2017/07/06 SIP「革新的燃焼技術」第3回公開シンポジウム

ガソリン燃焼チーム クラスター大学17（ノック抑制班）

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温度分布制御型マイクロフローリアクタを用いた低温酸化反応に関する研究

目　　的

多段酸化反応からの冷炎の分離抽出法及び定在冷炎の特性について調べる

背景
- 高効率の燃焼器開発には着火特性の理解が必要
- 多段着火で生じる冷炎の特性およびメカニズムに対する理解は不十分

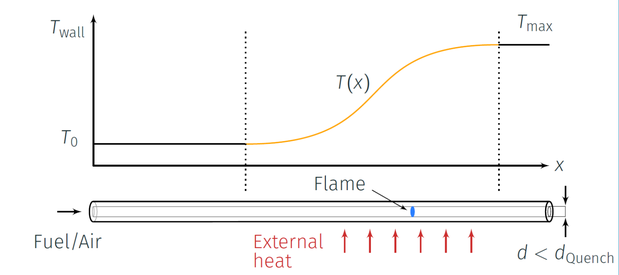
解決手段
- 温度分布制御型マイクロフローリアクタを冷炎に適応

→ 冷炎の定在化が可能

研　究　方　法

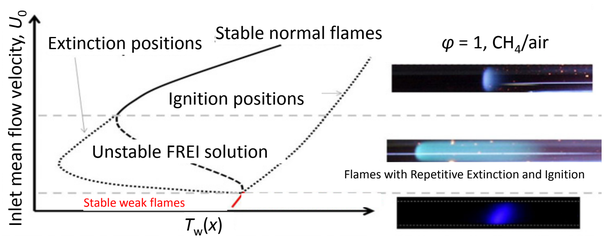
温度分布制御型マイクロフローリアクタ(MFR)[1][2]
- 消炎直径以下の石英管を外部熱源(H_2/air flame)によって加熱
- 層流かつ圧力一定

→ 気相温度は壁面温度に強く依存し，定常な温度分布を得られる



流入流速に応じた火炎応答 [1][2]
- 3つの解分岐（火炎応答）
- 低流入流速において着火解を示すweak flameが存在

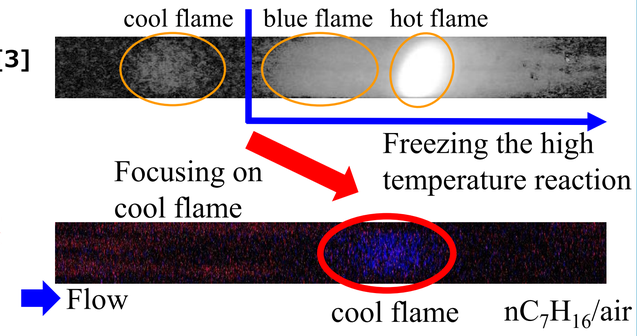
→ weak flameにより，着火過程の定常な観察が可能



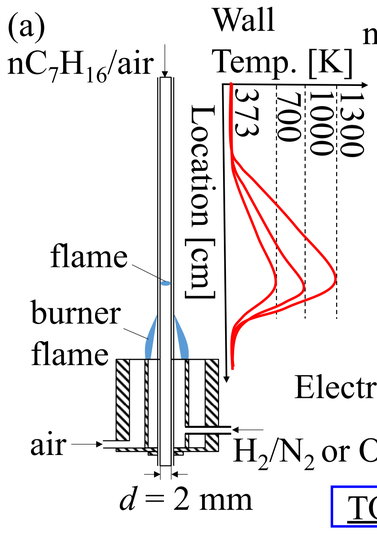
weak flameにおける多段酸化反応[3]
- MFRでは三段反応が生じる

→ 3つの反応帯は一般的な多段酸化反応を分離，定在化したもの

→ 冷炎のみを対象とした詳細な観察が可能



主な研究成果（手法）



実験条件
- 混合気：*n*-ヘプタン/空気
- 流入流速：V = 2 cm/s
- 圧力：P = 1 atm
- 当量比　：ϕ = 1

撮影条件
- CHフィルタ付デジタル一眼レフカメラ
- 長時間露光(5 ~ 30 分)

