TSINGHUA-PRINCETON-COMBUSTION INSTITUTE

2022 SUMMER SCHOOL ON COMBUSTION

COMBUSTION IN MICROGRAVITY AND MICROSCALE

Kaoru Maruta

Tohoku University

July 14-15, 2022

TSINGHUA-PRINCETON-COMBUSTION INSTITUTE

2022 SUMMER SCHOOL ON COMBUSTION

<table>
<tr><th colspan="6">Schedule</th></tr>
<tr><th>Beijing Time</th><th>July 11 (Mon.)</th><th>July 12 (Tue.)</th><th>July 13 (Wed.)</th><th>July 14 (Thu.)</th><th>July 15 (Fri.)</th></tr>
<tr><td>08:00 ~ 11:00</td><td></td><td></td><td>Mechanism Reduction and Stiff Chemistry Solvers
Tianfeng Lu
VMN: 52667557219</td><td></td><td>Mechanism Reduction and Stiff Chemistry Solvers
Tianfeng Lu
VMN: 52667557219</td></tr>
<tr><td>*10:00 ~ 12:00</td><td></td><td>Virtual Poster Session
10:00~12:00
VMN: 388239275</td><td></td><td>Virtual Lab Tour
10:00~12:00
VMN: 231842246</td><td></td></tr>
<tr><td>14:00 ~ 17:00 Session I</td><td colspan="3">Fundamental of Flames
Suk Ho Chung
VMN: 42399313194</td><td colspan="2">Combustion in Microgravity and Microscale
Kaoru Maruta
VMN: 71656262918</td></tr>
<tr><td>14:00 ~ 17:00 Session II</td><td colspan="2">Soot
Markus Kraft
VMN: 39404905340</td><td></td><td colspan="2">Current Status of Ammonia Combustion
William Roberts
VMN: 80506726244</td></tr>
<tr><td>19:00 ~ 22:00 Session I</td><td colspan="5">Combustion Chemistry and Kinetic Mechanism Development
Tiziano Faravelli
VMN: 35989357660</td></tr>
<tr><td>19:00 ~ 22:00 Session II</td><td colspan="4">Combustion Fundamentals of Fire Safety
José Torero
VMN: 57002781862</td><td></td></tr>
</table>

Note:

[1]Session I and Session II are simultaneous courses.

[2]VMN: Voov Meeting Number

Guidelines for Virtual Participation

1. General Guidelines

- Tencent Meeting software (腾讯会议) is recommended for participants whose IP addresses locate within Mainland China; Voov Meeting (International version of Tencent Meeting) is recommended for other IP addresses. The installation package can be found in the following links:

  a) 腾讯会议
  https://meeting.tencent.com/download/

  b) Voov Meeting
  https://voovmeeting.com/download-center.html?from=1001

- All the activities listed in the schedule are “registrant ONLY” due to content copyright.
- To facilitate virtual communications, each participant shall connect using stable internet and the computer or portable device shall be equipped with video camera, speaker (or earphone) and microphone.

2. Lectures

- The lectures are also “registrant ONLY”. Only the students who registered for the course can be granted access to the virtual lecture room.
- To enter the course, each registered participant shall open the software and join the conference using the corresponding Voov Meeting Number (VMN) provided in the schedule; only participants who show unique identification codes and real names as “**xxxxxx-Last Name, First Name**” will be granted access to the lecture room; the identification code will be provided through email.
- During the course, each student shall follow the recommendation from the lecturer regarding the timing and protocol to ask questions or to further communicate with the lecturer.
- For technical or communication issues, the students can contact the TA in the virtual lecture or through emails.
- During the course, the students in general will not be allowed to use following functions in the software: 1) share screen; 2) annotation; 3) record.

3. Lab Tour

- The event will be hosted by graduate students from Center for Combustion Energy, Tsinghua University and live streamed using provided Voov Meeting Number.
- During the activity, the participants will not be allowed to use following functions in the software: 1) share screen; 2) annotation; 3) record.
- Questions from the virtual participants can be raised using the chat room.

4. Poster Session

- The event will be hosted by the poster authors (one Voov Meeting room per poster) and live streamed using provided Voov Meeting Number.
- During the activity, the participants will not be allowed to use following functions in the software: 1) share screen; 2) annotation; 3) record.
- Questions from the virtual participants can be raised using the chat room or request access to audio and video communication.

Teaching Assistants

- **Fundamentals of Flame (Prof. Suk Ho Chung)**

  TA1: Hengyi Zhou (周恒毅); zhouhy19@mails.tsinghua.edu.cn

  TA2: Xinyu Hu (胡馨予); hxy21@mails.tsinghua.edu.cn

- **Combustion Chemistry and Kinetic Mechanism Development (Prof. Tiziano Faravelli)**

  TA1: Shuqing Chen (陈舒晴); chen-sq19@mails.tsinghua.edu.cn

  TA2: Jingzan Shi (史京瓒); sjz21@mails.tsinghua.edu.cn

- **Current Status of Ammonia Combustion (Prof. William Roberts)**

  TA1: Yuzhe Wen (温禹哲); wyz20@mails.tsinghua.edu.cn

  TA2: Haodong Chen (陈皓东); chd20@mails.tsinghua.edu.cn

- **Soot (Prof. Markus Kraft)**

  TA1: Yuzhe Wen (温禹哲); wyz20@mails.tsinghua.edu.cn

  TA2: Haodong Chen (陈皓东); chd20@mails.tsinghua.edu.cn

- **Combustion Fundamentals of Fire Safety (Prof. José Torero)**

  TA1: Xuechun Gong (巩雪纯); gxc19@mails.tsinghua.edu.cn

  TA2: Weitian Wang (王巍添); wwt20@mails.tsinghua.edu.cn

- **Combustion in Microgravity and Microscale (Prof. Kaoru Maruta)**

  TA1: Hengyi Zhou (周恒毅); zhouhy19@mails.tsinghua.edu.cn

  TA2：Xinyu Hu (胡馨予); hxy21@mails.tsinghua.edu.cn

- **Mechanism Reduction and Stiff Chemistry Solvers (Prof. Tianfeng Lu)**

  TA1: Shuqing Chen (陈舒晴); chen-sq19@mails.tsinghua.edu.cn

  TA2: Jingzan Shi (史京瓒); sjz21@mails.tsinghua.edu.cn

Tsinghua-Princeton-Combustion Institute, 2022 Summer School on Combustion
July 11-15, 2022

Combustion in Microgravity and Microscale
Part 1: Flame basics

Kaoru MARUTA
Institute of Fluid Science
Tohoku University

東北大学
流体科学研究所
丸田　薫

Introduction

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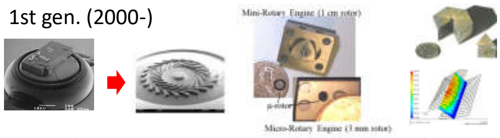
Introduction

Combustion in microgravity

Intense international collaboration since 1990's-

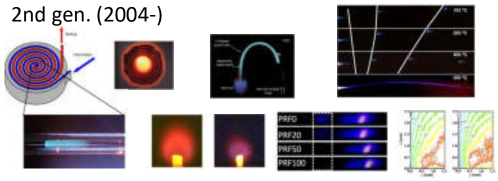
Combustion in microscale

1st gen. (2000-)



Mainly for power generation based on liquid fuels, U.S.

2nd gen. (2004-)



Applications + Combustion science

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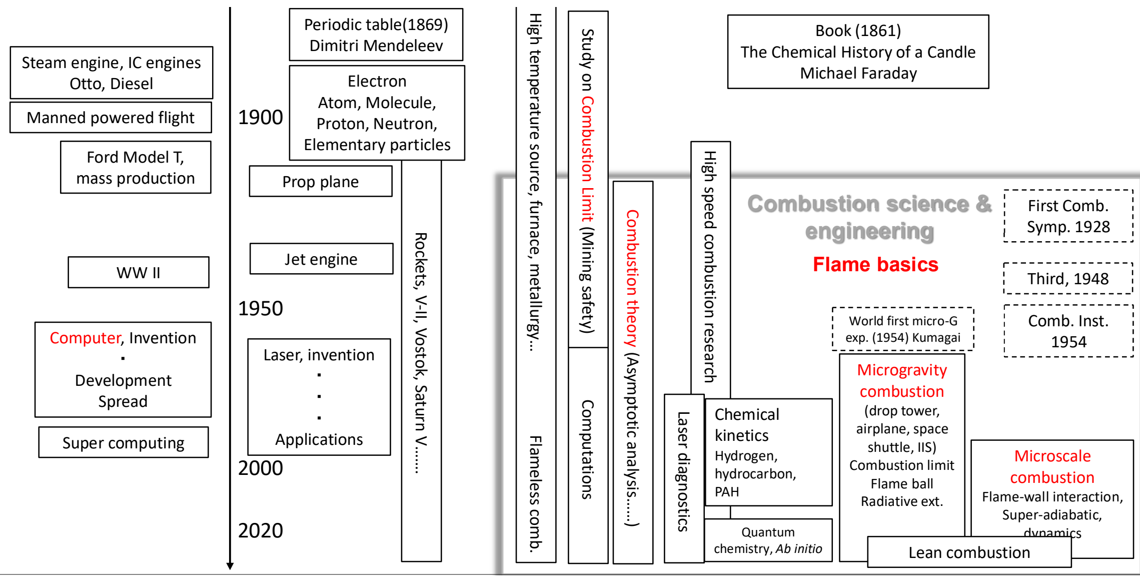
Science and technology developments and progress of combustion research



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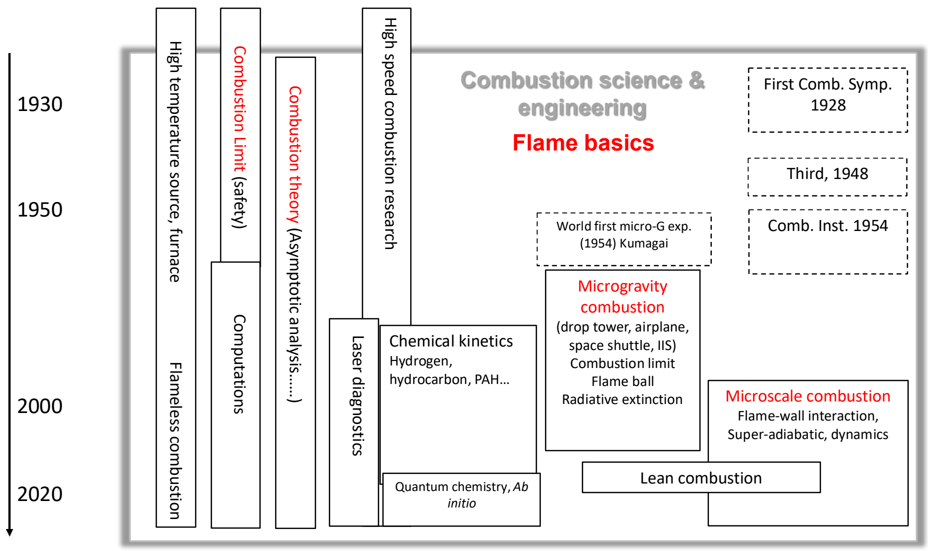
Progress of combustion research



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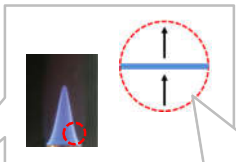
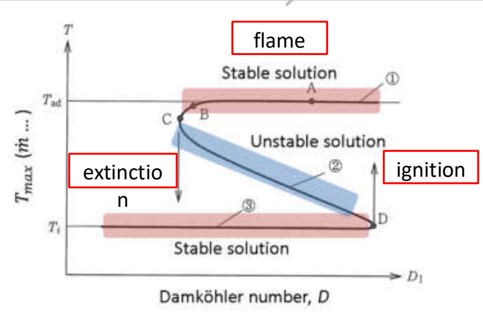
Flame basics

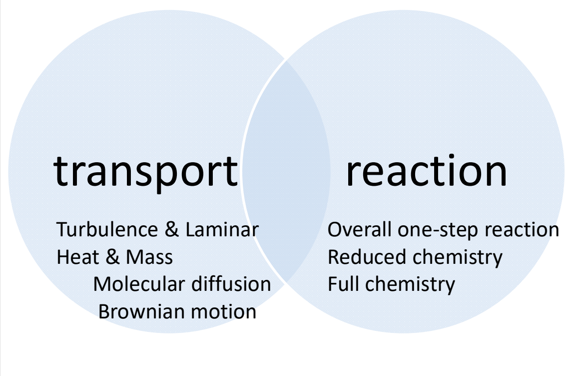


Adiabatic flame
Non-adiabatic flame
Super-adiabatic flame

Cool, blue (warm)
& hot flames



S-curve (Fendell curve)



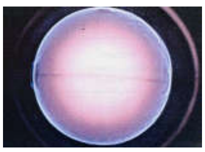
Flame basics

- Outline
- S-curve
- Premixed flame
- Flame characteristics
- Non-premixed flame

Flame classification

*

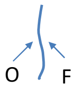
*

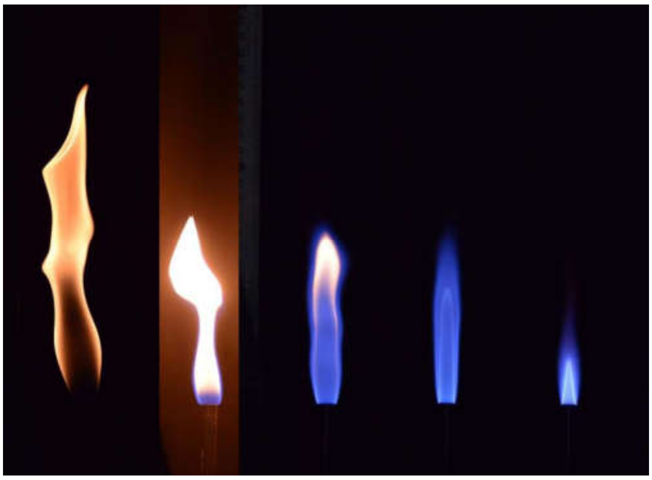


- Premixed and non-premixed (diffusion) flames
- Laminar and turbulent flames

*: www.nasa.gov

Premixed and non-premixed flame



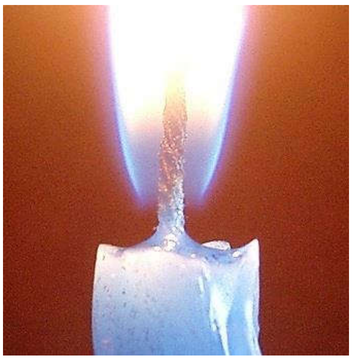


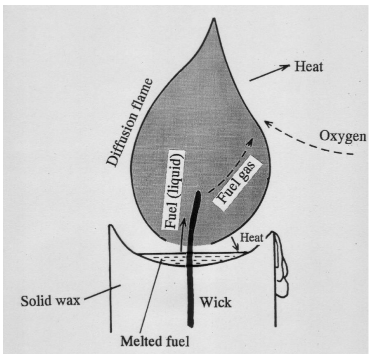
Non-premixed flame
(Diffusion flame)

Premixed flame

**: Energy dynamics laboratory

Phenomena in a candle flame





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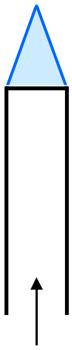
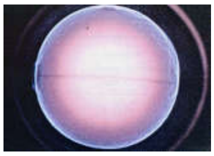
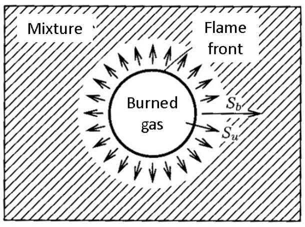
Stabilized and propagation flames







