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Study on cetane number dependence of diesel surrogates/air weak flames in a micro flow reactor with a controlled temperature profile

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Background

For modeling chemical kinetics of a fuel,
experimental data are obtained by,

- shock tube
- RCM
- flow reactor

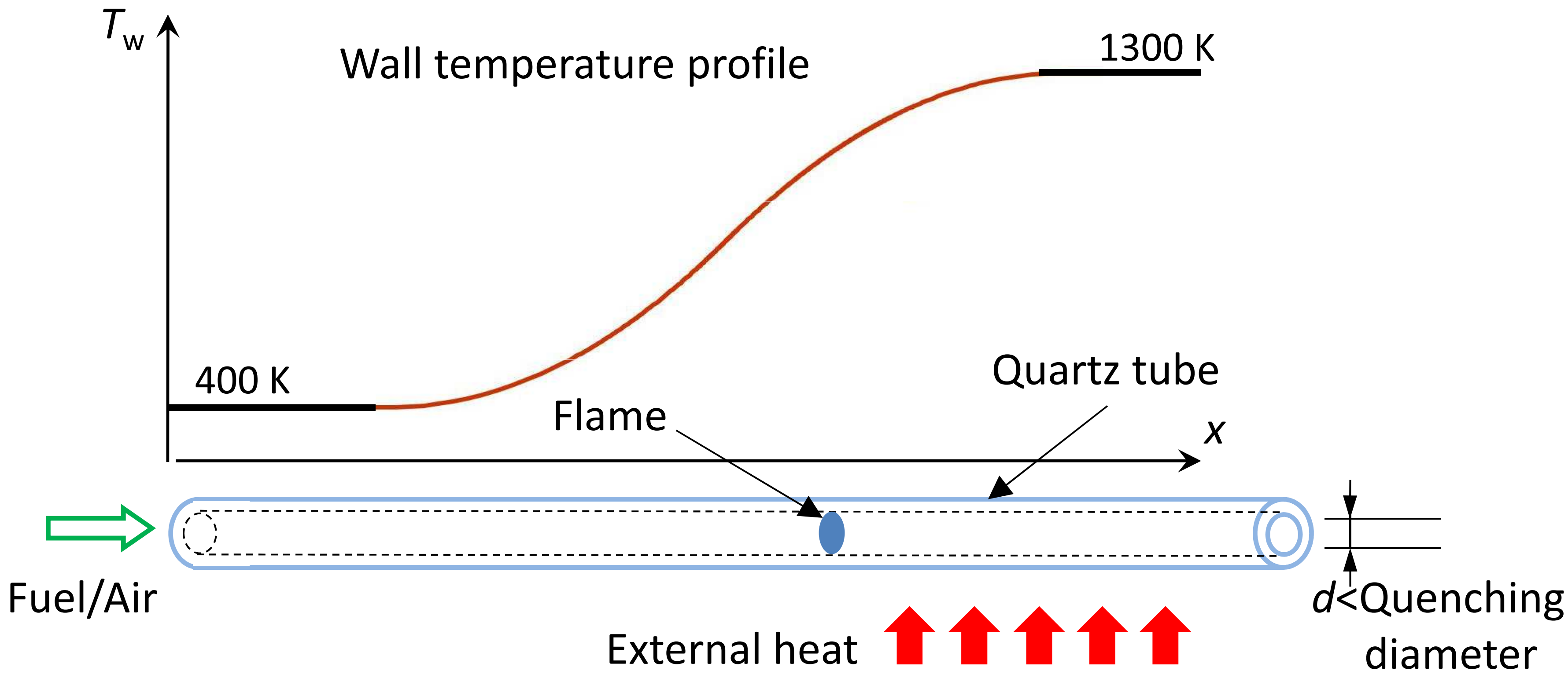
Targeted fuels are extended to large hydrocarbons

Diesel fuels (C10-16): Low vapor pressure

↓

- Difficult to form homogeneous mixture gas
- Only a few data were reported for low vapor pressure fuels