数値計算条件
- PREMIX[4] をベースとした一次元定常計算コード[1]

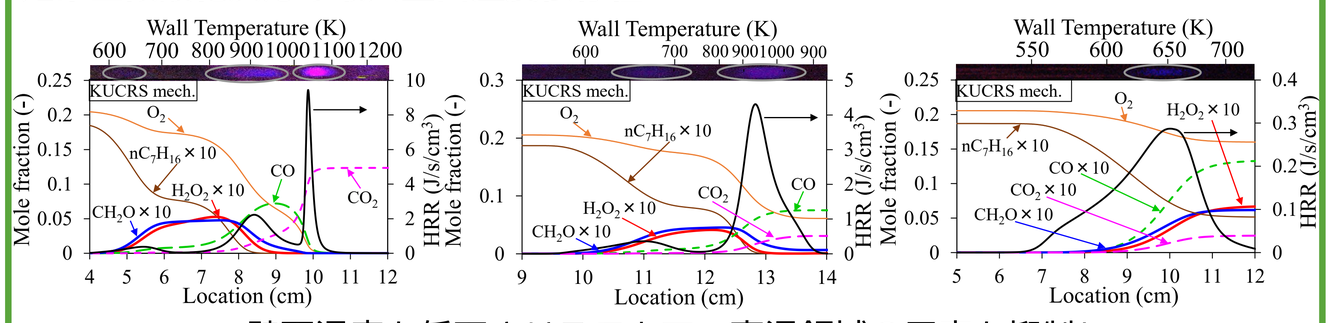
→ エネルギー方程式に気層と壁面との熱伝達項を追加

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

- 反応機構：
  KUCRS mech. (373化学種, 1072素反応)[5]
  LLNL mech. (654化学種, 2827素反応)[6]
  MFL mech. (140化学種)[7]