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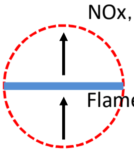
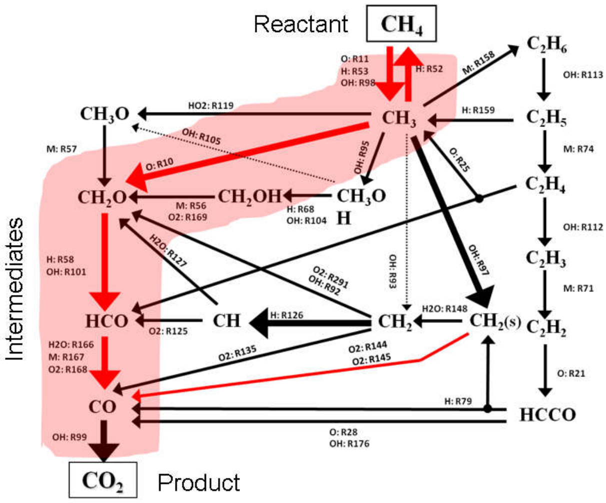
Flame and elementary reactions, methane reaction path

Product gases
CO_2, H_2O, CO, NOx, N_2, ・・・



Flame (flame front)

Reactants
CH_4, O_2, N_2



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Laminar and turbulent premixed flames

Laminar flame
(Direct photo)

Turbulent premixed flame (Schlieren image)

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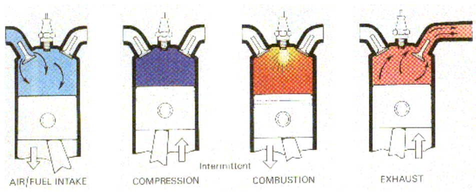
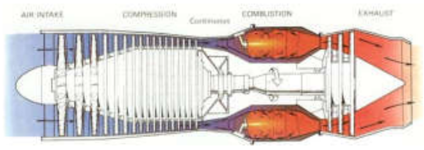
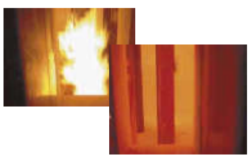
Combustion in practical devices





The Jet Engine, Rolls-Royce, 1992



- Turbulent combustion
- Reciprocating engines

Premixed combustion in Otto-cycle engine (Spark-Ignited engine, Gasoline engine)

Auto-ignited non-premixed (or partially premixed) combustion in Diesel engine (Compression ignition engine)

- Gas turbine engine

Different types of GT, Premixed and non-premixed combustion

- Furnace, incinerator

Mostly non-premixed, specific combustion-mode (Mild combustion)

Moderate or Intense Low oxygen Dilution (MILD) combustion

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Flame basics

- Outline
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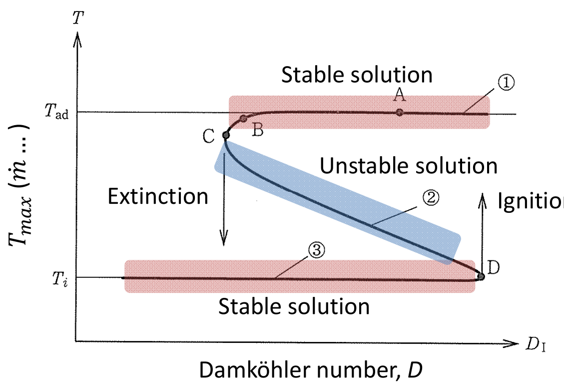
S-curve (Fendell curve)



$$D = \frac{Flow\ residence\ time}{Chemical\ time}$$

- Time scales of transport and chemical reaction
- Extensively applicable to various phenomena, e.g., candle flame, burner flame, counterflow flame, supersonic combustion, etc.

Fendell, F.E., J. Fluid Mech. 21(2) 281 (1965).
Liñán, A., Acta Astro. **1**(7) 1007 (1974).

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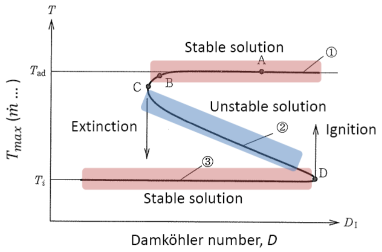
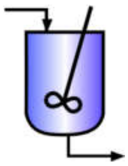
Chemical reactor and combustion



- Ignition
- Combustion
- Extinction



CSTR

Continuous stirred-tank reactor

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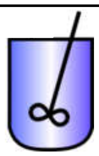
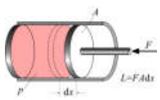
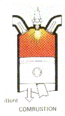
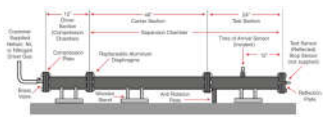
Analogy between combustor and reactor





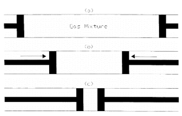


Batch



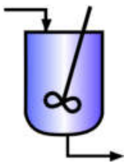
The Modal Shop, Inc., 2017 **Shock tube**

RCM



rapid compression machine

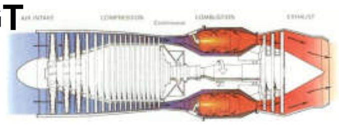
Meere et al., J. Eng. Math. 44: 57, 2002.



CSTR

Dagaut, ICFD 2016

GT



The Jet Engine, Rolls-Royce, 1992

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Time scales of reactive fluids

Chemical time		Physical time
NO formation	1 s
	10^{-2}s	Flow time
Product formation H_2O	10^{-4}s	Transport time: Molecular, Turbulent (Physical interest)
Radical formation H	10^{-6}s
Radical formation H_2O_2 quasi-steady state?	10^{-8}s	Radiation transfer ? quasi-steady state
	10^{-10}s	DNS Time-step

Ju, ICFD, 2008

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Time scales of chemical reactions

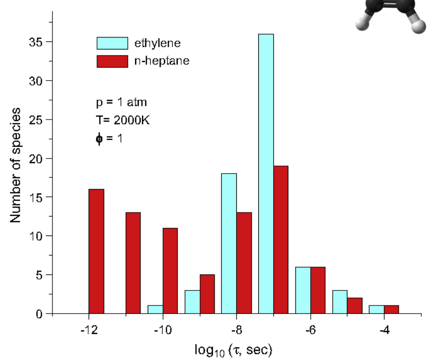
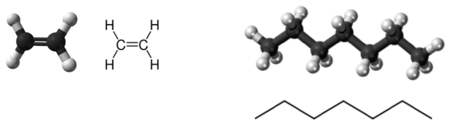


Fig. Histogram of species time scales in PSR with fixed temperature and residence time of 1 ms for a 33-species mechanism for ethylene and a 78-species mechanism for *n*-heptane, respectively.



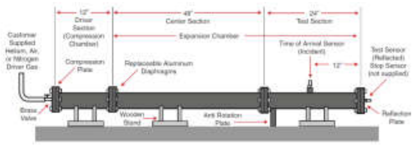
- Distributions of ignition time scale (Residence time @1 ms, 2000 K)
- Pico-sec〜milli-sec or even longer

Lu et al., Prog. Energ. Comb. Sci. 35: 192 (2009).

Seeking for “ideal” ignition phenomena

Batch

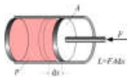
ST



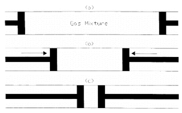
The Modal Shop, Inc., 2017

High Purity Photolysis Shock Tube (NASA Tube), Stanford Univ.

Kinetics Shock Tube (KST), Stanford Univ.



RCM



Meere et al., J. Eng. Math. 44: 57, 2002.
http://c3.nuigalway.ie

Chemical kinetics modeling

Homogeneous rector
0D model
Senkin, 1988
Lutz, A. et al.

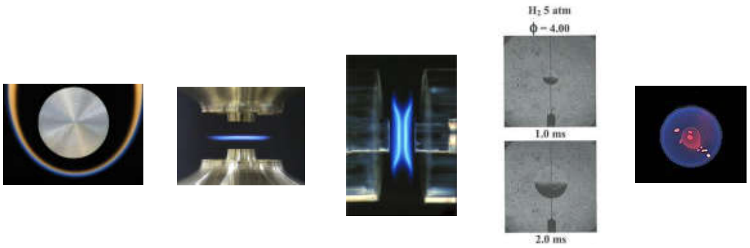
Equil (Equilibrium)
STANJAN*
JANAF Table**

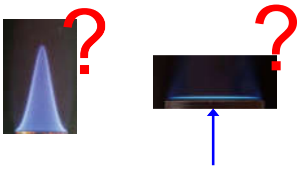
*STANJAN: Stanford and its connection with the JANAF thermochemical data tables

**JANAF thermochemical tables of the Joint Army-Navy-NASA-Air Force (JANNAF) Interagency Propulsion Committee

NIST-JANAF Thermochemical Tables: https://janaf.nist.gov/

Seeking for “ideal” flames



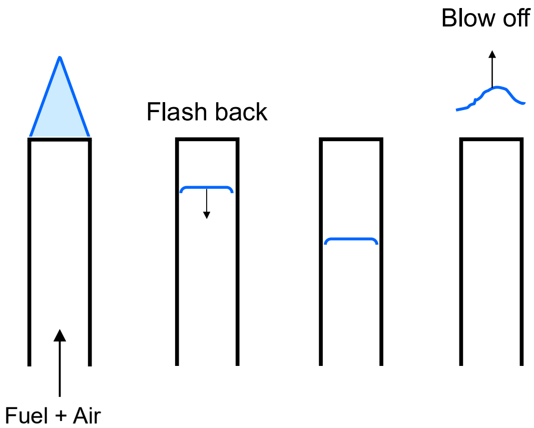


- Difficult to establish ideal (probably one-dimensional, adiabatic) flames without influences of external factors
- Detailed data from ideal flames are essential for establishing computational tools, precise kinetics, etc.

Flame basics

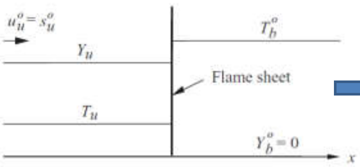
- Outline
- S-curve
- Premixed flame
- Flame characteristics
- Non-premixed flame

Bunsen flame



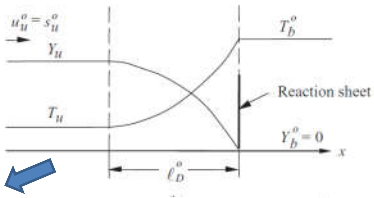
Flame propagation, laminar burning velocity, flame quench, extinction, blow off, flame structure

Laminar premixed flame (Deflagration wave)



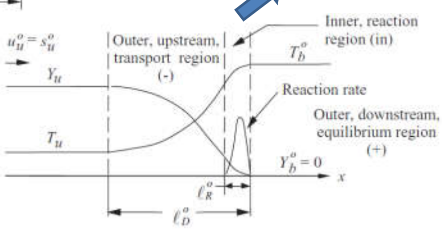
(Rankine-Hugoniot Relations,
→ detonation and deflagration waves)

- Flame is interface separating unburned and burned gases, thermodynamic equlibrium



- Transport in preheat zone, diffusion processes of mass and heat
- Reaction sheet, source of heat and sink of reactant
- If Le =1, Y and T profiles are mirror images

- Preheat and Reaction zones



Law, C.K., Combustion Physics, 2006.

1-D steady propagating flame

Governing equation for steady, isobaric, adiabatic one-dimensional flame propagation

Continuity
$$\dot{M} = \rho u A,$$

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

Species
$$\dot{M}\frac{dY_k}{dx} + \frac{d}{dx}(\rho A Y_k V_k) - A\dot{\omega}_k W_k = 0, \qquad (k = 1, \dots, K),$$

Equation of state
$$\rho = \frac{p\overline{W}}{RT}$$

Forward rate coefficient
$$k_f = AT^{\beta}\exp\left(\frac{-E_A}{RT}\right)$$

PREMIX, CHEMKIN

For further details, refer, e.g., Poinsot, Theor. Num. Comb.


```
! GRI-Mech Version 3.0 7/30/99  CHEMKIN-II format
! See README30 file at anonymous FTP site unix.sri.com, directory gri;
! WorldWideWeb home page http://www.me.berkeley.edu/gri_mech/ or
! through http://www.gri.org , under 'Basic  Research',
! for additional information, contacts, and disclaimer
ELEMENTS
O  H  C  N  AR
END
SPECIES
H2     H      O      O2     OH     H2O    HO2    H2O2
C      CH     CH2    CH2(S) CH3    CH4    CO     CO2
HCO    CH2O   CH2OH  CH3O   CH3OH  C2H    C2H2   C2H3
C2H4   C2H5   C2H6   HCCO   CH2CO  HCCOH  N      NH
NH2    NH3    NNH    NO     NO2    N2O    HNO    CN
HCN    H2CN   HCNN   HCNO   HOCN   HNCO   NCO    N2
AR     C3H7   C3H8   CH2CHO CH3CHO
END
!THERMO
! Insert GRI-Mech thermodynamics here or use in default file
!END
REACTIONS
2O+M<=>O2+M                              1.200E+17   -1.000       .00
H2/ 2.40/ H2O/15.40/ CH4/ 2.00/ CO/ 1.75/ CO2/ 3.60/ C2H6/ 3.00/ AR/  .83/
O+H+M<=>OH+M                             5.000E+17   -1.000       .00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+H2<=>H+OH                              3.870E+04    2.700    6260.00
O+HO2<=>OH+O2                            2.000E+13     .000       .00
O+H2O2<=>OH+HO2                          9.630E+06    2.000    4000.00
O+CH<=>H+CO                              5.700E+13     .000       .00
O+CH2<=>H+HCO                            8.000E+13     .000       .00
O+CH2(S)<=>H2+CO                         1.500E+13     .000       .00
O+CH2(S)<=>H+HCO                         1.500E+13     .000       .00
O+CH3<=>H+CH2O                           5.060E+13     .000       .00
O+CH4<=>OH+CH3                           1.020E+09    1.500    8600.00
O+CO(+M)<=>CO2(+M)                       1.800E+10     .000    2385.00
   LOW/ 6.020E+14     .000    3000.00/
H2/2.00/ O2/6.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/3.50/ C2H6/3.00/ AR/ .50/
O+HCO<=>OH+CO                            3.000E+13     .000       .00
O+HCO<=>H+CO2                            3.000E+13     .000       .00
O+CH2O<=>OH+HCO                          3.900E+13     .000    3540.00
O+CH2OH<=>OH+CH2O                        1.000E+13     .000       .00
O+CH3O<=>OH+CH2O                         1.000E+13     .000       .00
O+CH3OH<=>OH+CH2OH                       3.880E+05    2.500    3100.00
O+CH3OH<=>OH+CH3O                        1.300E+05    2.500    5000.00
O+C2H<=>CH+CO                            5.000E+13     .000       .00
O+C2H2<=>H+HCCO                          1.350E+07    2.000    1900.00
O+C2H2<=>OH+C2H                          4.600E+19   -1.410   28950.00
O+C2H2<=>CO+CH2                          6.940E+06    2.000    1900.00
O+C2H3<=>H+CH2CO                         3.000E+13     .000       .00
O+C2H4<=>CH3+HCO                         1.250E+07    1.830     220.00
O+C2H5<=>CH3+CH2O                        2.240E+13     .000       .00
O+C2H6<=>OH+C2H5                         8.980E+07    1.920    5690.00
O+HCCO<=>H+2CO                           1.000E+14     .000       .00
O+CH2CO<=>OH+HCCO                        1.000E+13     .000    8000.00
O+CH2CO<=>CH2+CO2                        1.750E+12     .000    1350.00
```

GRI-Mech 3.0 (1999)

GRI-Mech 3.0, <http://www.me.berkeley.edu/gri_mech/>.

