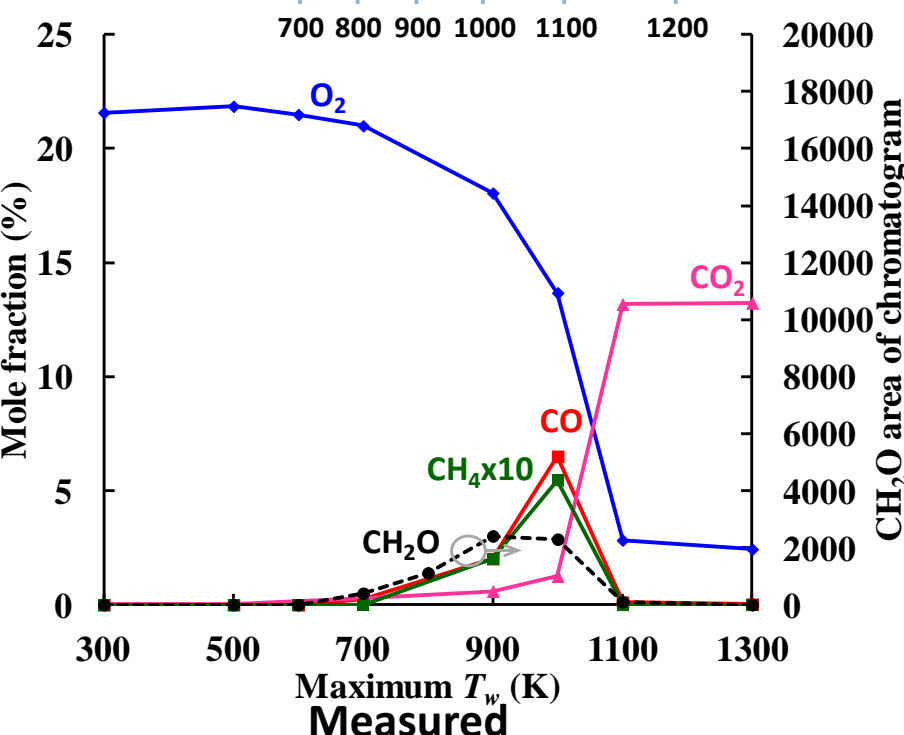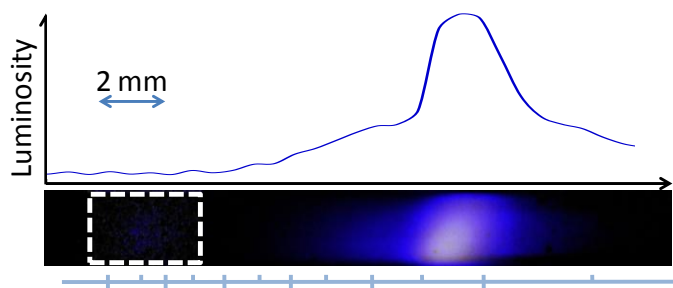
Measured