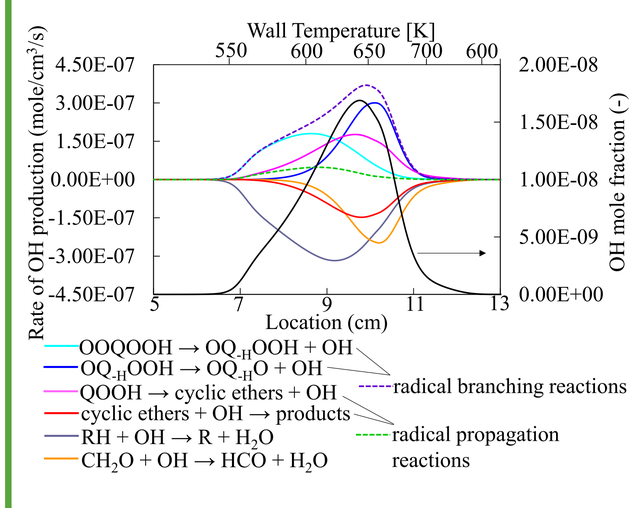
主　な　研　究　成　果

定常三段酸化反応の最大壁面温度依存性



壁面温度を低下させることで，高温領域の反応を抑制し，
三段反応から抽出した冷炎のみに注目することが可能

OH生成及び消費に寄与度の高い素反応とOHモル分率分布との関係性

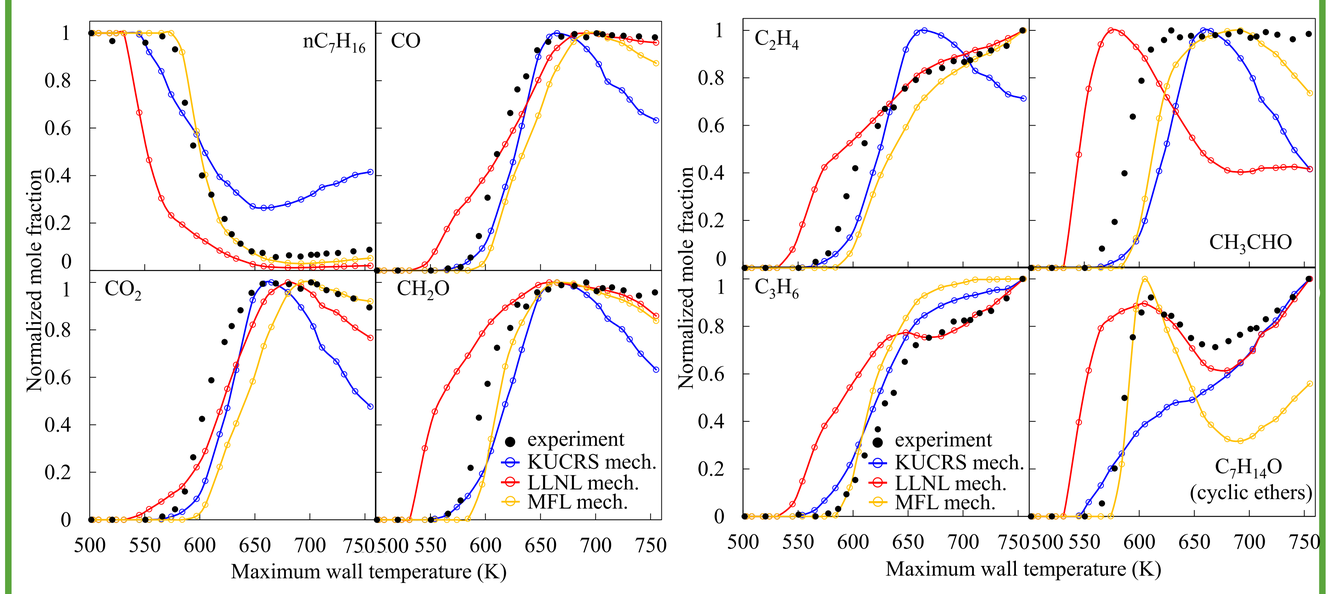


- OHは主にradical branching pathより生成
- OHは主に燃料消費反応によって消費
- radical branching pathによる正味のOH生成量とOHモル分率分布の概形はよく一致

→ radical branching pathと燃料消費反応との間でradical chain cycleが形成

Radical branching pathと冷炎形成には強い相関がある

化学種計測を通じた冷炎の化学構造



- 570 K付近から低温酸化反応が開始
- 600 K付近からモル分率分布はほぼ一定値
- 反応が開始する温度域を除いて，主要化学種においては反応機構は実験結果を定性的に再現
- C_2H_4, C_3H_6 のモル分率分布は単調増加
- C7H14Oの概形は極大，極小値を持つ
- 反応が開始する温度域，分布概形，最大値をとる温度域の3点を再現する反応機構はない

MFRを用いた化学種計測により，低温酸化を対象とした反応機構の予測精度の向上

今年度の取組及び研究計画

- 化学種計測結果をもとに反応モデルの検証

2016	2017	2018
質量分析の環境構築	反応モデルの検証	EGR条件の検証

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[1] K. Maruta et al., Proc. Combust. Inst., 30 (2005) 2429-2436.
[2] S. Minaev et al., Combust. Theor. Model., 11 (2) (2007) 187-203.
[3] A. Yamamoto et al., Proc. Combust. Inst., 33 (2011) 3259-3266.
[4] R.J. Kee, et al., Sandia National Laboratories Report, (1985) No. SAND85-8240.
[5] A. Miyoshi, J. Phys. Chem. A, 115 (15) (2011) 3301−3325.
[6] M. Mehl et al., Proc. Combust. Inst., 33 (1) (2011) 193−200.
[7] Diesel_nheptane_chem_MFL2015, Model Fuel Library, CHEMKIN-PRO v17.2. (2016).