53 species

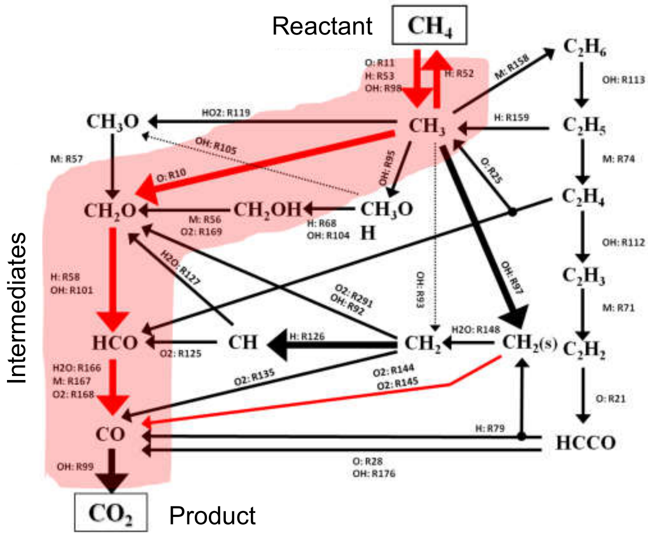
327 reactions

$$k_{f_i} = A_i T^{\beta_i}\exp\left(\frac{-E_i}{R_c T}\right)$$

+
Transport data
Thermodynamic data

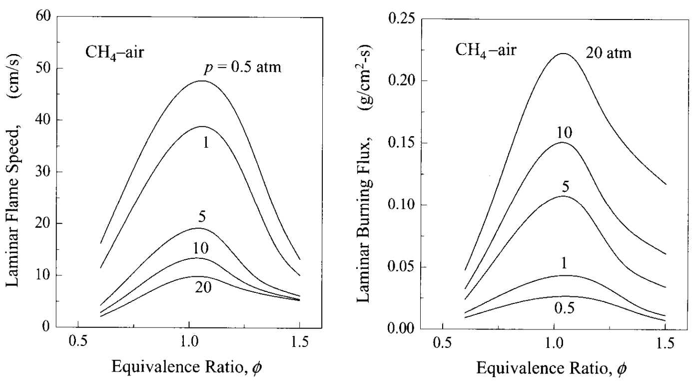
Cont'd

Example of reaction path, methane oxidation



Laminar burning velocity and burning flux

$$CH_4 + 2O_2 \leftrightarrow 2H_2O + CO_2$$

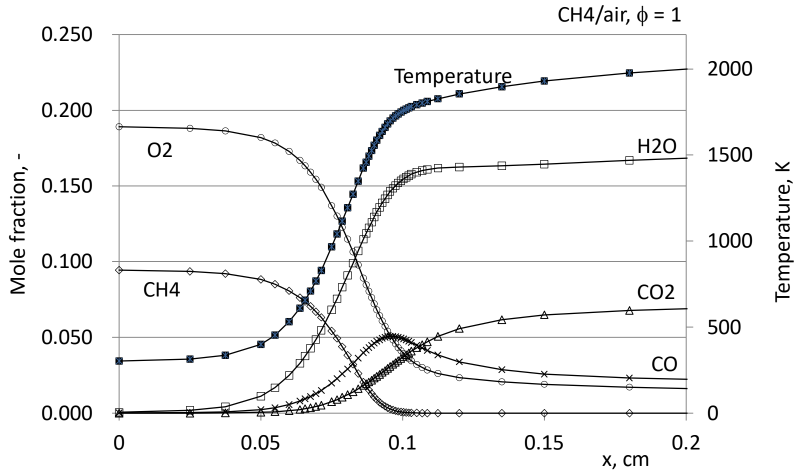


(a) Laminar flame speed, S_L

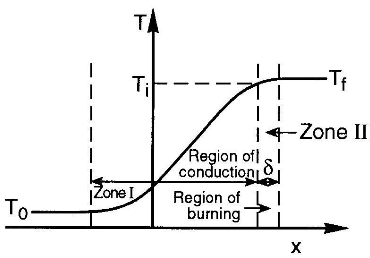
(b) Laminar burning flux, ρS_L

Figures: Law, C.K., Combustion Physics, 2006.

Structure of laminar one-dimensional premixed flame



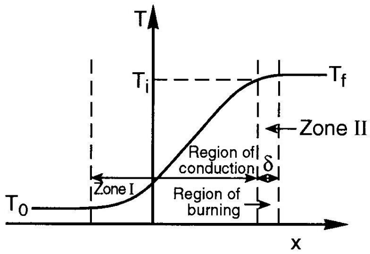
Approximate analysis, Mallard-Le Chatelier, 1880's



- Region of conduction (ZONE I) and region of burning (ZONE II)
- Intuitive recognition for reaction zone thickness, laminar burning velocity

Glassman, Combustion, 1987.

Approximate analysis, Mallard-Le Chatelier, 1880's



Incoming flow speed = reaction rate

$$\rho_u S_L = \dot{\omega}\delta$$

Temperature increase of unburned gas is due to conduction heat from reaction zone

$$\rho_u S_L c_p (T_i - T_0) = \lambda \left(\frac{T_f - T_i}{\delta} \right)$$

Delete δ

$$S_L = \sqrt{\frac{\lambda}{\rho_u c_p} \frac{(T_f - T_i)}{(T_i - T_0)} \frac{\dot{\omega}}{\rho_u}} \sim \sqrt{\alpha \frac{\dot{\omega}}{\rho_u}}$$

Delete $\dot{\omega}$

$$\delta \sim \frac{\alpha}{S_L}$$

α : thermal diffusivity

$$\alpha = \frac{\lambda}{\rho C_p}$$

$\dot{\omega}$: overall one-step reaction

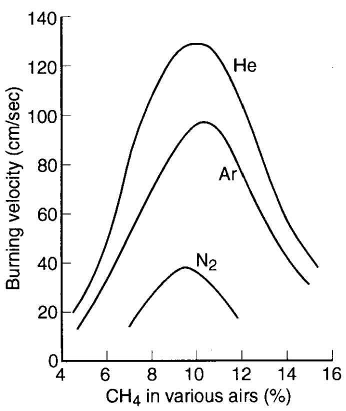
$$\dot{\omega} = Ap^N \exp\left(\frac{-E}{RT_f} \right)$$

Pressure dependence of S_L

$$S_L \sim (p^{N-2})^{\frac{1}{2}}$$

Glassman, Combustion, 1987.

Laminar flames with different inert gas



- Thermal diffusivities of Ar and N_2 approximately equal
- Since Ar is monoatomic gas, its specific heat is lower than N_2.
- Since heat release is the same, flame temperature, $T_{f,\,Ar} > T_{f,\,N2}$
- Ar and He are both monoatomic and thus their flame temperatures are equal, however, thermal diffusivity of He is much larger than Ar. Consequently, S_L of He case is much larger than Ar.

Clingman et al., Symp. (Int.) Combust. 4, 310, (1953).

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Simplification of governing equations

Zeldovich, Williams, Clavin,
Liñán, Matalon,
Poinsot, T., Theoretical and
Numerical Combustion, 3rd eds.

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Simplification of governing equations

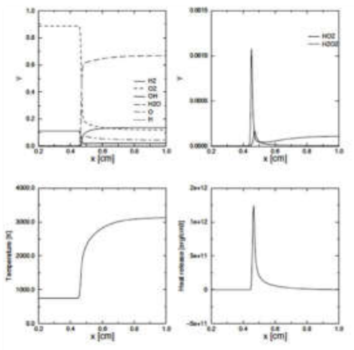
A one-dimensional steady problem in a coordinate system fixed to a flame

$$\rho u = \text{constant} = \rho_1 S_L$$

$$\frac{\partial}{\partial x}(\rho(u + V_k)Y_k) = \dot{\omega}_k$$

$$\rho C_p u \frac{\partial T}{\partial x} = \dot{\omega}'_T + \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) - \frac{\partial T}{\partial x}\left(\rho \sum_{k=1}^{N} C_{p,k} Y_k V_k\right)$$

Example of CHEMKIN computation for H2/O2 flame.



No momentum equation:
Extensively used for solving problem with a large number of species numerically. Used in software packages as CHEMKIN, COSILAB, CANTERA, FLAME MASTER, etc.

For intuitive understandings, simpler equations are useful and have been widely used.

Zel'dovich, Y.B. (1941), Spalding, D.B. (1957)

T. Poinsot, Princeton SS Lecture note, 2015.

Simplification of governing equations

Additional assumptions

An overall one-step reaction in lean flame is assumed. Expression of fuel reaction rate is written as follows.

$$\dot{\omega}_F = \boxed{A} Y_F \boxed{Y_O}\, e^{-\frac{T_a}{T}}$$

Assumed as nearly constant in lean flame

$$\dot{\omega}_F = \boxed{A'} Y_F e^{-\frac{T_a}{T}}$$

Instead of N species fractions, tracking only: Y_F. if Y_o=const. is assumed.

Assuming all Lewis numbers equal to unity $\quad Le = \frac{\alpha}{D} \quad$ where $\alpha = \frac{\lambda}{\rho C_p}$

$$\rho u = \text{constant} = \rho_1 u_1 = \rho_1 S_L$$

$$\rho_1 S_L \frac{dY_F}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_F}{dx}\right) + \dot{\omega}_F$$

$$\rho_1 C_p S_L \frac{dT}{dx} = \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) - Q\dot{\omega}_F$$

Can be simply solved -> extensively used in Combustion Theory, Williams, Linan, Clavin, Matalon…

T. Poinsot, Princeton SS Lecture note, 2015.

Simplification leads to "master equation" of LPF

Non-dimensionalization $\quad Y = Y_F / Y_F^1 \qquad \theta = \frac{C_p(T - T_1)}{Q Y_F^1} = \frac{T - T_1}{T_2 - T_1}$

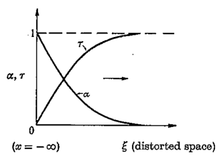


FIGURE 1. Temperature and fuel concentration profiles in flame. →, direction of flow; ----, asymptote.

Spalding, D.B., Proc. Roy. Soc. London. Ser. A 240(1220) 83 (1957).

$$\rho_1 S_L \frac{dY_F}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_F}{dx}\right) + \dot{\omega}_F \qquad / Y_F^1$$

$$\rho_1 C_p S_L \frac{dT}{dx} = \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) - Q\dot{\omega}_F \qquad / C_p(T_2 - T_1)$$

$$\rho_1 S_L \frac{d(Y+\theta)}{dx} = \frac{d}{dx}\left(\lambda \frac{d(Y+\theta)}{dx}\right)$$

If Le = 1 $\quad D = \frac{\lambda}{\rho C_p}$

$\theta + Y = 1 \qquad$ Chemical enthalpy + sensible enthalpy = Constant

$$\rho_1 s_L \frac{d\theta}{dx} = \frac{d}{dx}\left(\frac{\lambda}{c_p}\frac{d\theta}{dx}\right) - \underbrace{\boxed{B_1\left(T_1 + \theta(T_2 - T_1)\right)^{\beta_1} \rho (1-\theta) \exp\left(-\frac{T_{a1}}{T_1 + \theta(T_2 - T_1)}\right)}}_{\dot{\omega}_T}$$

Expressed by only one variable: reduced temperature, progress variable

T. Poinsot, Princeton SS Lecture note, 2015.

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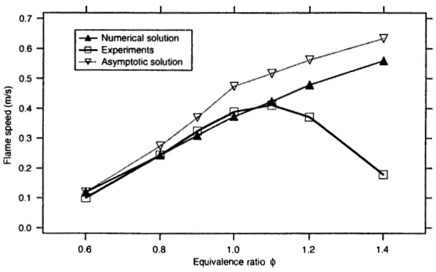
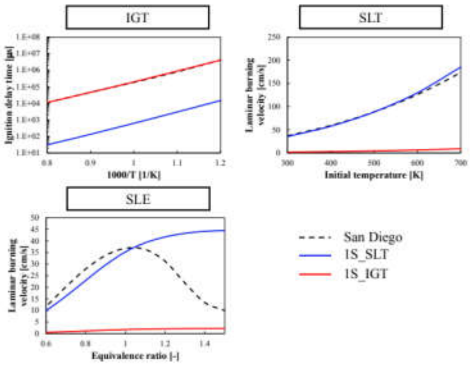
Capability and limit of simplified models



Flame speed of CH4/air mixture

Poinsot and Veynante, Theoretical and Numerical Combustion



in cm^3-mol-cal-sec units

Symbol	Reaction	A	E
1S_IGT	(1-R1) $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$	5.40E+12	36600
1S_SLT		3.30E+15	38000

Variable transport and thermal properties with overall one-step chemistry, Sasaki, unpublished.

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Flame characteristics and related topics

- Laminar burning velocity
- Adiabatic flame temperature

- Flame stretch
- Flame quench
- Flammability limits
- Quenching diameter
- Excess enthalpy combustion
- Flame instability

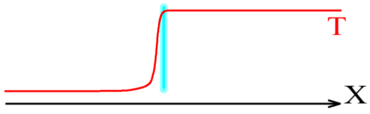
- MILD combustion
- Micro-scale combustion

Moderate or Intense Low oxygen Dilution (MILD) combustion

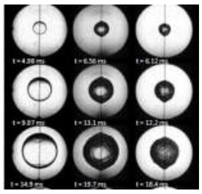
Adiabatic one-dimensional premixed flame

- Ideal flame is hard to realize because…
- Effect of heat loss
- Effect of flow non-uniformity
- Effect of wall (Thermal and chemical)
- Intrinsic flame instabilities

- Thus, measurement of laminar burning velocity needs various ideas & technique
- Laminar burning velocity → (eigenvalue of the governing equations) essential for chemical time determination, kinetics developments, etc.

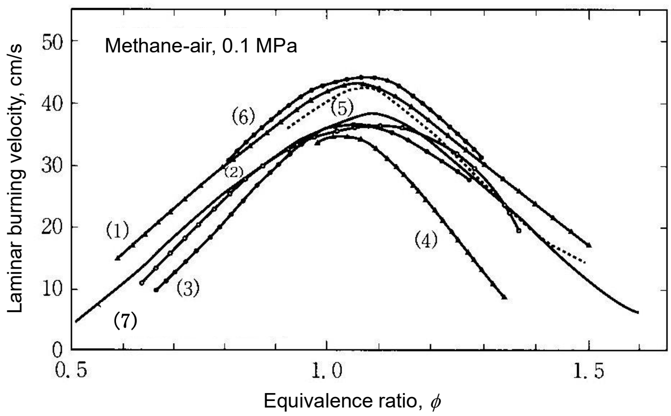


Adiabatic 1D planar premixed flame



Lowry, W., et al., J. Eng. Gas Turb. Power **133**: 091501 (2011).

Laminar burning velocity, methane-air flame



(1),(4),(7) Chamber (2) Flat flame (3) Propagating tube (5),(6) Burner flame

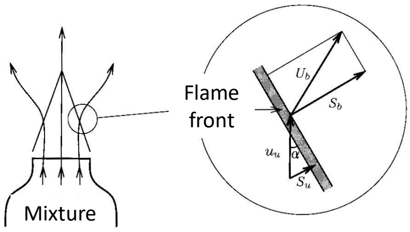
Fundamentals of Combustion Phenomena, Ohm. 2001 in Japanese.

Measurements of laminar burning velocity

- Burner method
- Flat flame
- Outwardly propagating spherical flame
- Counterflow flames

Bunsen flame and laminar burning velocity

Kobayashi lab., TOHOKU U.