Micro flow reactor with a controlled temperature profile



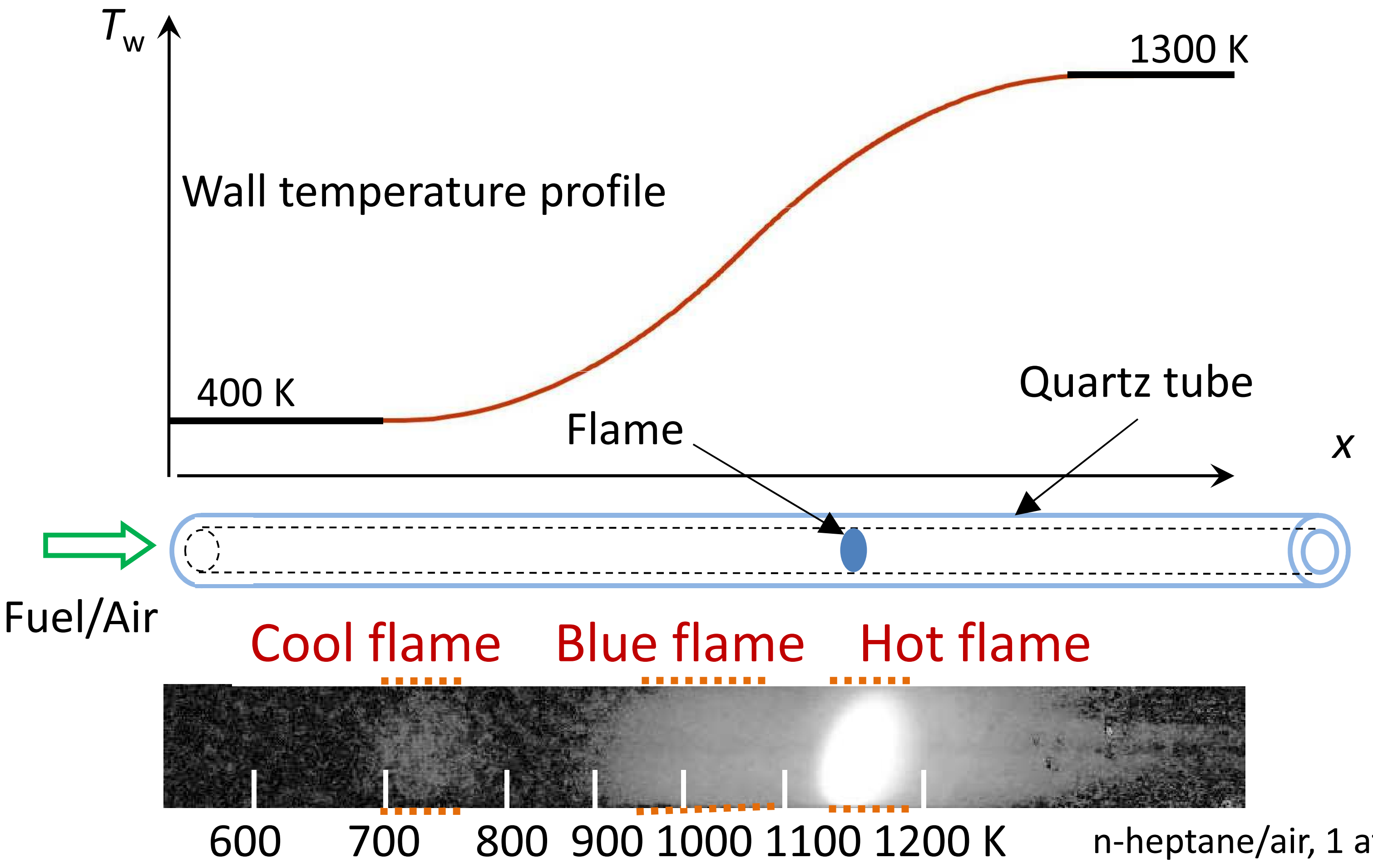
- Laminar flow
- Constant pressure

  Investigate combustion phenomena in simple conditions

- Controlled steady temperature

  Observe oxidation process at wide temp. range (400-1300 K)

Previous works: weak flame (flame in low inlet velocity)



n-heptane/air, 1 atm
Yamamoto et al., PCI 33

- Gas-phase temperature ≒ wall temperature
- Weak flames exist at specific temperatures

Fuel oxidation process can be observed in weak flames

Diesel surrogates and Cetane number (CN)

CN

Cetane number

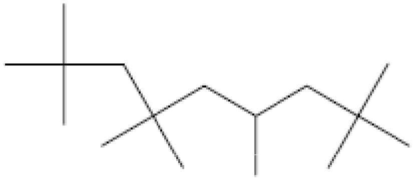
Ignitibility of diesel fuel

n-cetane ($C_{16}H_{34}$) 100

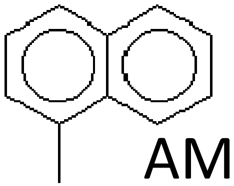
n-decane ($C_{10}H_{22}$) 76

High ignitibility

n-heptane ($C_{7}H_{16}$) 53



iso-cetane ($C_{16}H_{34}$) 15



AMN : a-methylnaphthalene ($C_{11}H_{10}$) 0

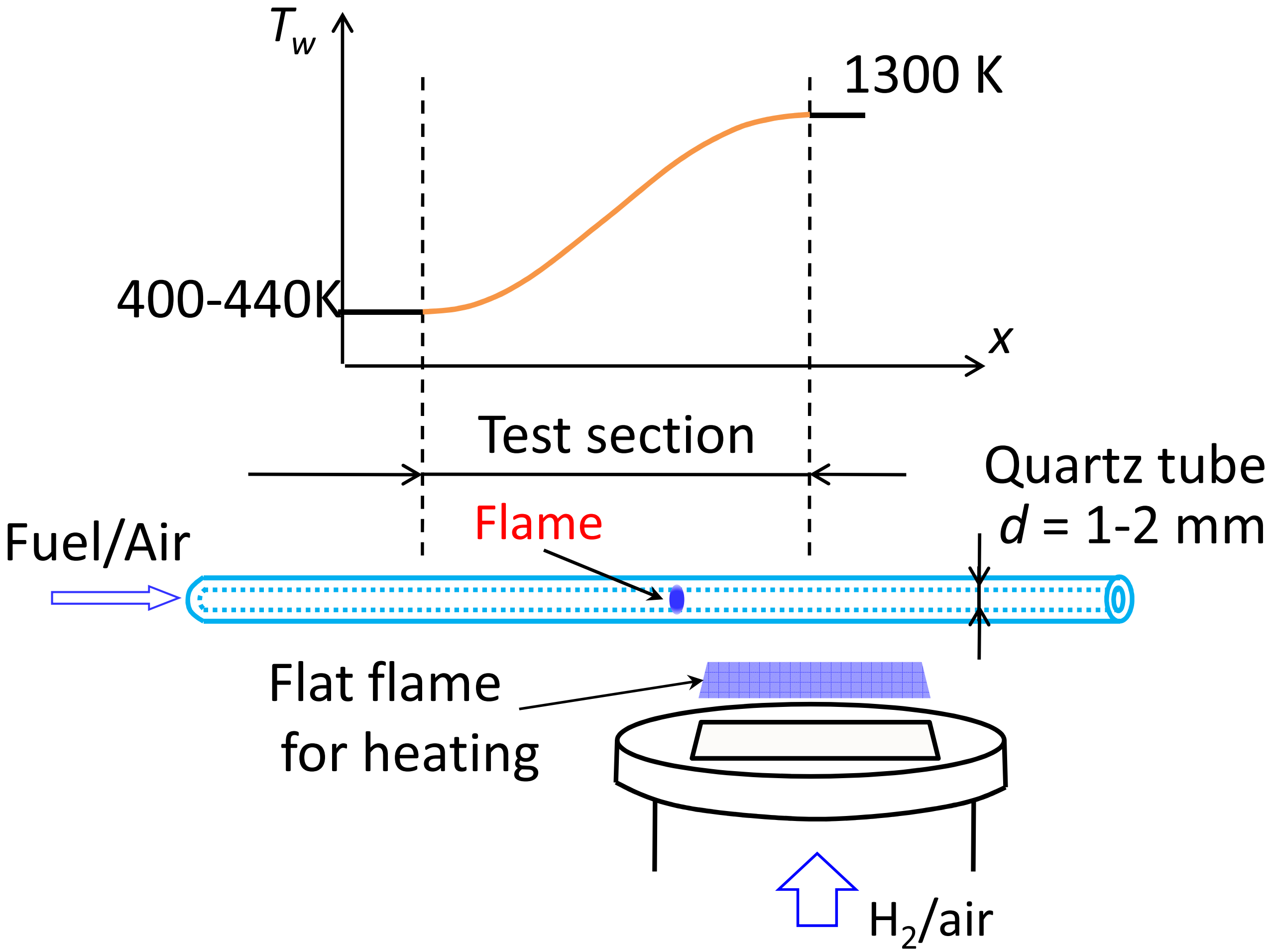
How the flames in our reactor respond to Cetane number?

Objectives

Investigate oxidation process of diesel surrogate

- Weak flame response to Cetane number
- Gas analysis for clarifying flame structure

Experimental setup



External heat source: H_2/air burner

Inlet temperature: 400-440 K depending on applied fuels

Flame images were taken by CH-filtered digital still camera

Computational method

◆Computational code: PREMIX based 1D steady code[1]

•Gas-phase energy equation

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

Heat transfer to the wall

◆Chemical kinetics models

•C8-16 n-alkane [2] (2115 species 8157 reactions)
• iso-cetane[3] (1114 species 4469 reactions)
• n-heptane [4] (561 species 2539 reactions)

developed by LLNL

•substituted aromatic[5] (158 species 1049 reactions) developed by Pitsch et al.