SIP 革新的燃焼技術 Innovative Combustion Technology bridging to....

2017/07/06 SIP「革新的燃焼技術」第3回公開シンポジウム

ガソリン燃焼チーム クラスター大学17 （ノック抑制班）

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The reactivity of ultra-lean gasoline surrogate/air weak flames in a micro flow reactor with a controlled temperature

1 Objective

Background
- New automotive engines are developed to increase efficiency and decrease CO_2
- Ultra-lean combustion of gasoline can lead to higher efficiency
- Engine knocking can occur and must be avoided

➔ Reactivity of ultra-lean mixtures must be well understood

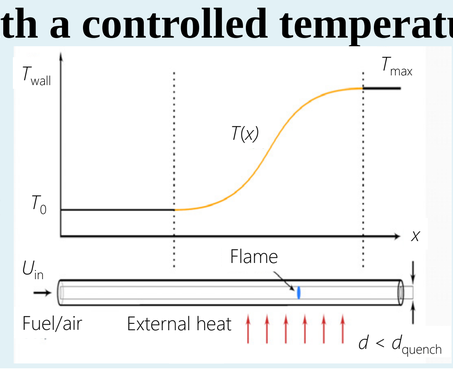
Challenges
- Ultra-lean combustion usually limited to high temperature/pressure regimes
- Common approaches use transient methods (RCM, Shock tube)

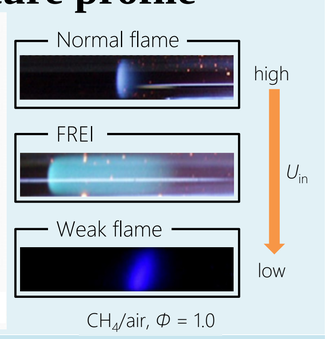
Solution
- Investigation by **micro flow reactor with controlled temperature profile** (MFR)
- Allows for investigation at atmospheric and elevated pressures and temperatures
- Enables steady state investigation
- Easy and reliable method to evaluate fuel reactivity

2 Principle

Micro flow reactor with a controlled temperature profile[1][2]

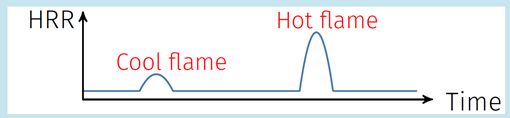
- Steady *T*-profile
- Laminar flow
- Constant pressure
- **Flame pattern dependent on flow velocity**
- Weak flame represents ignition





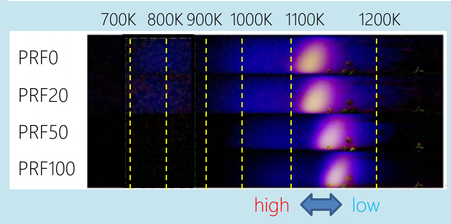
Weak flames
- Spatially separated flames
- Cool, blue and hot flames
- *T* can be identified
- Reactivity can be evaluated
- Ultra-lean combustion possible

Conventional



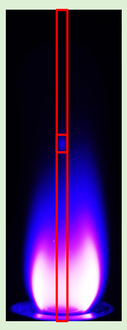
MFR

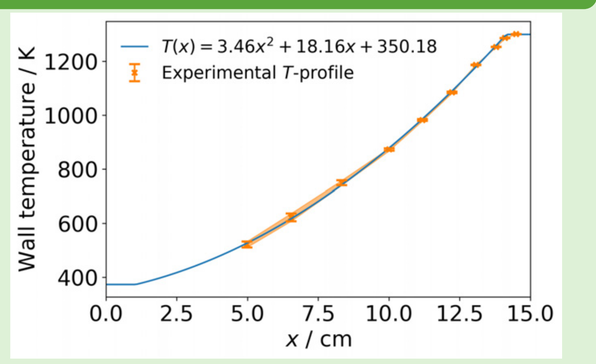
$\Phi = 1.0$
$U_{in} = 2.0$ cm/s



[3]