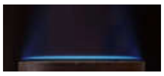


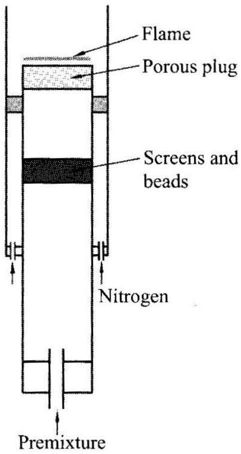
- Flame propagate to flow stream with angle α
- Laminar burning velocity could be obtained from α and U_u

$$S_u = U_u \sin \alpha$$

Fundamentals of Combustion Phenomena, Ohm. 2001 in Japanese.

Burner stabilized flat flame

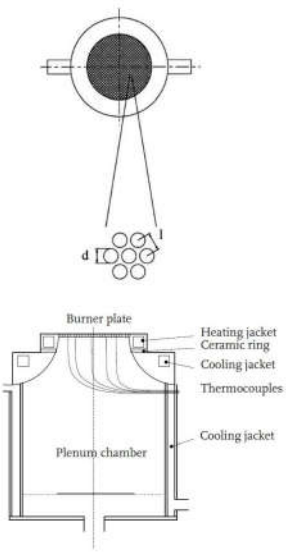




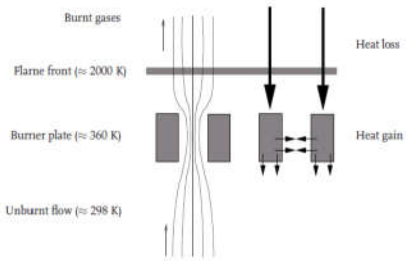
- Flame is stabilized above porous material where flow velocity profile is flat
- Once flame is stabilized, local flow velocity could be equal to laminar burning velocity
- Effect of heat loss from flame to porous material could not be ignored
- Effect of buoyancy is significant at low flow velocity

Figure: Law, C.K., Combustion Physics, 2006.

Modern flat flame burner



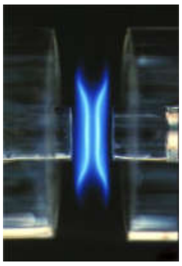
- Effect of heat loss to the burner plate could be canceled
- High fidelity measurement of laminar burning velocity by flat flame is enabled

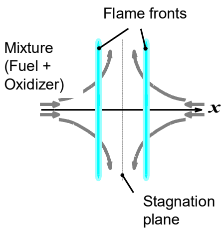


L.P.H. de Goey et al., Eindhoven TU, 2011-

Counterflow premixed twin flames

Commonly used basic flame geometry,
general characterization of flame





- One dimensional flame
- No conductive heat loss
- Flow could be characterized by an unique parameter
  – stretch rate

  → Flame stretch!

Counterflow premixed flame and laminar burning velocity

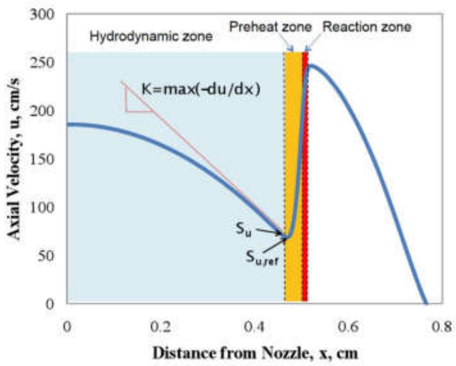


Fig. Axial velocity profile along the stagnation streamline and definition of the strain rate and reference flame speed.

Egolfopoulos et al., Prog. Energ. Combust. Sci. 43 (2014) 36.

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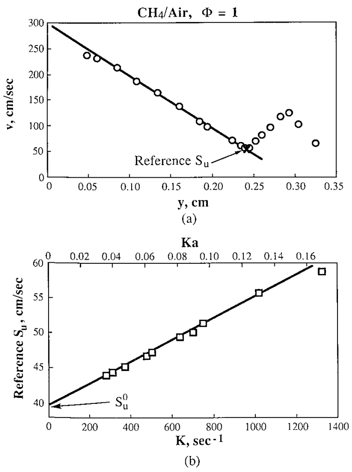
Counterflow premixed flame and laminar burning velocity



- Local minimum of axial velocity profile corresponds to burning velocity at given stretch rate
- Linear extrapolation to zero stretch rate provides stretch-free laminar burning velocity of given mixture

Law, Symp. (Int.) Combust. 22, 1381, (1988).

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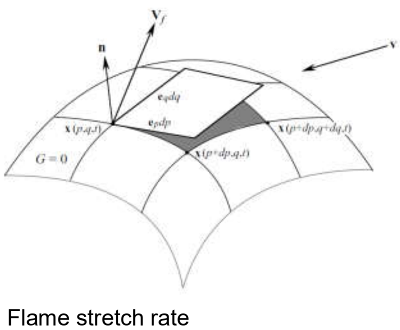
Stretch rate



Flame stretch rate

$$\kappa = \frac{1}{A}\frac{dA}{dt}$$

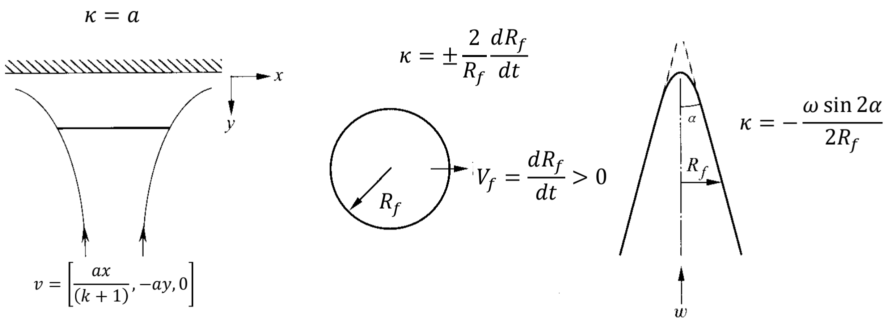
$$\kappa = \nabla_t \cdot \boldsymbol{V}_f + \left(\boldsymbol{V}_f \cdot \boldsymbol{n}\right)(\nabla \cdot \boldsymbol{n})$$

- Effects of flow non-uniformity, flame curvature, and flame/flow unsteadiness can be described by the single parameter
- Three factors for flame stretch are aerodynamic strain, flame curvature and flame motion

Chung and Law, CNF 55(1), 123-125, 1984.
Matalon, CST 31(3-4), 169-181, 1983.

Law, C.K., Combustion Physics, 2006.

Examples of stretched flames



(a) Forward stagnation flame

(b) Outwardly propagating spherical flame

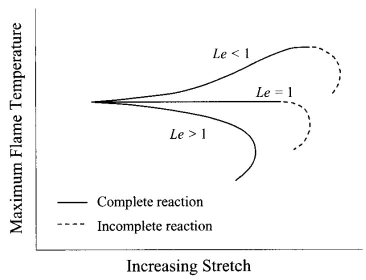
(c) Axisymmetric Bunsen flame

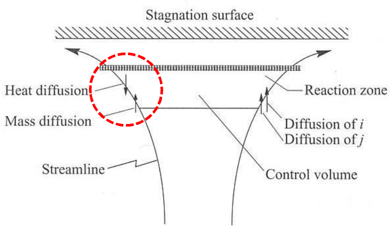
Figures: Law, C.K., Combustion Physics, 2006.

Flame stretch and Lewis number effect

- Lewis number: ratio of mass and thermal diffusions

$$Le = \frac{\alpha}{D} \quad \text{where} \quad \alpha = \frac{\lambda}{\rho C_p}$$





With the increase of stretch rate, flame temperature increases if Le < 1 and decreases if Le > 1

Figures: Law, C.K., Combustion Physics, 2006.

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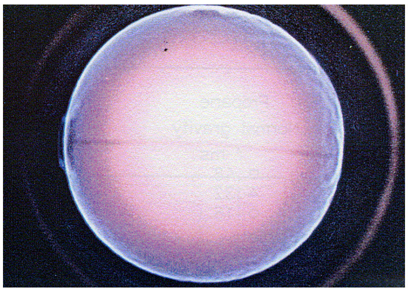
Outwardly propagating spherical flame



CH4/air, ϕ=0.65

- If a quiescent mixture is ignited, outwardly propagating spherical flame is observed
- When the size of the spherical flame is small, effect of the pressure increase can be negligible
- Laminar burning velocity can be measured if the effect of flame stretch is considered
- Applicable to high pressure

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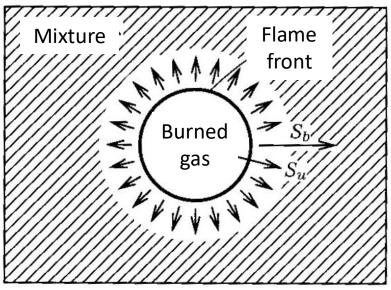
Outwardly propagating spherical flame

Commonly used basic flame geometry
Simple but essential flame physics involved



$$S_u = \left(\frac{\rho_b}{\rho_u}\right) S_b$$

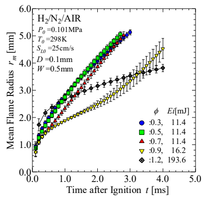
Need to consider the effects of other factors, e.g., ignition energy, stretch rate, etc.

- Estimating relative flame speed S_u to the mixture from nominal flame velocity S_b
- Density ratio was estimated from temperature ratio
- Need to consider the effects of other factors, in particular, effect of flame radius

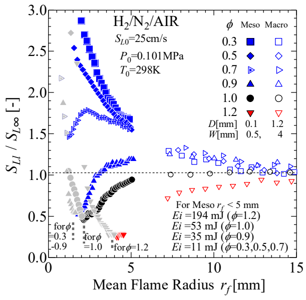
→ Flame stretch!

Derivation of LBV from outwardly propagating spherical flame

Experimental results, H2/N2/Air



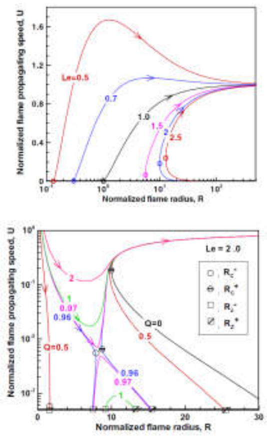
$$k = \frac{2}{R_f}\frac{dR_f}{dt}$$



Figures: courtesy of Prof. Nakahara of Ehime U.

Nakahara, M., et al., PCI 34, 703 (2013).

Theoretical prediction



Chen, Burke, Ju, PCI 33, 1219 (2011).

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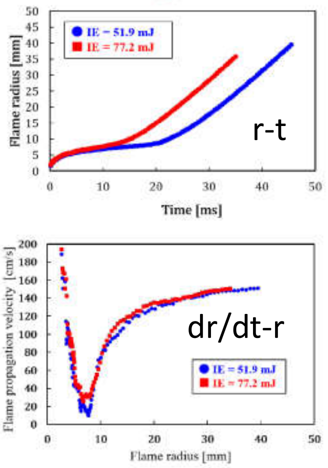
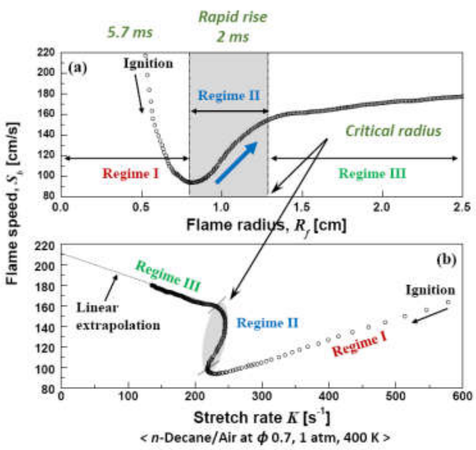
Derivation of LBV from outwardly propagating spherical flame

Experiments, iso-octane/air, ϕ = 0.80, Le > 3



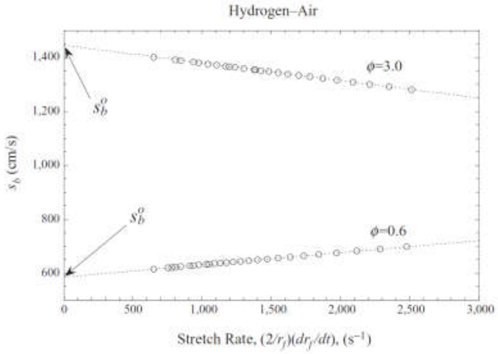


$$k = \frac{2}{R_f}\frac{dR_f}{dt}$$

Figures: Ju, Y., Princeton SS, 2017.

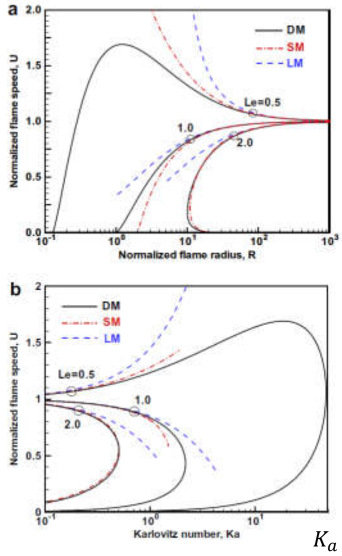
Determination of laminar burning velocity

linear extrapolation



$$k = \frac{2}{R_f}\frac{dR_f}{dt}$$

Figure: Law, C.K., Combustion Physics, 2006.



$$K_a = 2U/(aR)$$

Chen, Z., et al. (2009) Proc. Combust. Inst. 32(1): 1253.

Variation of measured laminar flame speeds

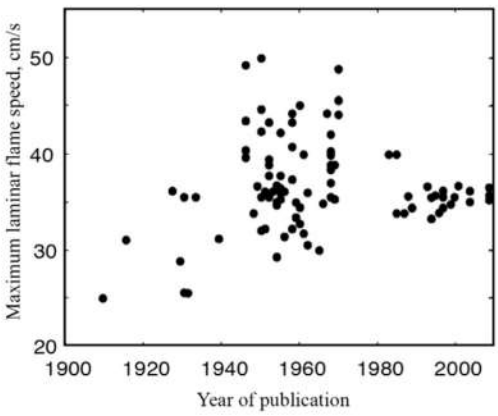


Fig. Variation of measured maximum laminar flame speeds of CH_4/air mixtures at standard conditions as a function of year of publication

Egolfopoulos et al., Prog. Energ. Combust. Sci. 43 (2014) 36.