Computed

Measured species profiles are in good agreement with computed ones

Comparison of computed species profiles:
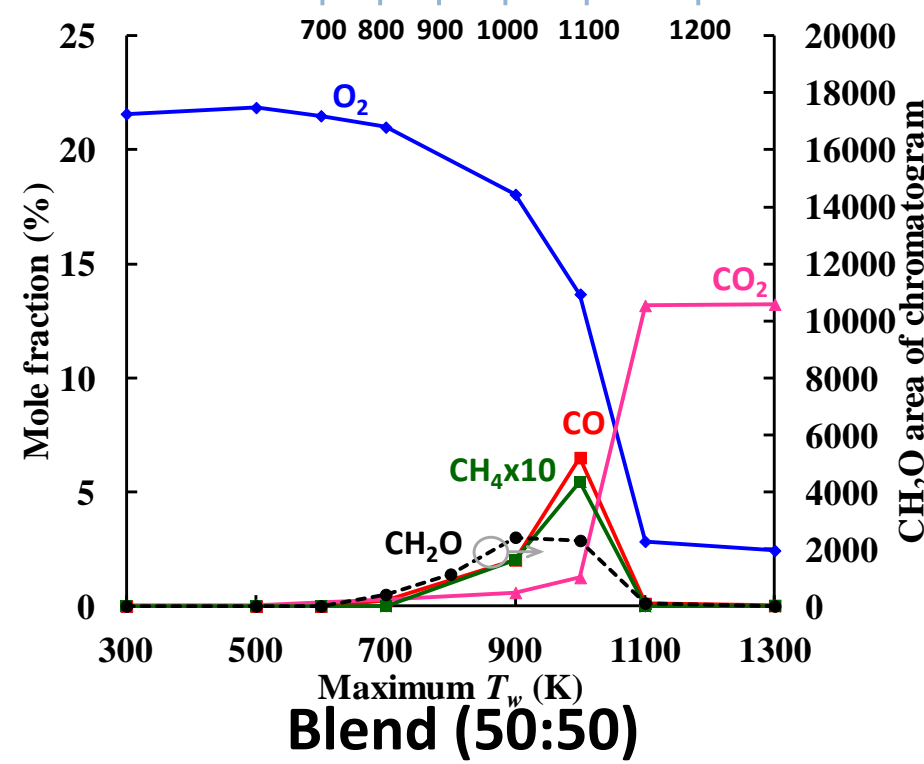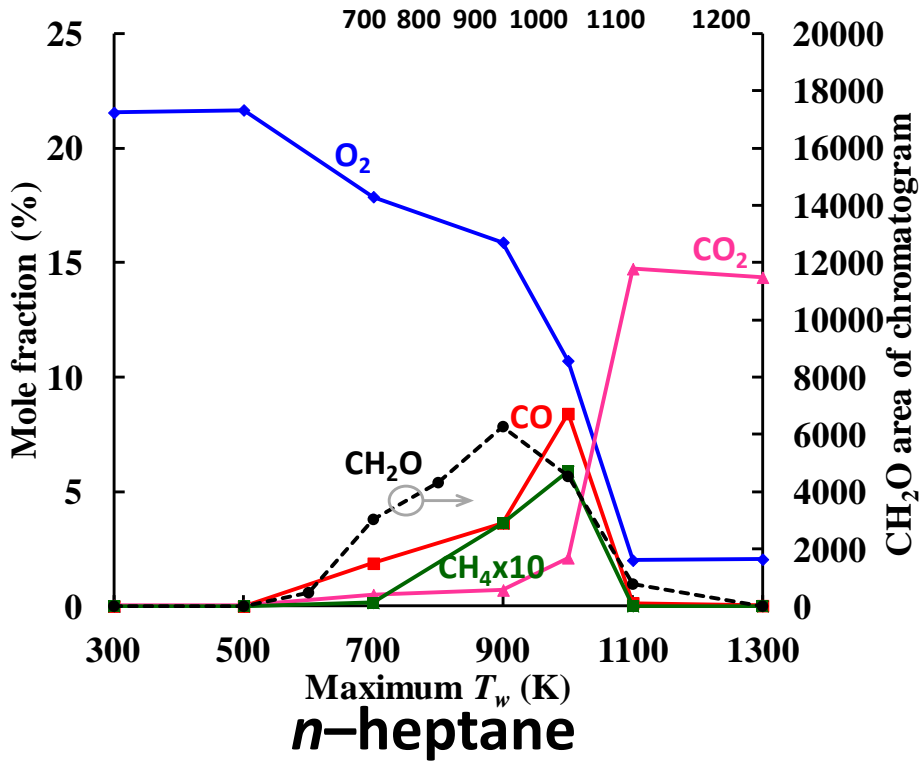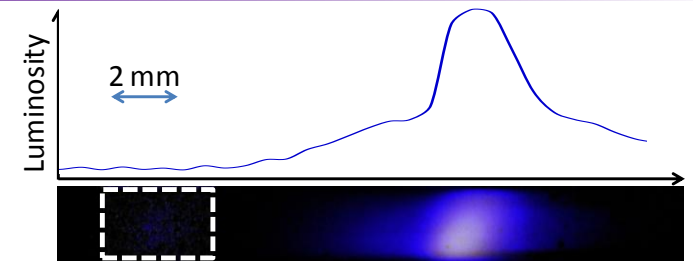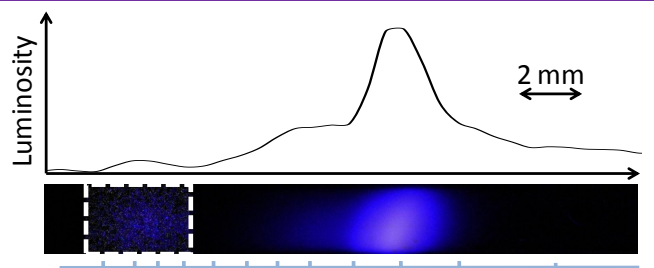## *n*–heptane and N$_2$-diluted *n*–heptane
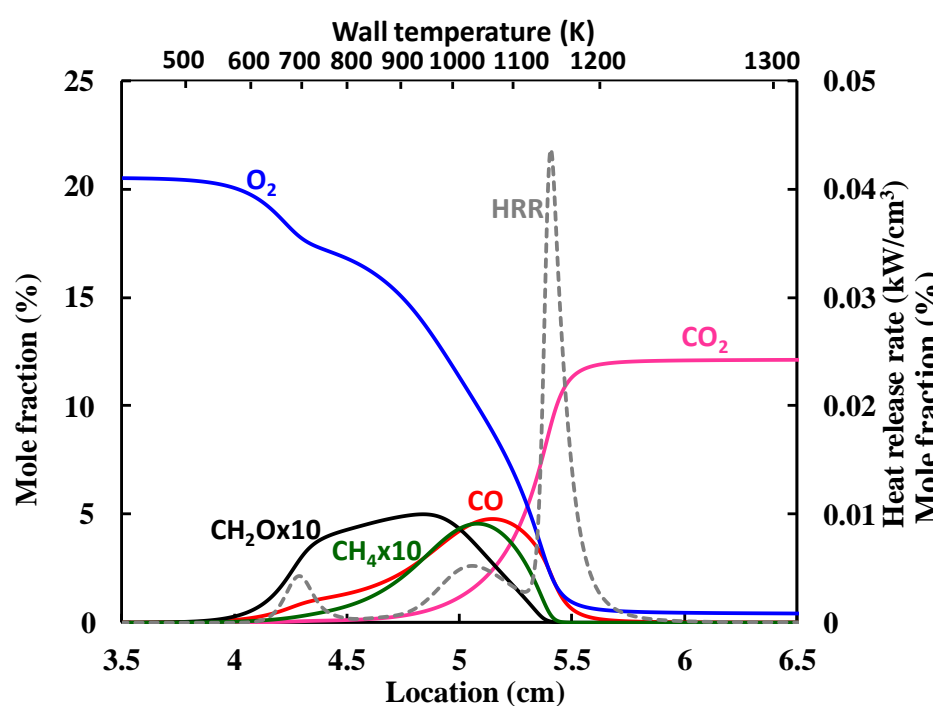
n–heptane