3 Results





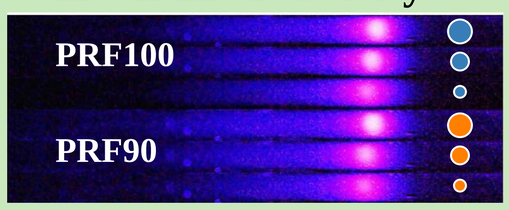
$$\dot{M}\frac{dT}{dx}-\frac{1}{c_p}\frac{d}{dx}\left(\lambda A\frac{dT}{dx}\right)+\frac{A}{c_p}\sum_{k=1}^{K}\rho Y_k V_k c_{pk}\frac{dT}{dx}+\frac{A}{c_p}\sum_{k=1}^{K}\dot{\omega}_k h_k W_k-\frac{A}{c_p}\frac{4\lambda Nu}{d^2}(T_w-T_g)=0$$

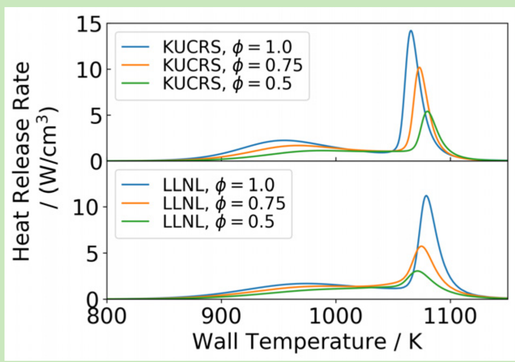
Experiment

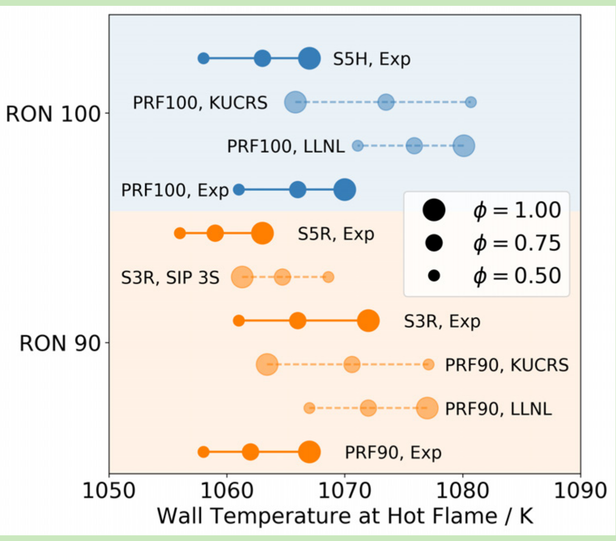
Vertical-type MFR
- Mixing in heated tank
- Long exposure times + CH filter
- Broad *T* profile
- High reproducibility

Numerical simulations
- PREMIX[4] 1-D steady code
- Additional term for heat transfer with wall[1]
- Detailed SIP mechanisms[5]