Tools for combustion and ignition reaction modeling

CHEMKIN
https://www.ansys.com/products/fluids/ansys-chemkin-pro

CANTERA
https://cantera.org/index.html

KAUST CloudFlame
https://cloudflame.kaust.edu.sa/home

NASA CEA
https://www1.grc.nasa.gov/research-and-engineering/ceaweb/topicshome/

GASEQ
http://www.gaseq.co.uk/

Tools in Colorado State University
http://navier.engr.colostate.edu/code/

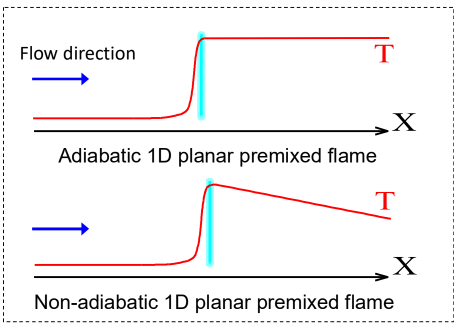
Flame basics

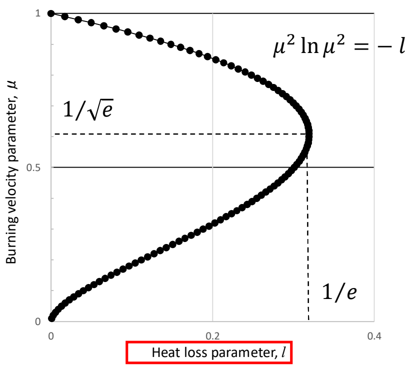
- Outline
- S-curve
- Premixed flame
- Flame characteristics
- Non-premixed flame

Flame characteristics

- Flame quench
- Flammability limits
- Quenching diameter
- Excess enthalpy combustion
- Flame instability

Theory of flame quench, thermal

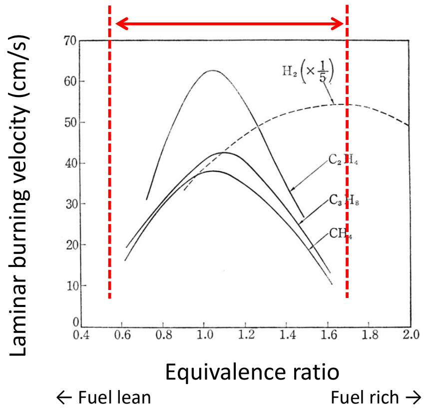




$$\lambda \frac{d^2T}{dx^2} - mc_p \frac{dT}{dx} = -\omega q^o + \boxed{L}$$

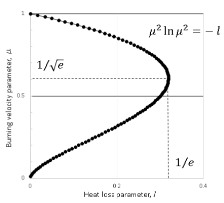
Zel'dovich, Y.B., *Zhurn. Eksp. Teoret. Fiz.* 11, 159 (1941).
Spalding, D.B., Proc. Royal Soc., Ser. A 240(1220) 83 (1957).
Clavin, P., Acta Astronautica 3(3): 223 (1976).
Williams, F.A., Combustion Theory, 1985.

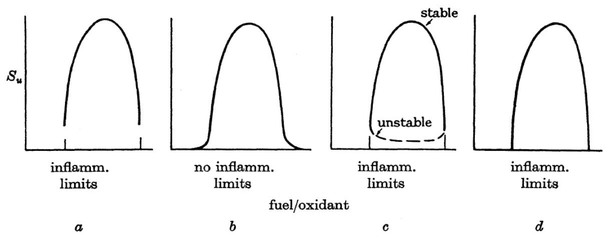
Fundamental flammability limits



- Mixture is only flammable within a certain range of the equivalence ratio
- What is the mechanism of fundamental flammability limits?

Flame quench and fundamental flammability limit





Burning velocity against mixture ratio.
a, experimental findings;
b, prediction of all theories neglecting heat losses;
c, prediction of present theory, taking account of heat losses;
d, prediction of Weinberg's theory, neglecting heat losses and radicle-generation other than branching reaction.

Spalding, D.B., Proc. Royal Soc., Ser. A 240(1220) 83 (1957).

What is the loss mechanism?
The question of a long time; solved by microgravity experiments in 1990's. ➡ Microgravity

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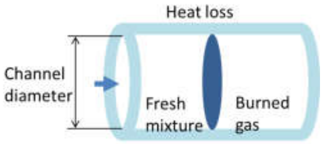
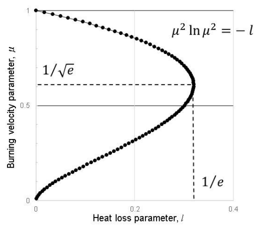
Quenching diameter



$$d_q = 2\sqrt{e\beta Nu}\,\delta_f$$

$$H = \frac{(Heat\,loss)}{(Heat\;generation)} = \frac{c_p(T_f - T_u)\omega(\pi d^2/4)\delta_f}{\pi d \delta_f h(T_f - T_u)} = 4Nu\delta_f^2/d^2$$

- Determined from the ratio of heat generation and heat loss
- Analogy with flammability limit



$$\lambda \frac{d^2T}{dx^2} - mc_p \frac{dT}{dx} = -\omega q^o + L$$

Microscale combustion

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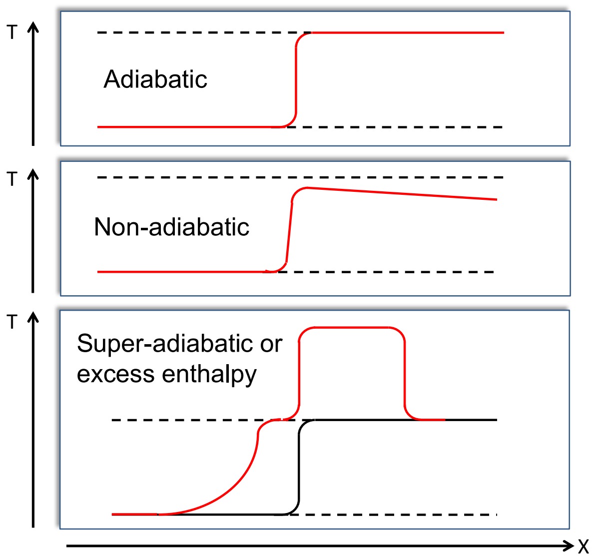
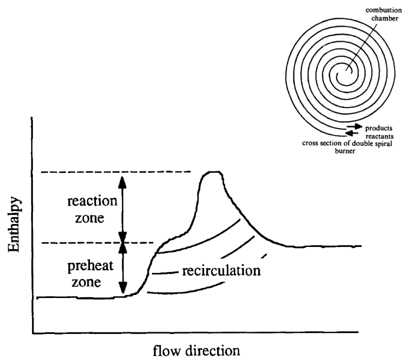
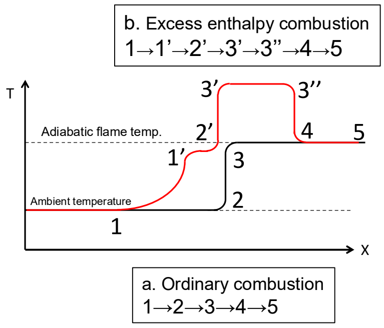
Adiabatic, non-adiabatic & super-adiabatic flames



- Adiabatic flame
- Non-adiabatic flame
- Third status is “super-adiabatic or excess enthalpy flame” and it would be better for higher thermal efficiency

Super-adiabatic or excess enthalpy combustion





Weinberg, F.J., *Combustion temperatures: The future ?*, Nature **233,** 239 (1971).

Weinberg, F.J., Symp. (Int.) Combust. 15(1) 1 (1975).

- Higher maximum temperature than adiabatic flame temperature
- Wider flammability limits
- Fuels with low calorific values applicable

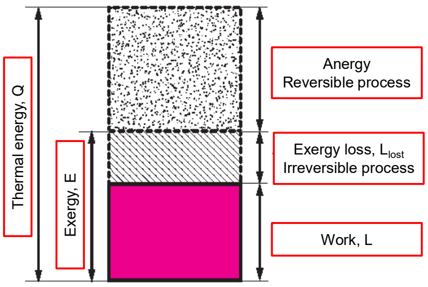
➡ Super-adiabatic
Flameless

Exergy (or availability)

Exergy efficiency
Second law efficiency

Ratio of effective work
to total exergy

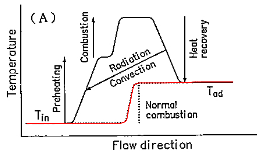
$$E_Q = L_{\max} = Q_H \eta_{\mathrm{Carnot}} = Q_H\left(1 - \frac{T_0}{T_H}\right)$$



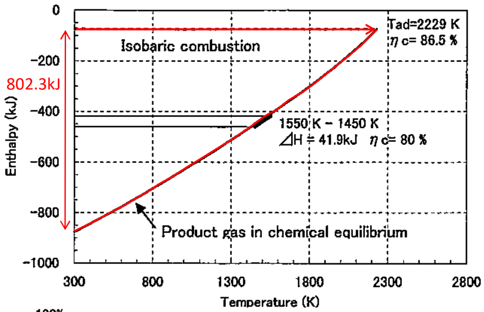
$\eta_{\mathrm{I}} = \frac{L}{Q}$ $\eta_{\mathrm{II}} = \frac{L}{E}$

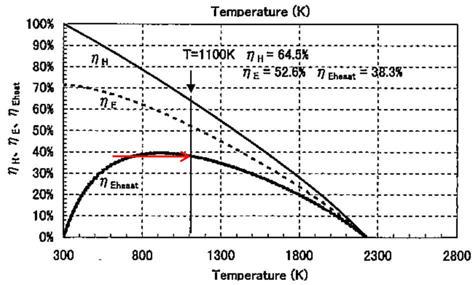
$$E_{\mathrm{flow}} = (H_1 - H_0) - T_0(S_1 - S_0) \quad (\mathrm{J})$$

Exergy efficiency of normal combustion



Normal combustion





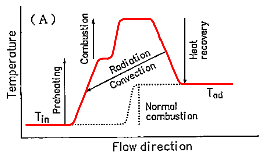
η_H: Ratio of the utilized thermal energy to the heat generation

η_E: Ratio of the utilized exergy to the fuel exergy

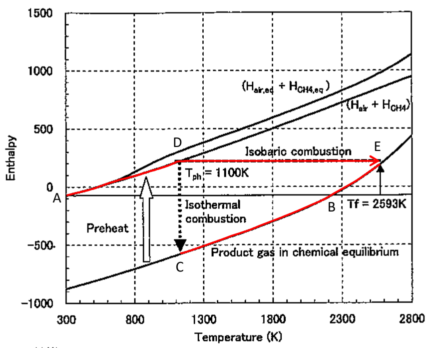
$\eta_{E\,heat}$: Ratio of the utilized exergy to the total exergy

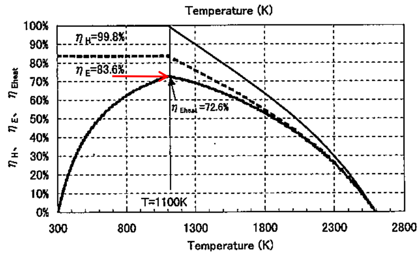
Yoshizawa, J Combust. Soc. Japan 50, 2008

Exergy efficiency of excess enthalpy combustion



Combustion with heat recirculation





η_H: Ratio of the utilized thermal energy to the heat generation

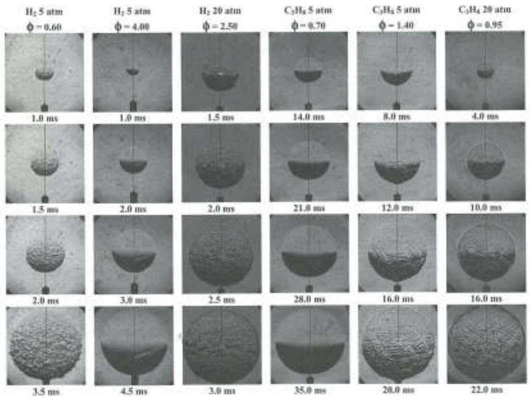
η_E: Ratio of the utilized exergy to the fuel exergy

$\eta_{E\,heat}$: Ratio of the utilized exergy to the total exergy

Yoshizawa, J Combust. Soc. Japan 50, 2008

Super-adiabatic
Flameless

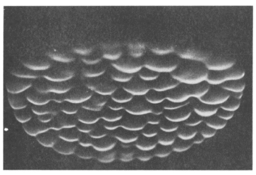
Spherical flames under intrinsic instabilities



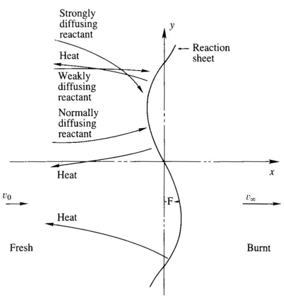
- Not all spherically propagating flames are ideal
- Some are wrinkled and cracked due to intrinsic instability
- Diffusive-thermal instability
- Hydrodynamic instability
- Acoustic instability

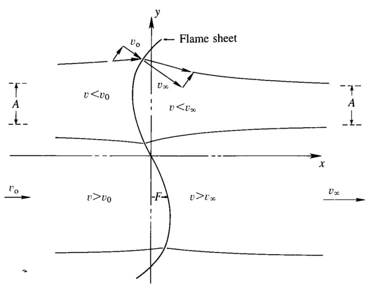
Law, C.K., Combustion Physics, 2006.

Flame instabilities, phenomenology



SABATHIER et al., *Prog. Aeronaut. Astronaut.* 76, 246 (1981).





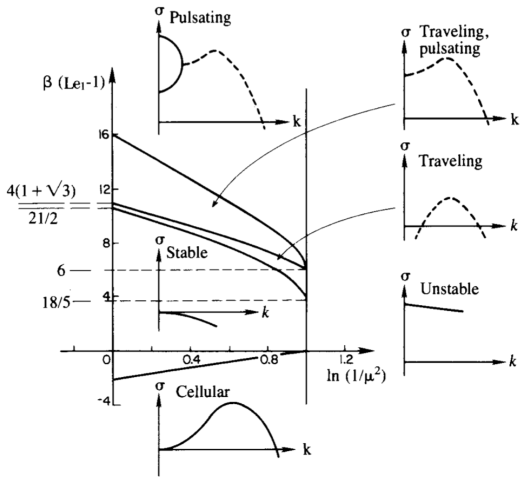
- Diffusive-thermal instability
- Hydrodynamic instability

Williams, Combustion Theory, 1985.

Theory

Sivashinsky, Acta Astronaut. 4, 1177 (1977).
Sivashinsky, Annu. Rev. Fluid Mech. 15, 179 (1983).
Clavin, PECS 11, 1 (1985).
Joulin and Clavin, Combust. Flame 35, 139 (1979).

Diffusive-thermal instability



- Depending on Lewis number and heat loss, various modes of diffusive-thermal instabilities are exhibited.
- Stability of each mode is indicated in the diagram.

Joulin, G. and Clavin, P., (1979) Combust. Flame 35: 139.
Williams, F. A., Combustion Theory., 1985

Flame basics

- Outline
- S-curve
- Premixed flame
- Flame characteristics
- Non-premixed flame

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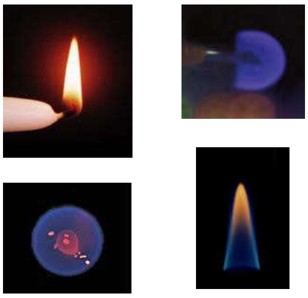
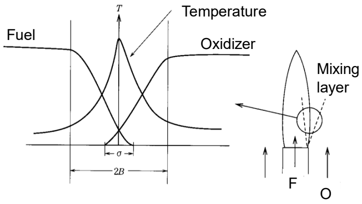
Non-premixed flames





- Fuel and oxidizer initially spatially separated
- If subsequent mixing is not sufficiently fast, the mixing and reaction occur in thin reaction zone
- Fuel and oxidizer are mainly transported thorough diffusion processes

Fundamentals of Combustion Phenomena, Ohm. 2001 in Japanese.

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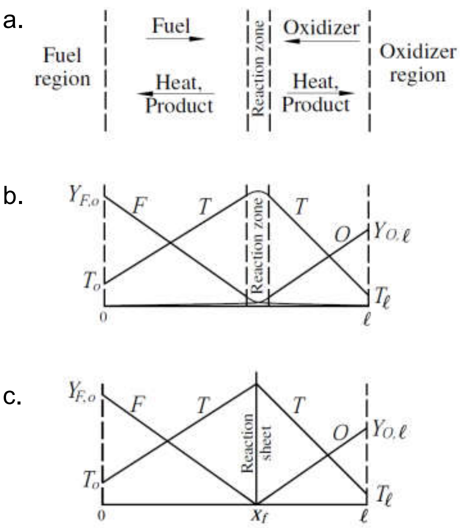
Non-premixed flames



Figures: Law, C.K., Combustion Physics, 2006.