*Estimated values are used for missing species in n-alkane and iso-cetane models due to lack of their transport database

◆Conditions

Same as the experiments; inlet velocity 3.0 cm/s, equivalence ratio 1, pressure 1 atm

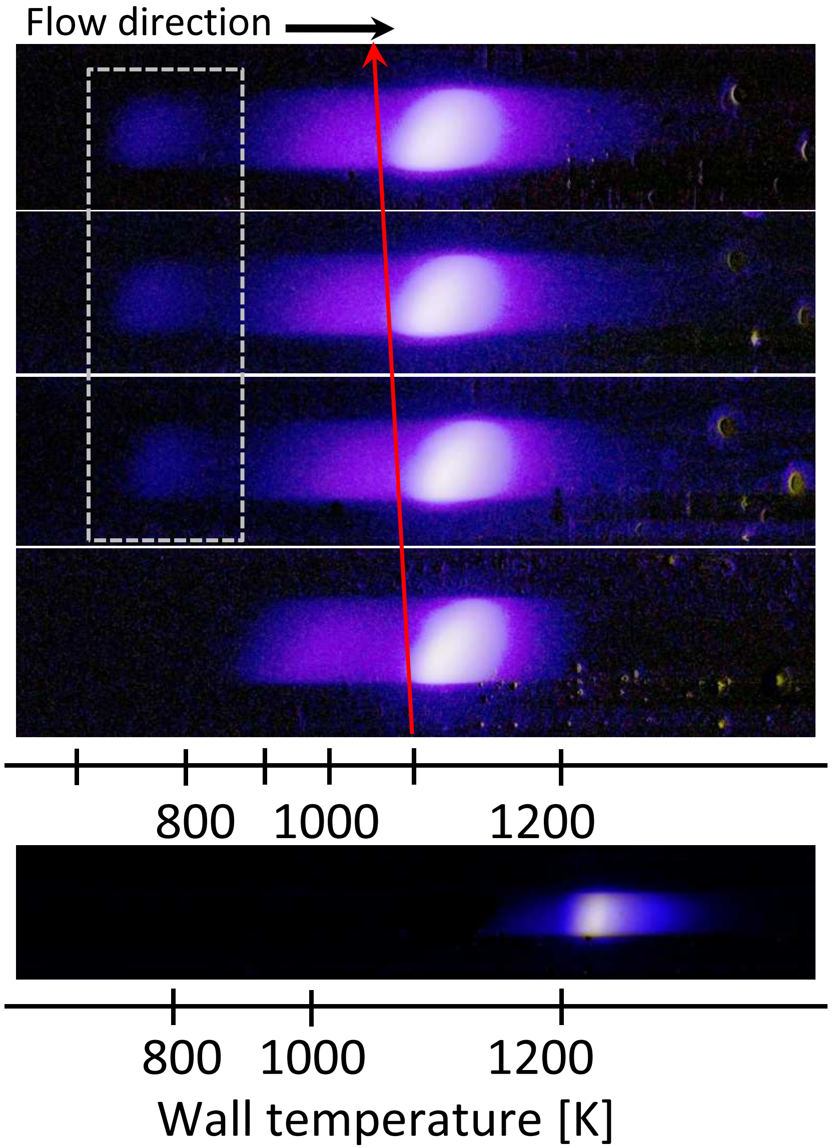
[1] K. Maruta, T. Kataoka, N.I. Kim, S. Minaev and R. Fursenko, Proc. Combust. Inst. 30 (2005) 2429-2436.
[2] C. K. Westbrook, W. J. Pitz, O. Herbinet, H. J. Curran, E. J. Silke, Combust. Flame. 156 (2009) 181–199.
[3] M. A. Oehlschlaeger, J. Steinberg, C. K. Westbrook, W. J. Pitz, Combust. Flame. 156 (2009) 2165–2172.
[4] H.J. Curran, P. Gaffuri, W.J. Pitz, C.K. Westbrook, Combust. Flame 114 (1-2) (1998) 149-177.
[5] K. Narayanaswamy, G. Blanquart, H. Pitsch, Combust. Flame. 157 (2010) 1879-1898.

Weak flames response to Cetane number

Comparison of weak flame images of
diesel surrogates

Weak flames of the various CN fuels

n-cetane
CN 100
n-decane
CN 76
n-heptane
CN 53
iso-cetane
CN 15
AMN
CN 0



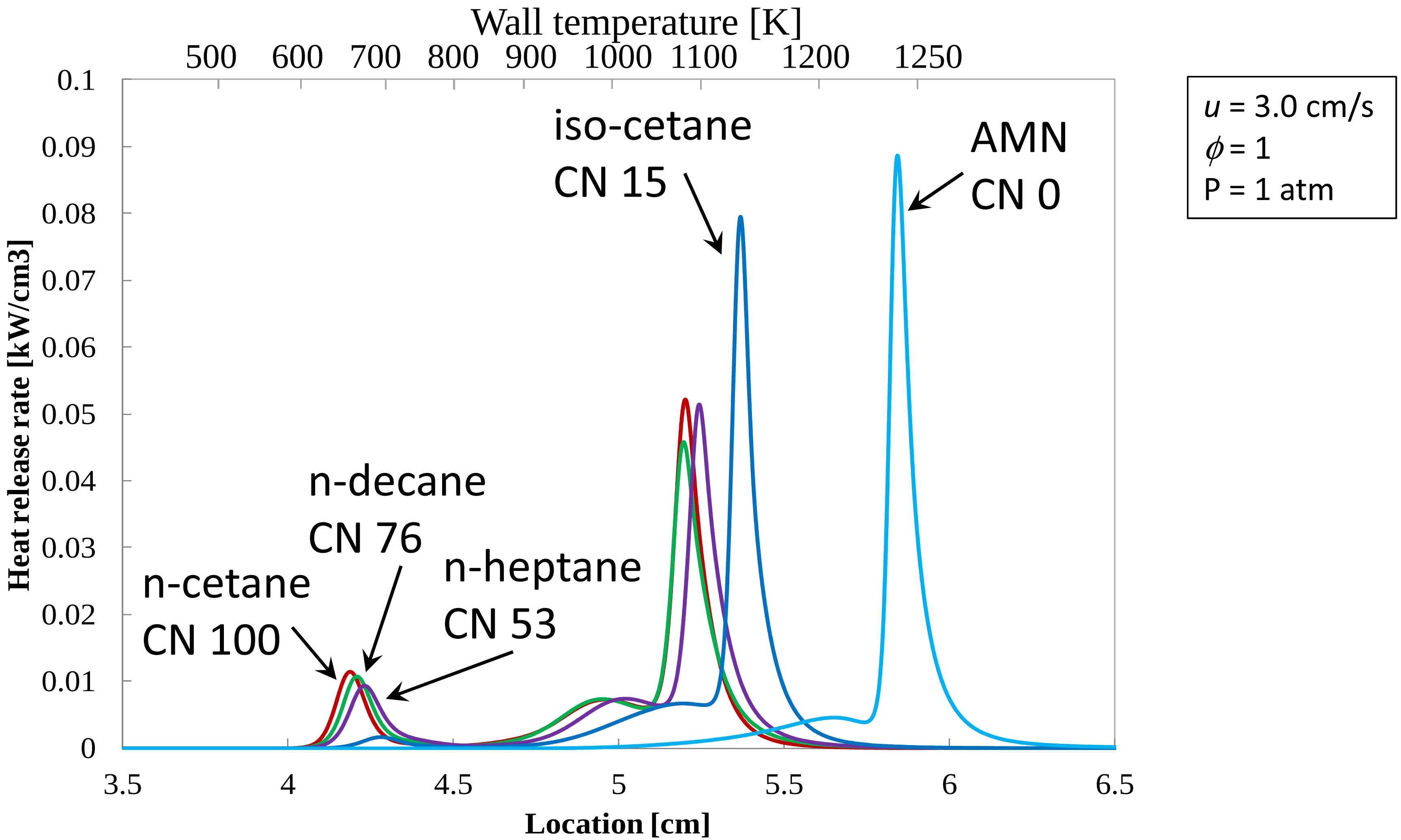
Cool flame
- Around 800 K
- In higher CN fuels