N$_2$-diluted *n*–heptane

The peak values of CH$_2$O, CO and CH$_4$ in N$_2$-diluted *n*–heptane (50:0) are almost half of those in pure *n*–heptane (100:0)

Comparison of measured species profiles: *n*–heptane vs blend

n–heptane

Blend (50:50)

- The peak value of CH$_2$O in blend is almost half of that in *n*–heptane → Toluene does not affect cool flame of *n*–heptane.
- The peak values of CO and CH$_4$ in blend are comparable with those in *n*–heptane → A small amount of toluene oxidizes at 1st hot flame
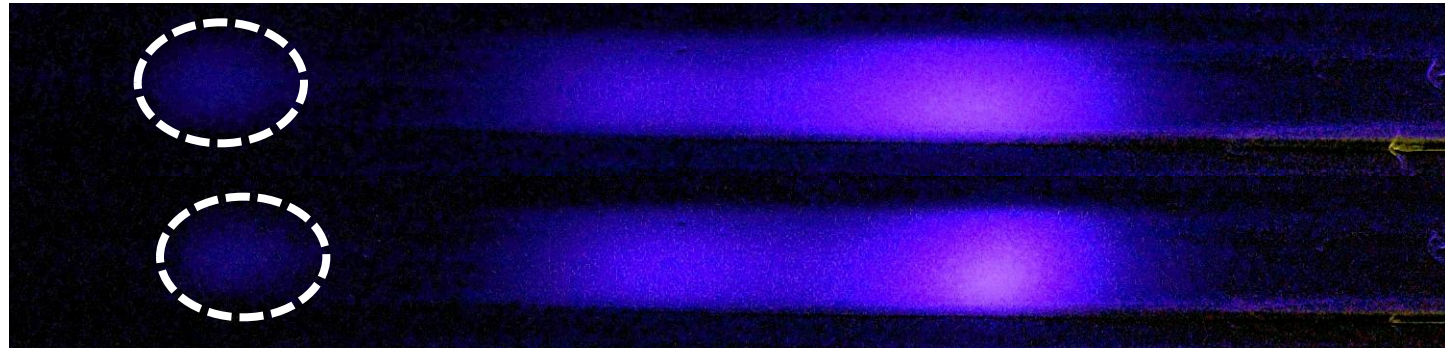
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Effect of toluene addition to *n*–heptane at elevated pressure

Flame images at P = 5 atm

Flow direction ➡

n–heptane

blend

n–heptane:toluene=**70:30**

Cool flame of blend shifts to higher temperature region than that of *n*–heptane

⬇

Toluene would inhibit low-temperature chemistry at elevated pressure

Conclusions

The methodology of a micro flow reactor with a controlled temperature profile has been employed for *n*–heptane, toluene, and blends.

• Toluene shows one weak flame while the model shows two peaks of heat release rate. Computed CO mole fraction at 1st hot flame is higher than measured one

• *n*–heptane, blend and toluene are in order of increasing wall temperature at 2nd hot flame

• Toluene does not affect cool flame at atmospheric pressure while wall temperature at cool flame shifts to higher temperature region at elevated pressure