- a. Typical configuration of non-premixed flame
- b. Fuel and oxidizer are transported through diffusion (+ convection). Since reactions occur at finite rate and reaction zone thickness is finite, some reactants are leaked
- c. Reaction of non-premixed flame often regarded as infinitely fast and thus reaction zone is regarded as a sheet and no leakage of reactants from there

Counterflow non-premixed flames

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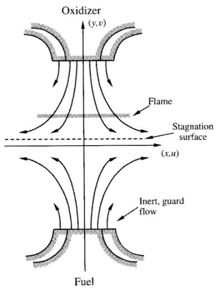
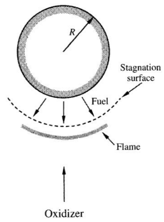
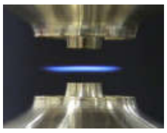


Tsuji burner



Figures: Law, C.K., Combustion Physics, 2006.



Energy Dynamics Lab. Tohoku U.

http://yoshidaweb.web.fc2.com

- Non-premixed flame established in counterflow field or in forward stagnation region in front of a porous cylinder (Tsuji burner)
- one-dimensional stretched flame for basic flame study, structure, extinction limits, etc.

Structure of counterflow non-premixed flame

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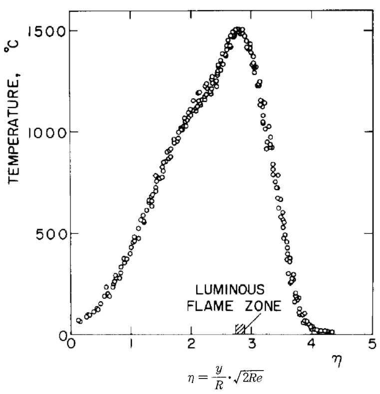
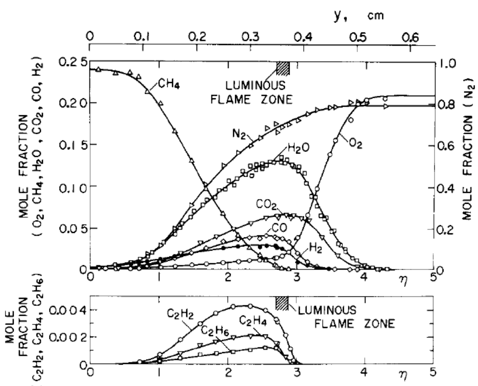
Stretch rate, 56 sec^{-1}



$\eta = \frac{y}{R} \cdot \sqrt{2Re}$



Temperature and species concentration profiles were measured.
Contribute to the development of computational code, e.g., CHEMKIN.

Tsuji, Yamaoka, Symp. (Int.) Combust. 13, 723, 1971.
Tsuji, H., Prog. Energ. Combust. Sci. 8(2), 93, 1982.

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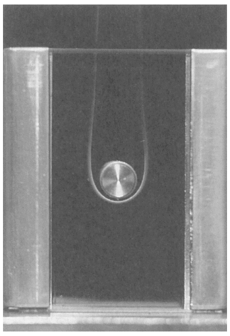
Prof. Tsuji

Tsuji burner



Non-premixed flame of methane and air stabilized in a forward stagnation region in front of a porous cylinder

Call for Nominations: Hiroshi Tsuji Early Career Researcher Award

Co-sponsored by Elsevier and The Combustion Institute

Released: 25 September 2017

Started in 2016, the Hiroshi Tsuji Early Career Researcher Award (co-sponsored by Elsevier and The Combustion Institute) is given every year to recognize an early career researcher who has made a significant contribution to advance their field of research, which should fall under the broad umbrella of fundamental or applied combustion or combustion-related fields. The winning researcher receives US$ 10,000 and the presentation of the award takes place at the biennial International Symposia on Combustion.

The award is named the Hiroshi Tsuji Early Career Researcher Award in recognition of Professor Tsuji's many important contributions to combustion science, most famously his invention and utilization of a stable counterflow burner configuration, the *Tsuji burner*. The configuration has influenced a vast number of fundamental studies and applications regarding flame structure, extinction, soot formation and other areas in laminar and turbulent combustion. It is also a foundational element for early career researchers coming to the field.

The award is proudly sponsored by Elsevier and The Combustion Institute.

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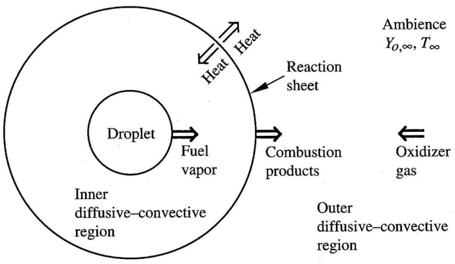
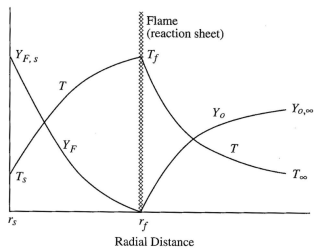
Droplet combustion, non-premixed flame





Similarity in non-premixed flames:
a flame in a forward stagnation region (Tsuji burner) and droplet combustion under quasi-steady assumption

Large flame radius -> low stretch rate
Small flame radius -> high stretch rate

Figures: Law, C.K., Combustion Physics, 2006.

Summary of part 1

After overviewing the history of combustion research, flame basics were introduced for discussing the microgravity and microscale combustion.

Scaling based on S-curve, premixed flame fundamentals including formulation, simple theory and flame stretch, flame characteristics, and non-premixed flame fundamentals were discussed.

Concept of adiabatic, non-adiabatic and super-adiabatic flames were revisited.

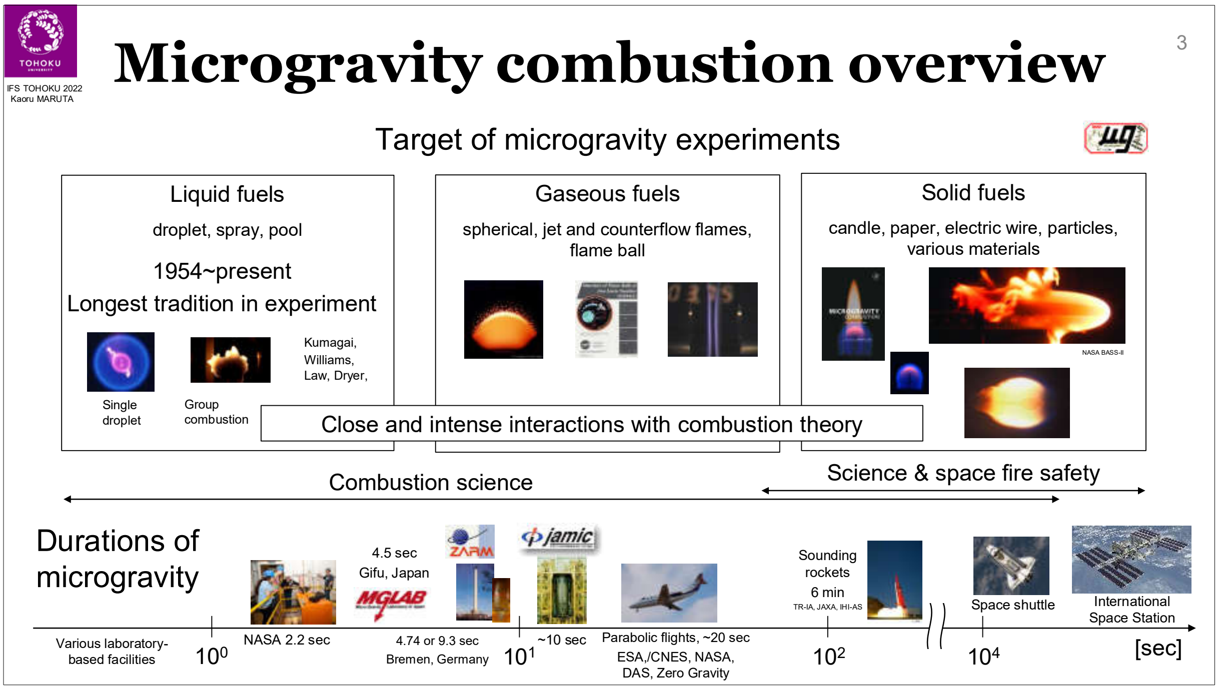
End of Part 1

Combustion in Microgravity and Microscale

Part 2: Microgravity combustion

Kaoru MARUTA
Institute of Fluid Science
Tohoku University

Introduction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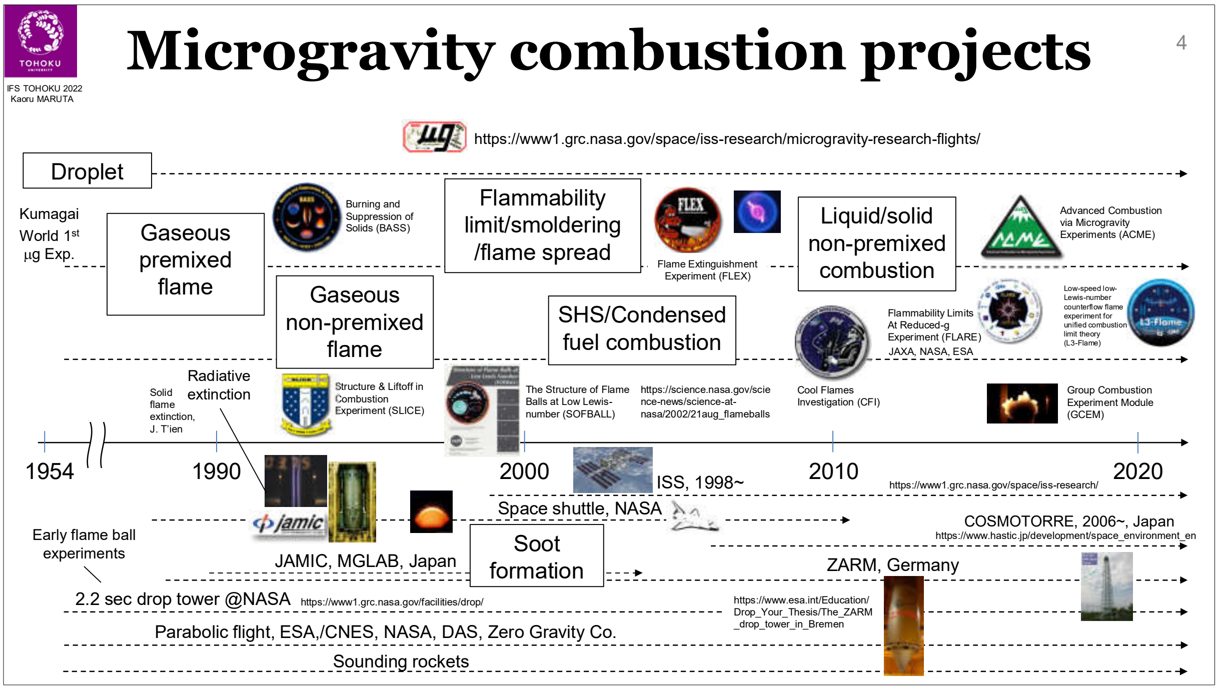
IFS TOHOKU 2022
Kaoru MARUTA
Microgravity combustion overview
3
Target of microgravity experiments
Liquid fuels
droplet, spray, pool
1954~present
Longest tradition in experiment
Single droplet
Group combustion
Kumagai, Williams, Law, Dryer,
Gaseous fuels
spherical, jet and counterflow flames, flame ball
Solid fuels
candle, paper, electric wire, particles, various materials
NASA BASS-II
Close and intense interactions with combustion theory
Combustion science
Science & space fire safety
Durations of microgravity
Various laboratory-based facilities
10^0
NASA 2.2 sec
4.5 sec
Gifu, Japan
MGLAB
ZARM
4.74 or 9.3 sec
Bremen, Germany
10^1
jamic
~10 sec
Parabolic flights, ~20 sec
ESA,/CNES, NASA, DAS, Zero Gravity
Sounding rockets
6 min
TR-IA, JAXA, IHI-AS
10^2
Space shuttle
10^4
International Space Station
[sec]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Microgravity combustion projects
4
https://www1.grc.nasa.gov/space/iss-research/microgravity-research-flights/
Droplet
Kumagai World 1st µg Exp.
Gaseous premixed flame
Burning and Suppression of Solids (BASS)
Flammability limit/smoldering /flame spread
Flame Extinguishment Experiment (FLEX)
Liquid/solid non-premixed combustion
Advanced Combustion via Microgravity Experiments (ACME)
Gaseous non-premixed flame
SHS/Condensed fuel combustion
Flammability Limits At Reduced-g Experiment (FLARE) JAXA, NASA, ESA
Low-speed low-Lewis-number counterflow flame experiment for unified combustion limit theory (L3-Flame)
Solid flame extinction, J. T'ien
Radiative extinction
Structure & Liftoff in Combustion Experiment (SLICE)
The Structure of Flame Balls at Low Lewis-number (SOFBALL)
https://science.nasa.gov/science-news/science-at-nasa/2002/21aug_flameballs
Cool Flames Investigation (CFI)
Group Combustion Experiment Module (GCEM)
1954
1990
2000
2010
2020
ISS, 1998~
https://www1.grc.nasa.gov/space/iss-research/
Space shuttle, NASA
COSMOTORRE, 2006~, Japan
https://www.hastic.jp/development/space_environment_en
Early flame ball experiments
JAMIC, MGLAB, Japan
Soot formation
ZARM, Germany
2.2 sec drop tower @NASA
https://www1.grc.nasa.gov/facilities/drop/
https://www.esa.int/Education/Drop_Your_Thesis/The_ZARM_drop_tower_in_Bremen
Parabolic flight, ESA,/CNES, NASA, DAS, Zero Gravity Co.
Sounding rockets

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Early reviews on microgravity combustion

The findings of the review highlight how buoyancy has impeded the rational development of combustion science, precluding observations of fundamental one-dimensional configurations, low Reynolds number flows and other limiting conditions.

- C.K. Law and G.M. Faeth - 1994

A review … is presented, with an emphasis on a discussion of the ways in which reduced-gravity experiments and modeling has led to new understanding. Comparison of time scales shows that the removal of buoyancy-induced convection leads to manifestations of other transport mechanisms, notably radiative heat transfer and diffusional processes such as Lewis number effects.

- P.D. Ronney - 1998

Early reviews on microgravity combustion:
1) Williams, F.A. (1990) Combustion phenomena in relationship to microgravity research, Microgravity Science and Technology 3(3), pp 154-161.
2) Law, C.K., Faeth, G.M. (1994), Opportunities and challenges of combustion in microgravity, PECS 20(1), 65-113.
3) Ronney, P.D. (1998), Understanding combustion processes through microgravity research, Symp. (Int.) Combust., 27(2), 2485-2506.
Review on gaseous combustion limits:
4) Ju, Y., Maruta, K., Niioka, T. (2001), Combustion limits, Applied Mechanics Reviews 54(3), pp. 257-277.

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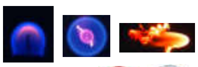
Featured topics of microgravity combustion

Condensed fuel combustion

From droplet to flame spread in various materials

Pioneer exp. 1954~



Kumagai, Williams, Law, Dryer

Flame ball

Zel'dovich, Buckmaster, Joulin, Ronney

Theory 1940's~
Experiments 1980's~

Counterflow flame/flammability limit

Theory 1950's~
Experiments 1990's~

Droplet combustion
Cool flame

Flame ball

Radiative extinction

Low Mach number
low Froude number
Low Reynolds number
Williams, Microgravity Sci. Tech. 3, 1990, 154.