Hot flame:
- CN 100-15: 1120-1150 K
- CN 0: over 1200 K

Higher CN fuels
react at lower temperature

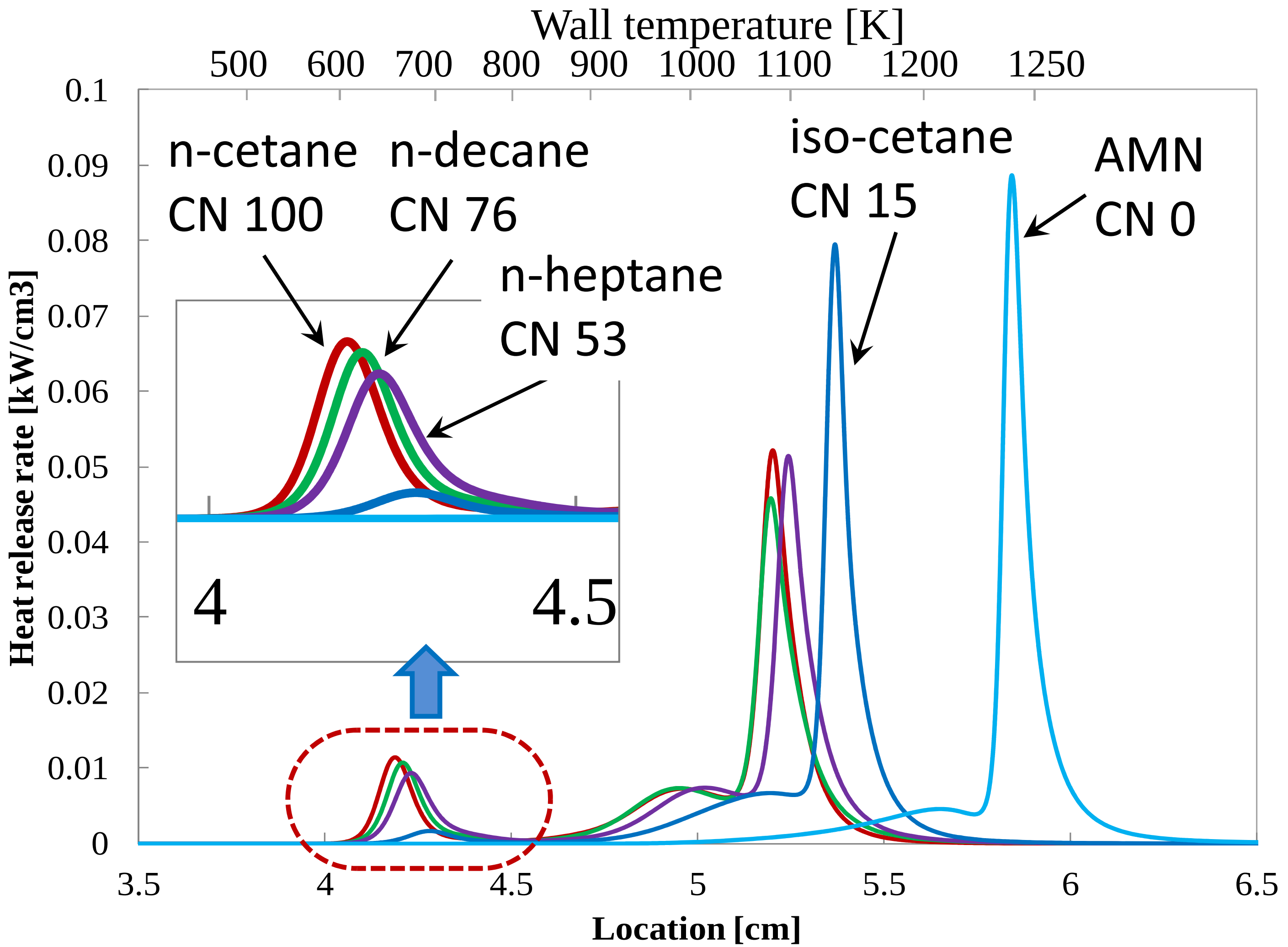
u = 3.0 cm/s
ϕ = 1
P = 1 atm
Exposure time : 2 minutes

Heat release rate (HRR) of the various CN fuels



- HRR peaks corresponds to the flame luminescence zones
- Sharp peaks in higher temp. range: Hot flames