Hot flame reactivity



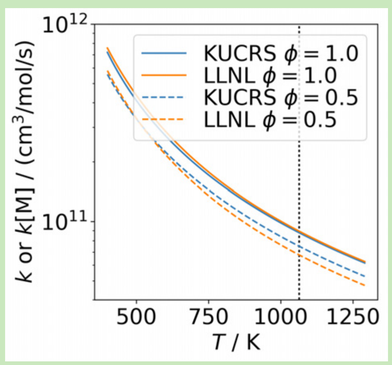




Three-body reaction: $H+O_2(+M)=HO2(+M)$

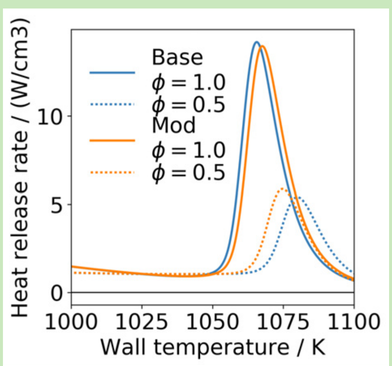
Chain Termination
- Competes with chain branching reaction: $H+O_2=OH+O$
- Strong influence on hot flame reactivity
- Different representation in various mechanisms

Rate constants



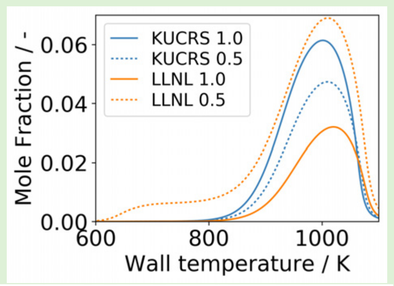
- Similar in stoich. case
- Different in lean case
- Influences Φ dependence

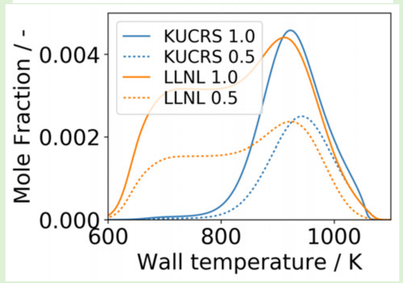
Modified mechanism



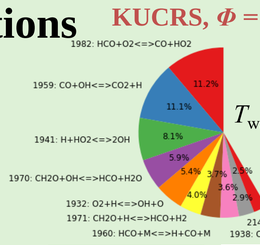
- Φ = 1.0 moves downstream
- Φ = 0.5 moves upstream
- Sensitive to third bodies

Effect of Φ in simulations

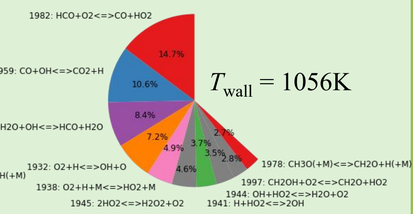


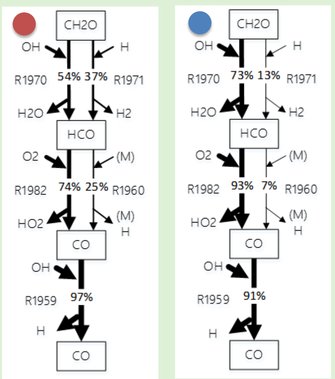


KUCRS, Φ = 1.0



KUCRS, Φ = 0.5





$CH_2O+1.25O_2 = CO_2+0.5H_2O+0.9OH+0.05O$

$CH_2O+1.05O_2 = CO_2+0.9H_2O+0.2OH$

KUCRS/SIP mech:
- Later fuel consumption
- Later interm. consumption
- Higher reactivity for Φ = 1.0

4 Outlook

2016	2017	2018
• PRF experiments and simulations • Comparison of reaction mechanisms	• Surrogate experiments and simulations • Identification of main reactions	• High pressure • EGR conditions • Compilation into reactivity index

High pressure
- Experiments and simulations under engine conditions
- Effect of equivalence ration under these conditions

Exhaust gas recirculation
- EGR up to 20%
- Effect of third bodies on reactivity

References

[1] K. Maruta, T. Kataoka, N. Kim, S. Minaev, R. Fursenko, *Proc. Combust. Inst.*, 30 (2005), 2429-2436.
[2] S. Minaev, K. Maruta, R. Fursenko, *Combustion Theory and Modelling*, Vol. 11 No. 2 (2007), 187-203.
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