Comprehensive review on microgravity combustion
Law & Faeth, PECS 20, 1994, 65.

Time scale analysis for stoichiometric and near-limit conditions,
Chemical, Buoyant, Conduction, Radiation
Ronney, Int. Symp. Combust. 27, 1998, 2485.

Combustion limits
Premixed flame, Dynamics and instability, Non-premixed flame, lifted and edge flames
Ju et al, Applied Mech. Reviews 54, 2001, 257.

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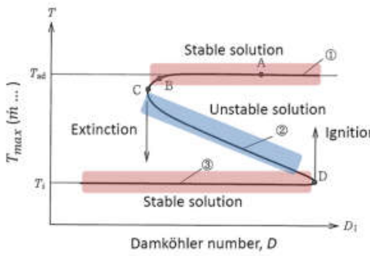
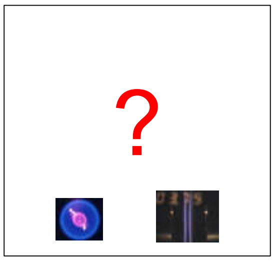
What happened on S-curve in microgravity?





Low Mach number
low Froude number
Low Reynolds number
Williams, Microgravity Sci. Tech. 3, 1990, 154.

Comprehensive review on microgravity combustion
Law & Faeth, PECS 20, 1994, 65.

Time scale analysis for stoichiometric and near-limit conditions,
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Ronney, Int. Symp. Combust. 27, 1998, 2485.

Combustion limits
Premixed flame, Dynamics and instability, Non-premixed flame, lifted and edge flames
Ju et al, Applied Mech. Reviews 54, 2001, 257.

Radiative extinction
Radiation reabsorption
…

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History: droplet combustion in microgravity

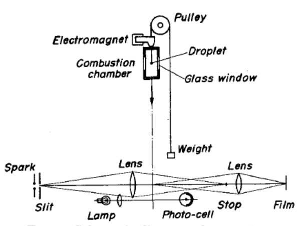


FIG. 1. Schematic diagram of apparatus.

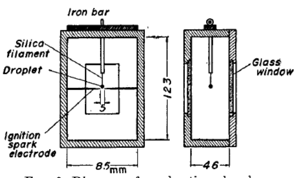


FIG. 2. Diagram of combustion chamber.

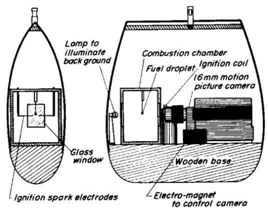


Figure 6. Schematic diagram of falling apparatus

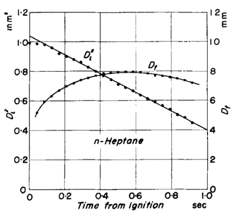
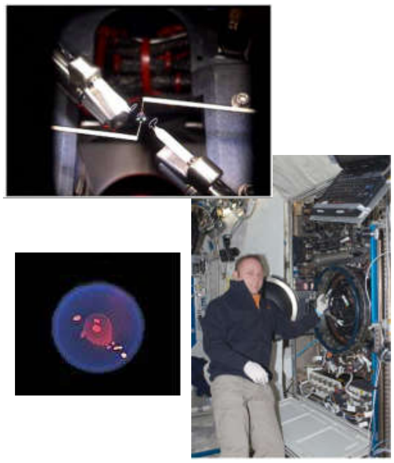


Figure 8. Variation of droplet diameter and flame diameter of spherically burning n-heptane droplet

- One of the representative fundamental non-premixed flames
- The world's first scientific experiments conducted under microgravity (1950's) by Seiichiro Kumagai of Univ. of Tokyo
- Prove D^2-law by providing high fidelity data

1) Kumagai, Isoda, Symp. (Int.) Combust. 6. 726 (1957). 2) Isoda, Kumagai, Symp. (Int.) on Combust. 7, 523 (1958).

Droplet combustion in Space



- Droplet combustion has been extensively contributed to the understandings of spray combustion to date
- Finally, cool burning flames of free droplet observed in International Space Station (ISS) in 2008-2009 (Prof. F.A. Williams of UCSD & collaborators)

Nayagam, V., et al., Combust. Flame 159(12): 3583 (2012).
Nayagam, V., et al., Combust. Flame 162(5) 2140 (2015).

http://jacobsschool.ucsd.edu/news/news_releases/release.sfe?id=1548
https://www.youtube.com/watch?v=qQQ1OHW1_F4
https://www.youtube.com/watch?v=BxxqCLxxY3M

Microgravity combustion:

Flammability limit and near-limit flames

- History
- Counterflow flames
- Flame ball
- Near-limit flames with complicated combined effects

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History of study on combustion limits

1800 Requirement for fire safety in coal mines

1950 Basic limit theory presented

Flame ball was predicted

The world first experiment in microgravity (Kumagai)

Large variations on combustion limit study

Drop tower (NASA, JAMIC)

Lean burn

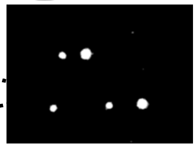
Space experiments

1990 Low speed counterflow flame

Flammability limit theory (Planar flame)

Flame ball

2000



2010 Unified combustion limit theory

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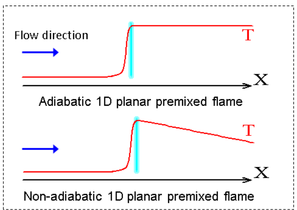
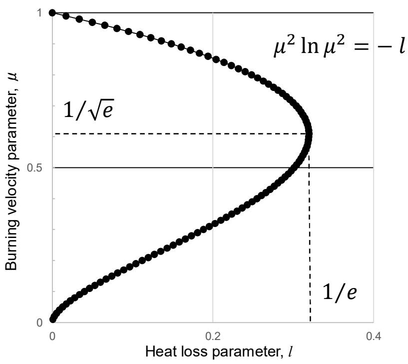
Flammability limit theory (1940's-)

Concept of flammability limit for one-dimensional planar flame



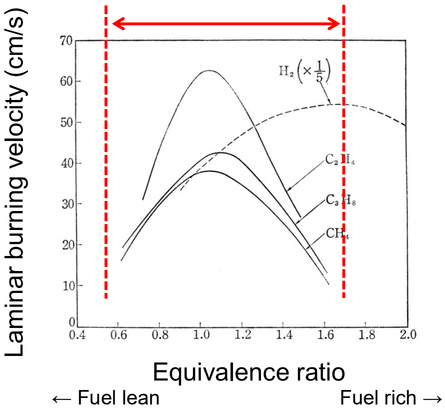


- Flammability limit may be induced by a certain heat loss
- What is loss mechanism?
- Conduction loss? Radiative loss? If adiabatic, no limit?

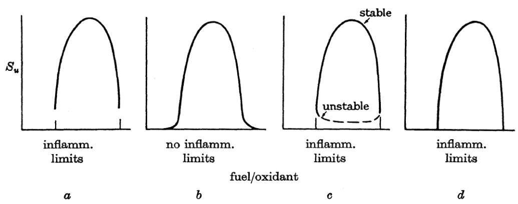
$$\lambda \frac{d^2T}{dx^2} - mc_p \frac{dT}{dx} = -\omega q^o + L$$

Zel'dovich, Y.B., *Zhurn. Eksp. Teoret. Fiz.* 11, 159 (1941).
Spalding, D.B., Proc. Royal Soc., Ser. A 240(1220) 83 (1957).
Clavin, P., Acta Astronautica 3(3): 223 (1976).
Williams, F.A., Combustion Theory, 1985.

What is the mechanism of fundamental flammability limit?



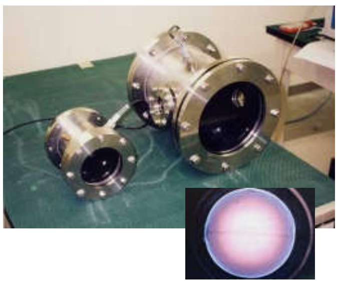
- Fact: mixture is only flammable within a certain range of equivalence ratio
- Loss mechanism?



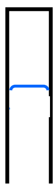
a, experiment; b, all theories neglecting heat losses; c, Spalding theory d, Weinberg theory neglecting heat losses and radicle-generation other than branching reaction.

Spalding, D.B., Proc. Royal Soc., Ser. A 240(1220) 83 (1957).

Conventional methods of combustion limit study



Constant volume chamber



Propagation tube

Fire safety in mines, “standard” propagation tube

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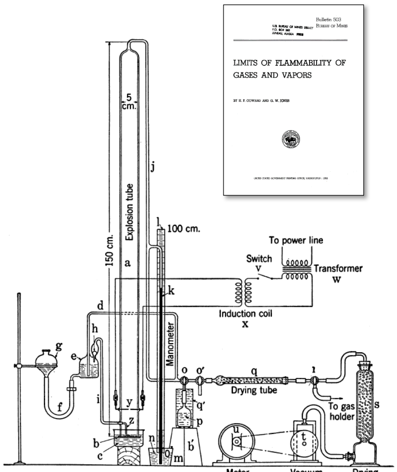

FIGURE 3.—Apparatus for Determining Limits of Flammability of Gases and Vapors.

TABLE 1.—*Limits of flammability of hydrogen in air in smaller vessels*

H_2-air

Dimensions of tube, cm. Diameter	Length	Firing end	Limits, percent Lower	Higher	Content of aqueous vapor	Reference No.
Upward Propagation of Flame						
7.5	150	Closed	4.15	75.0	Half-saturated	356
5.3	150	Open	4.19	74.6	Dried	94
5.3	150	do	[1] 4.12	[1] 74.3	do	94
5.3	150	do	[2] 4.17	[2] 74.8	do	94
5.0	150	Closed	4.15	74.5	Half-saturated	356
5.0	180	Open	4.0	72.0	Dried	133
4.8	150	do	4.0	73.8	do	38
4.5	80	Closed	[3] 4.1			56
4.5	80	do	3.9			57
2.5	150	Open	4.2		Dried	271
2.5	150	Closed	4.25	73.0	Half-saturated	356
2.5	96	do	4.1	72.8		98
2.2	45	do	3.9	73.0	Saturated	274
1.6	96	do	4.22	71.2		98
.8	96	do	5.1	67.9		98
Horizontal Propagation of Flame						
7.5	150	Closed	6.5		Half-saturated	356
5.0	150	do	6.7		do	356
2.5	150	do	7.15		do	356
2.5	150	Open	6.2		Saturated	271
2.5		do		71.4		273
.9	150	do	6.7	65.7	Saturated	276
Downward Propagation of Flame						
21.0	31	Open	9.3		Saturated	63
8.0	37	Closed	8.9	[4] 68.8	do	324
7.5	150	do	8.8	74.5	Half-saturated	356
7.0	150	do		74.5		115
6.2	33	Open	8.5		Saturated	95
6.0	120	do	9.45		Partly dried	325
6.0	120	Closed	9.3		do	325
6.0	120			[4] 68.0	do	325
5.3	150	Open	9.0		Dried	94

- Flame propagation tube, Bureau of Mines, US
- Flammability limits significantly differ in the upward and downward propagating H_2-air flames

COWARD, H.F. and JONES, G.W., *Limits of Flammability of Gases and vapors*, BUREAU OF MINES Bulletin 503, (1952).

Experiments by propagation tube CH_4-air

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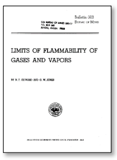

TABLE 11.—*Limits of flammability of methane in air, with upward*

Dimensions of tube, cm. Diameter	Length	Firing end	Limits, percent Lower	Higher
10.2	96	Closed	5.00	15.00
7.5	150	do	5.35	14.85
6.2	33	Open	5.45	13.5
6.0	200	Closed	5.40	14.8
5.3	150	Open	5.26	14.3
5.0	50	Closed		15.11
5.0	150	Open	5.40	14.25
5.0	180	do	5.24	14.02
5.0	180	do	5.33	13.80
4.7	100	do	5.3	14.3
4.0	100	Closed	5.5	14.1
2.7		Open	5.28	
2.5	150	do	5.5	
2.5	150	Closed	5.80	13.20
2.25	125	Open	5.48	

TABLE 13.—*Limits of flammability of methane in air, with downward*

Dimensions of tube, cm. Diameter	Length	Firing end	Limits, percent Lower	Higher
8.0	37	Closed	5.9	12.9
7.5	150	do	5.95	13.35
6.2	33	Open	6.3	
6.1	120		6.1	13.0
6.0	200	Closed	6.0	13.4
5.0	50	do	5.80	13.38
5.0	150	do	6.12	13.25
5.0	125	Open	5.85	
4.0	100	Closed	6.1	13.3
2.7		Open	5.84	
2.5	150	do	6.1	
2.5	150	Closed	6.30	12.80
2.25	125	Open	6.41	
2.2		Closed	5.6	13.6
1.9	40	do	6.1	12.8
1.9	40	do	6.15	12.0
.815		Open	6.25	
.515		do	7.03	

COWARD and JONES, BUREAU OF MINES Bulletin 503, (1952).

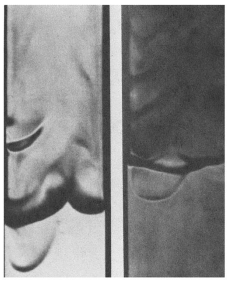

FIG. 5. Schlieren photographs of two downward propagating flames just prior to complete extinction. Notice the tongue of hot gas ahead of the main flame. This is a typical observation of the extinction process for a downward propagating flame.

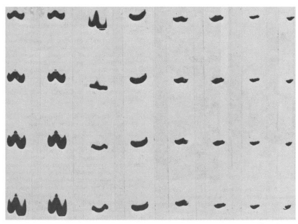

FIG. 6. Visible light photography of the extinction of a downward propagating flame. Notice that the final flame occupies only a small central portion of the tube. Even though the photos do not show it directly, this downward propagating flame was observed to rise in the tube just prior to extinction. Framing rate: 64 frames/second. Time is increasing from top to bottom and then from left to right.

- Flammability limits of the upward and downward propagating flames not significantly differ as hydrogen but still significant effects of the tube directions

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Microgravity combustion:

Flammability limit and near-limit flames

- History
- Counterflow flames
- Flame ball
- Near-limit flames with complicated combined effects

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Low-speed counterflow flames under microgravity

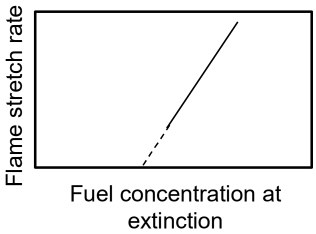
-~~Heat losses~~

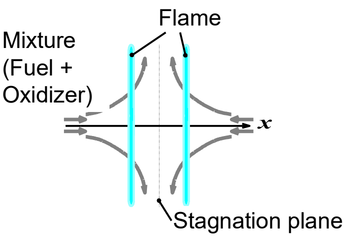
-~~Buoyancy~~

-Flame stretch

-~~Wall effect~~

-~~Curvature~~

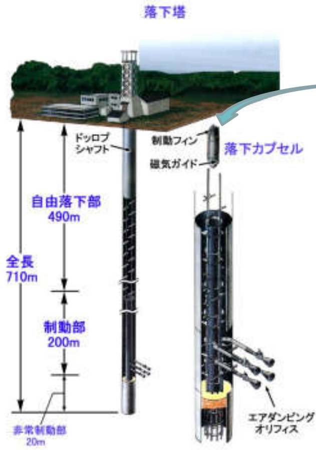




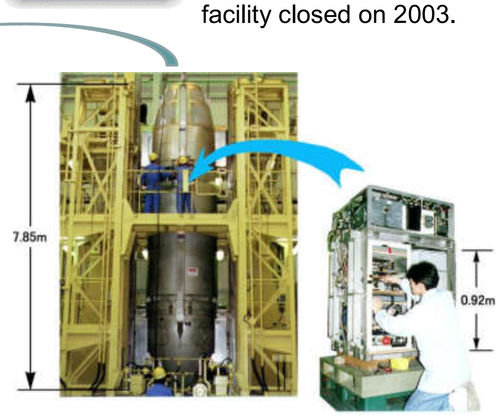
Concept
Law, Egolfopoulos, Symp. Int. Combust. 23, 413 (1990).