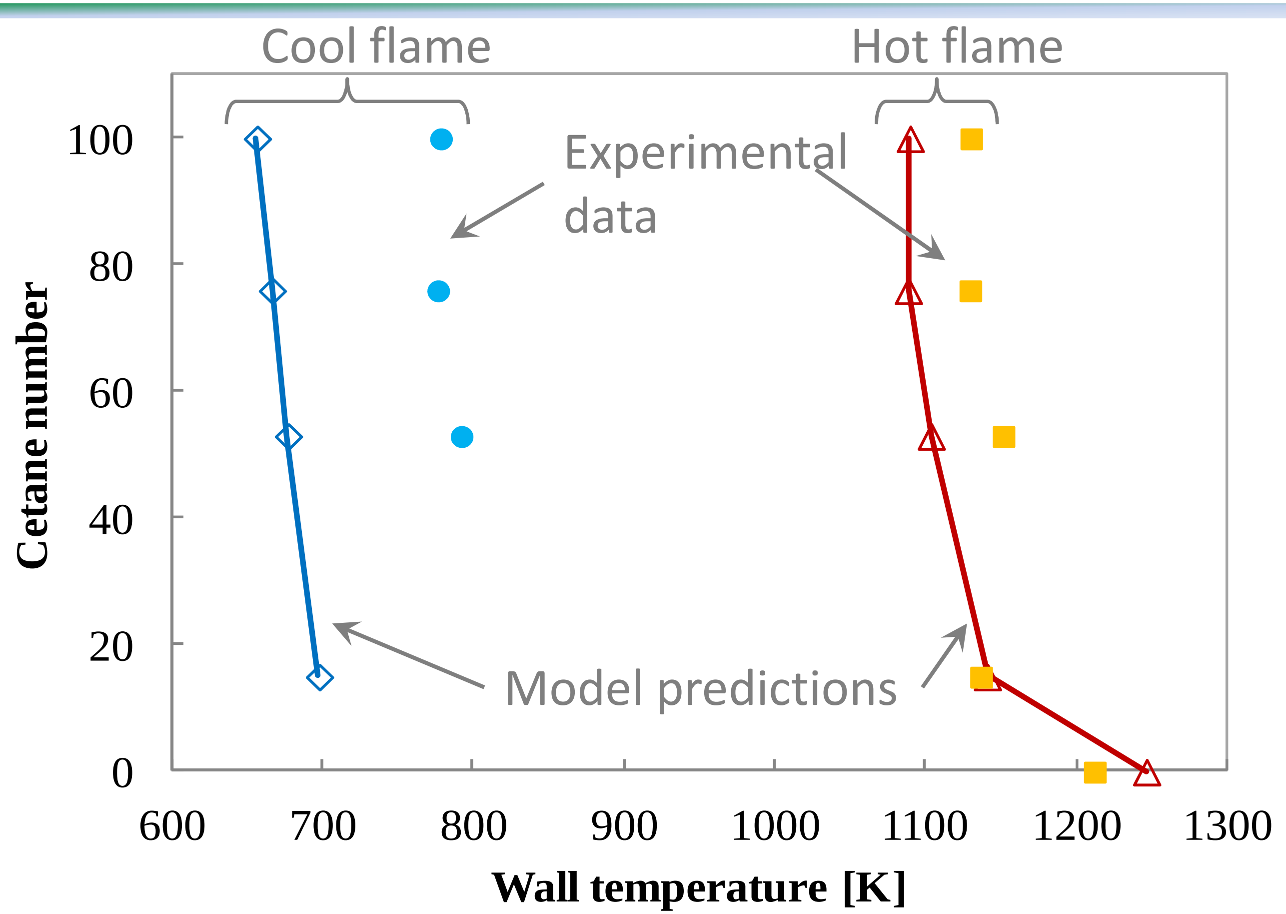
Heat release rate (HRR) of the various CN fuels



u = 3.0 cm/s
ϕ = 1
P = 1 atm

- Small peaks in low temp. range: Cool flames
- Found in CN 100-53 ⇨ Qualitative agreement to Experiments

Relationship of flame temperature and Cetane number

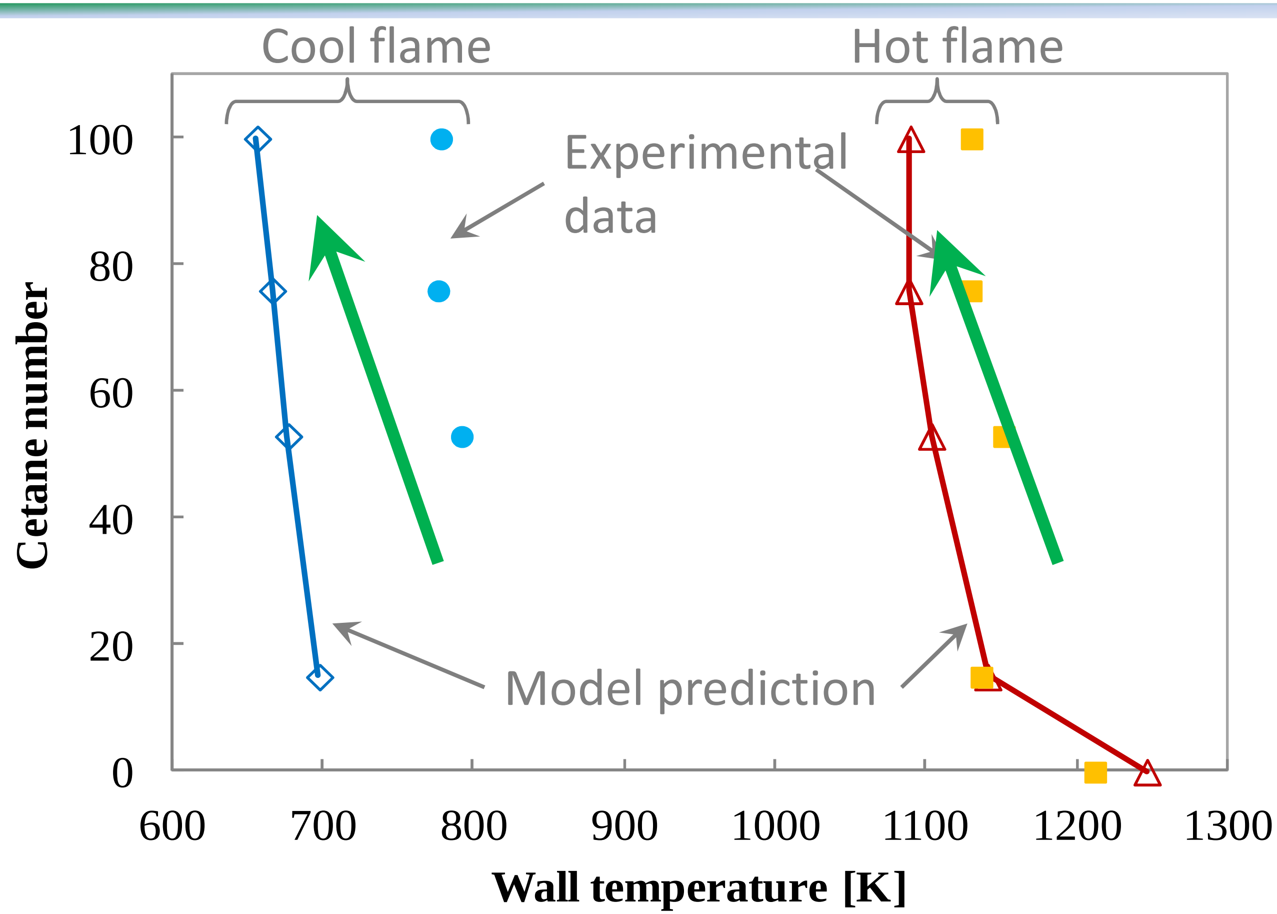


Comparison of temperature difference

Hot flame :	Within 30 K
Cool flame :	Models predict 100 K lower

Further studies for low temperature reaction are required

Relationship of flame temperature and Cetane number



Increasing CN, wall temperature decrease

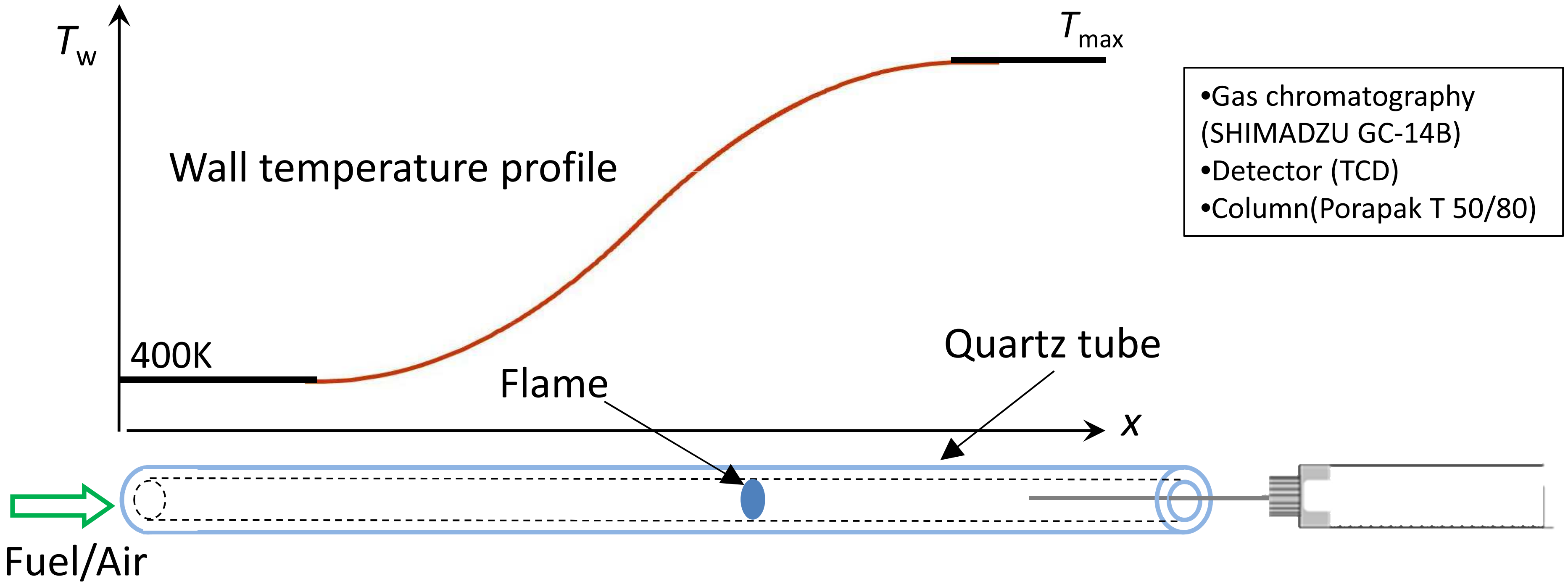
Higher CN, higher ignitability

Flame appearance in our reactor agree with Cetane rating

Flame structure of n-cetane and iso-cetane

Gas analysis for CH_2O

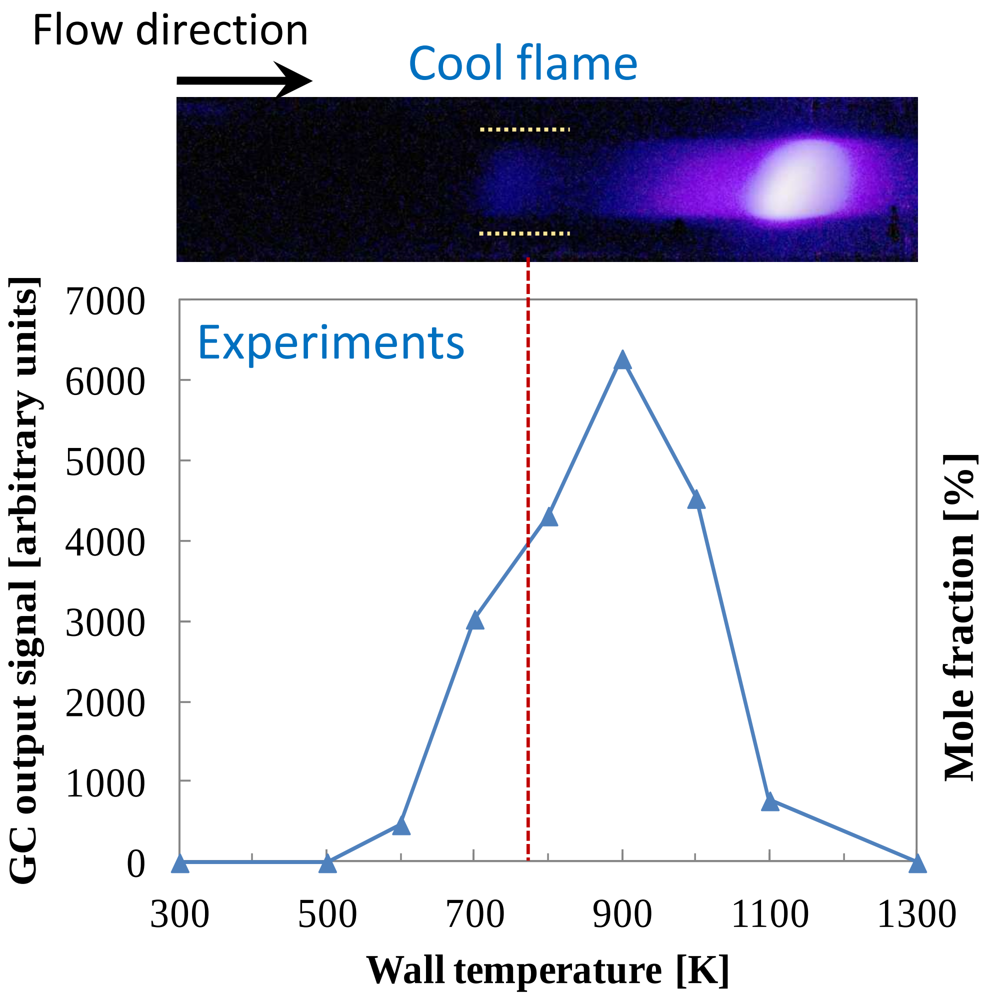
Gas analysis method



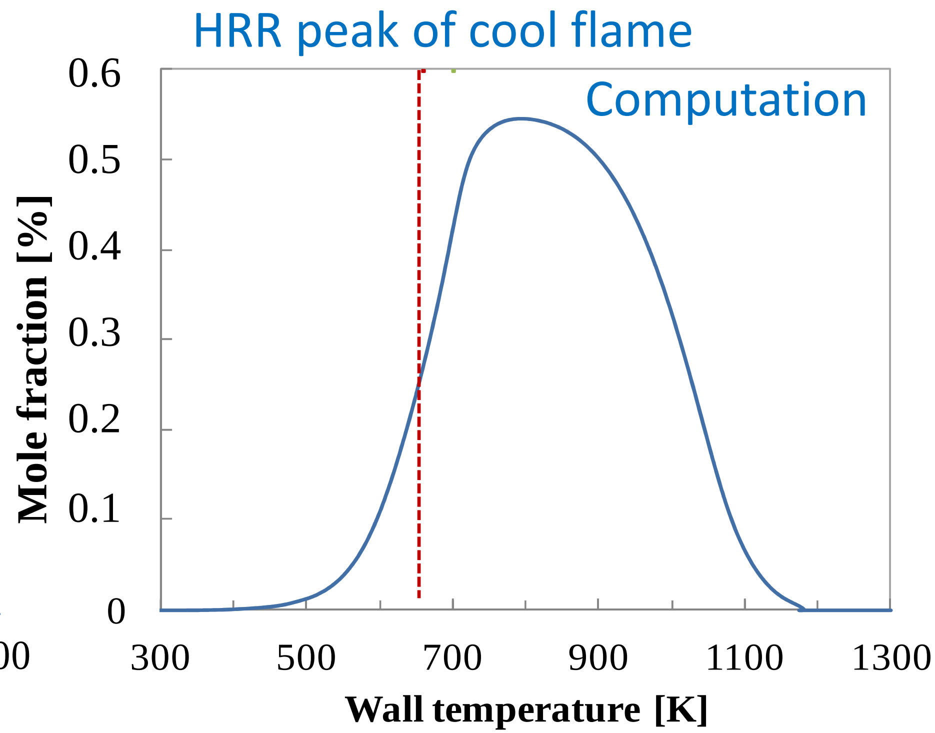
- •Gas chromatography (SHIMADZU GC-14B)
- •Detector (TCD)
- •Column(Porapak T 50/80)

- Extracting gas from tube exit, then analyzed by GC
- Target species: CH_2O = Typical product in cool flame
- Comparative validation with n-heptane whose cool flame is confirmed in a lot of studies

CH_2O profiles of n-heptane



n-heptane (C7H16)

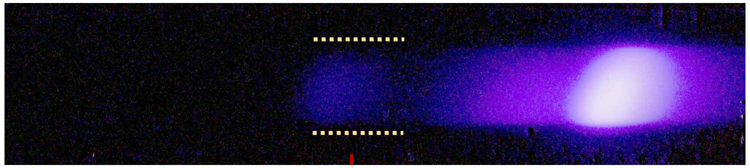


CH_2O is produced in cool flame

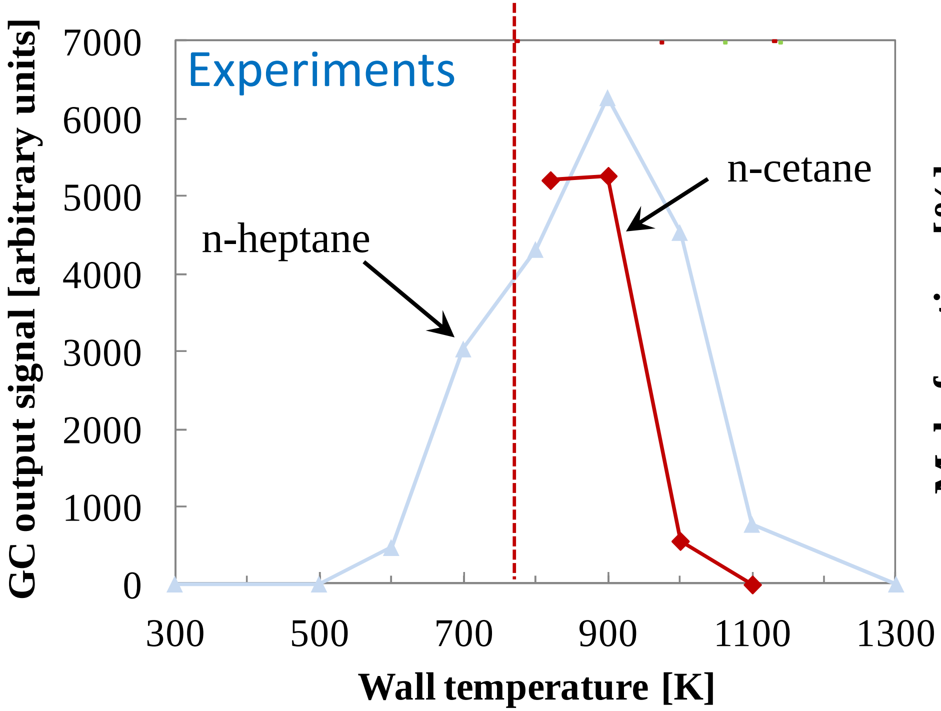
CH$_2$O profiles of n-cetane and n-heptane

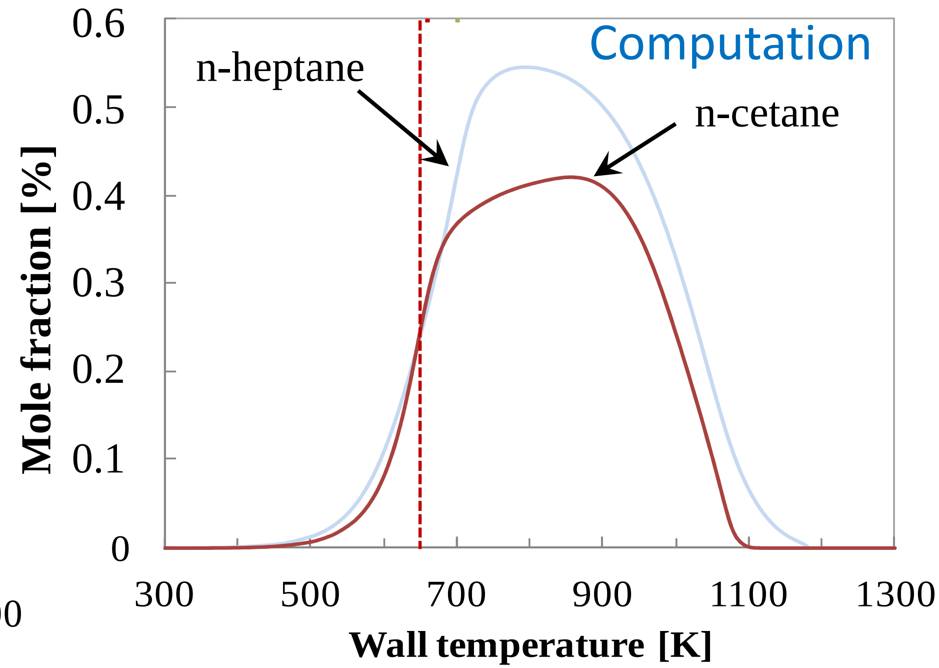
Flow direction

Cool flame



n-cetane (C16H34)



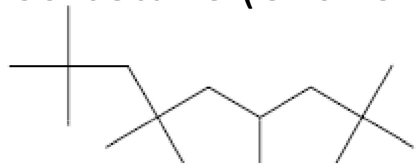


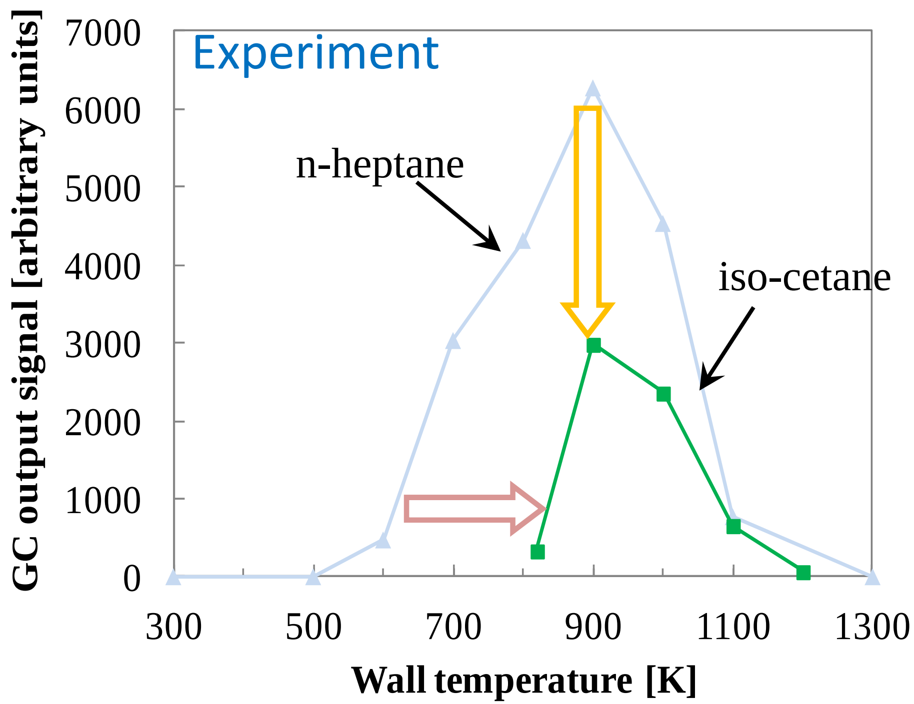
CH$_2$O is produced in cool flame

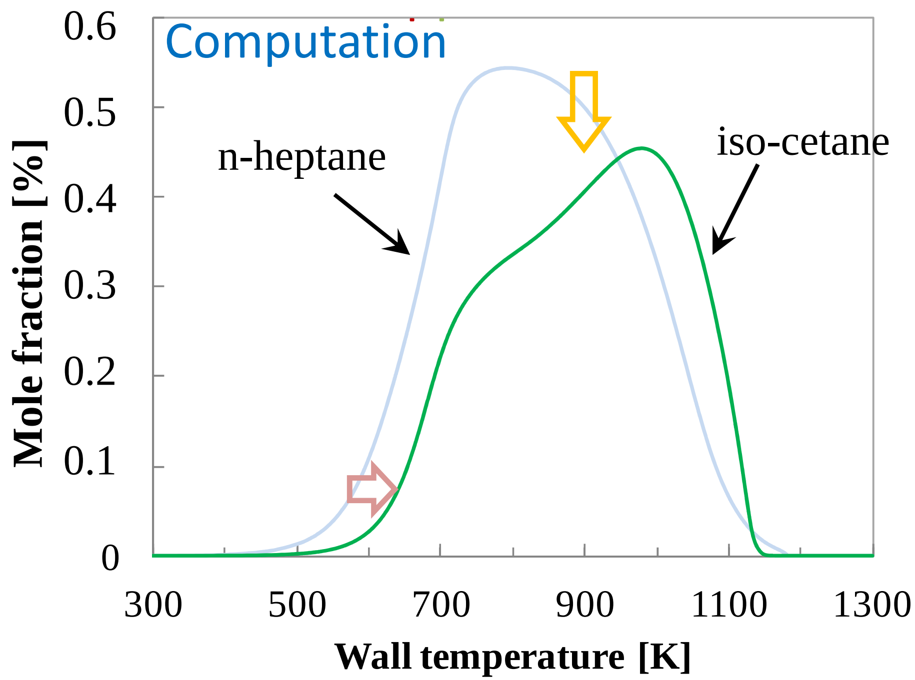
CH$_2$O profiles of n-cetane are similar to n-heptane

CH_2O profiles of iso-cetane and n-heptane

iso-cetane (C16H34)







Comparison to n-heptane	Experiment		Computation
CH_2O begin to produce at	200 K higher	⟺	50 K higher
Amount of CH_2O peak	50 %		80%

Numerical model overestimated CH_2O production

Blended fuel of n-cetane and iso-cetane

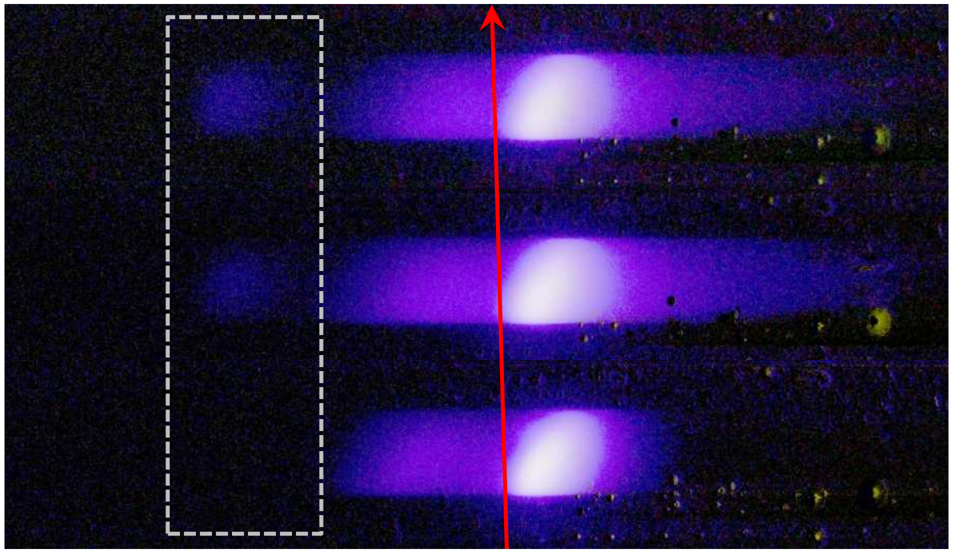
Cetane number variation

- Pure fuels with specific CN
- Blended fuels of two fuels

Pure n-cetane (CN 100)

Blended fuel (CN 76)

Pure iso-cetane (CN 15)



Increasing CN…

- Cool flames become stronger
- Hot flames shift to low temperature

Summary

Ignition and combustion characteristics of a gaseous diesel surrogates/air mixture were examined by micro flow reactor with a controlled temperature profile.

- Experimental data of low vapor pressure fuels are obtained in wide temperature range by the reactor
- Cool flames are observed in high Cetane number fuels in atmospheric pressure
- The weak flame trends corresponds to Cetane rating
- Model predictions agree well with experimental data except iso-cetane case

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