Microgravity experiments
Maruta, K., et al., Japanese Symp. Combust. 33, 137 (1995).
Maruta, K., et al., Symp. Int. Combust. 26, 1283 (1996).

Microgravity experiments at drop tower

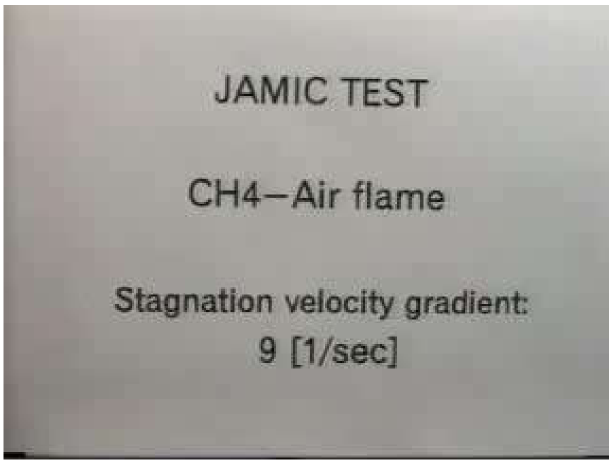


10 seconds microgravity during 490 meters free fall, facility closed on 2003.



Counterflow flame experiments in the ten-second drop tower, CH4/air

Counterflow twin flames at small stretch rates under microgravity (mid 90's)



Maruta et al., International Symposium on Combustion 26, (1996).

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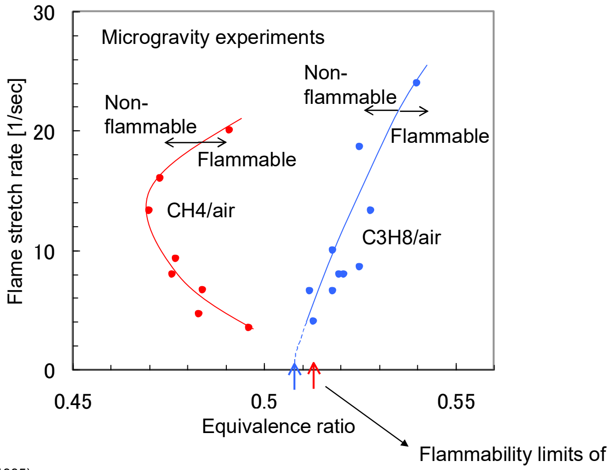
Results of microgravity experiments

C-shaped curve for CH_4 **(unexpected!)**

and monotonic curve for C_3H_8



Maruta, et al., Japanese Symp. Combust. 33, 137 (1995).
Maruta, Yoshida, Ju, Niioka, Symp. Int. Combust. 26, 1283 (1996).

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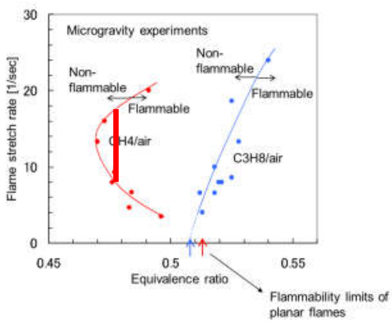
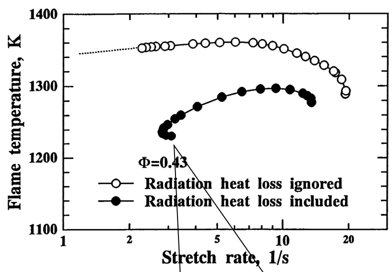
Experimental C-shaped extinction curve and radiative extinction



Maruta, et al., Japanese Symp. Combust. 33, 137 (1995).
Maruta, Yoshida, Ju, Niioka, Symp. Int. Combust. 26, 1283 (1996).

Computations:
Sung and Law, Symp. Int. Combust. 26, 865 (1996).



Another extinction limit appeared when radiative heat transfer is considered

Guo, Ju, Maruta, Niioka, Liu, Combust. Flame 109(4) 639 (1997).

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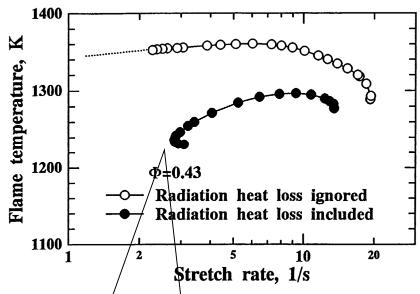
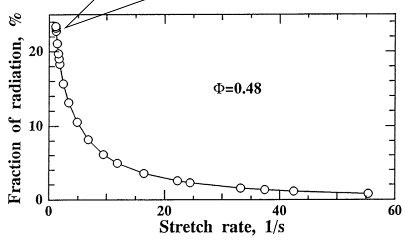
Experimental C-shaped extinction curve and radiative extinction



Despite low flame temperature, volume effect makes the role of radiative heat loss dominant



Another extinction limit appeared when radiative heat transfer is considered

$$r_f = \int_{-L}^{L} q_r dy \Big/ \int_{-L}^{L} \sum_{k=1}^{KK} h_k \omega_k M_k dy$$

Guo, Ju, Maruta, Niioka, Liu, Combust. Flame 109(4) 639 (1997).

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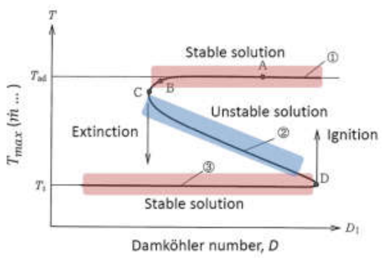
S-curve and radiative extinction



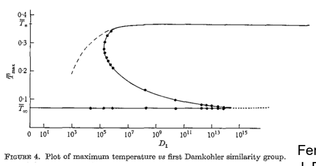
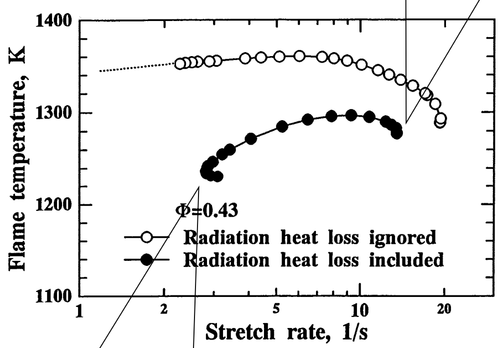


FIGURE 4. Plot of maximum temperature vs first Damkohler similarity group.

Fendell, F. E. (1965), J. Fluid Mech. 21: 281.

Conventional low Da extinction at high stretch



Another extinction appeared at low stretch

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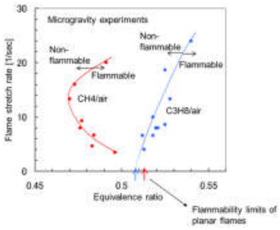
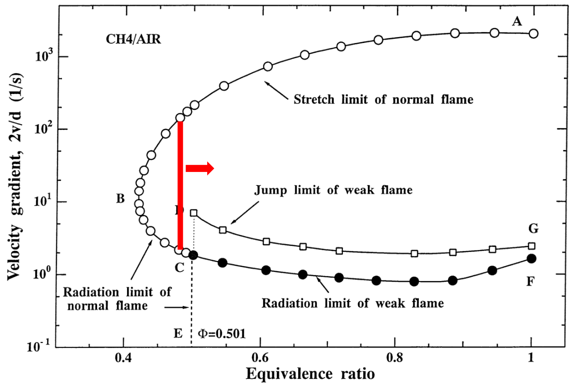
Experimental C-shaped extinction curve and comprehensive "G-curve"





Ju, Guo, Maruta, J. Fluid Mech. 342 (1997)
Maruta et al., Int. Symp. Combust. 27 (1998)

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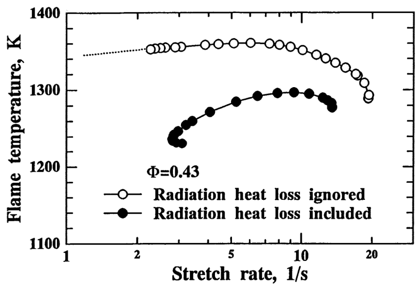
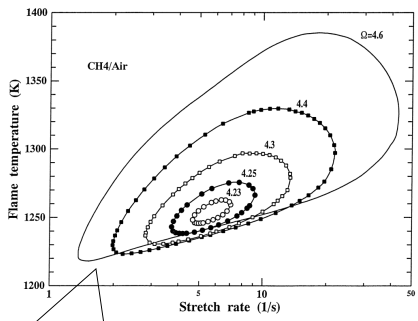
Experimental C-shaped extinction curve and comprehensive "G-curve"





If equivalence ratio was changed, island responses with different size were appeared

Ju, Guo, Maruta, J. Fluid Mech. 342 (1997)

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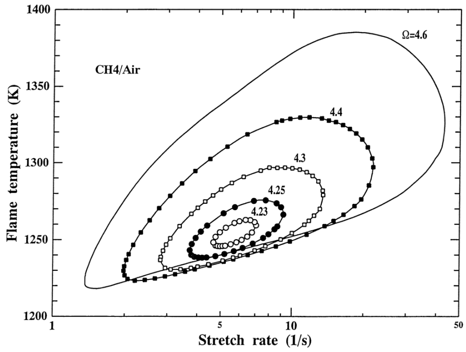
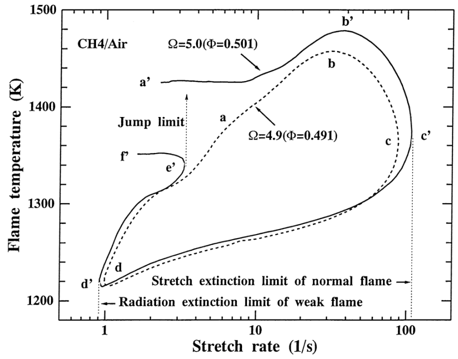
Experimental C-shaped extinction curve and comprehensive "G-curve"





Ju, Guo, Maruta, J. Fluid Mech. 342 (1997)

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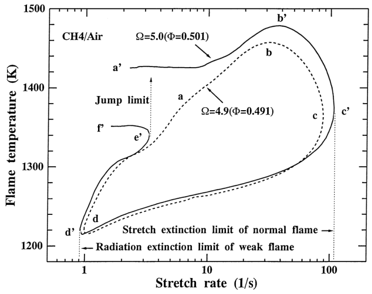
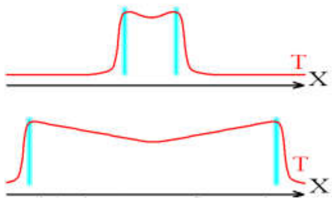
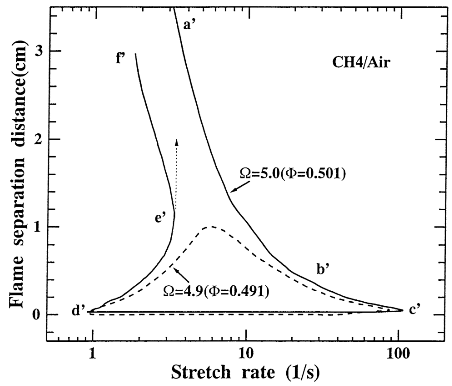
Experimental C-shaped extinction curve and comprehensive "G-curve"





Non-adiabatic (counterflow twin flames)

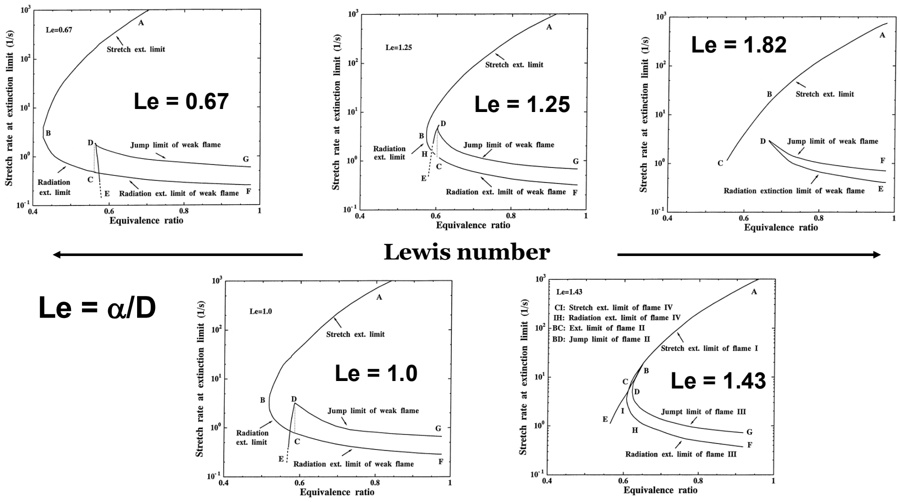


Flame separation distance

Ju, Guo, Maruta, J. Fluid Mech. 342 (1997).
Buckmaster, J., Combust. Theory Model. 1(1): 1 (1997).

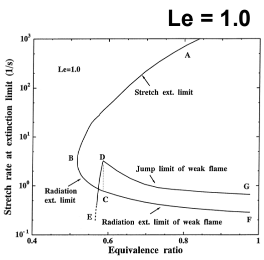
Effects of Lewis number on extinction curves

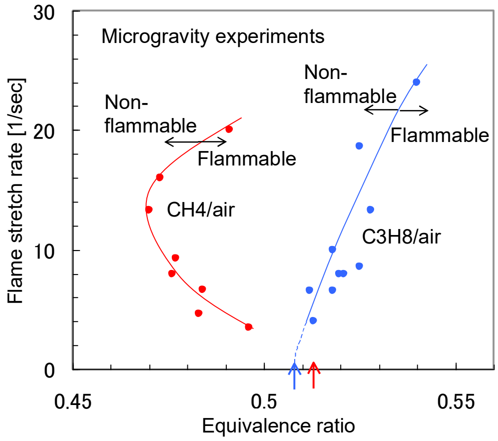
G- to K-shaped transformation

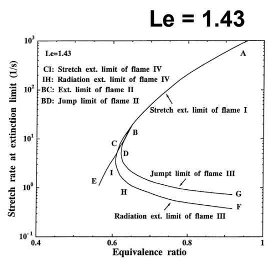


Ju, Guo, Maruta, Niioka, Combust. Flame 113, 603 (1998).

Flammability limits of planar flames obtained but sublimit mixture is flammable …







- Limit of planar flame ≠ “flammability limit”
- Definition?

Maruta, et al., Japanese Symp. Combust. 33, 137 (1995).
Maruta, Yoshida, Ju, Niioka, Symp. Int. Combust. 26, 1283 (1996).
Ju, Guo, Maruta, Niioka, Combust. Flame 113, 603 (1998).

Flame physics of flammability limits

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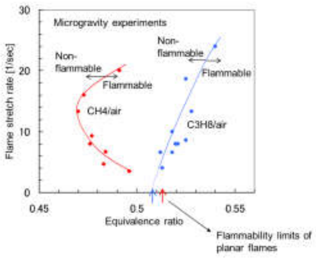


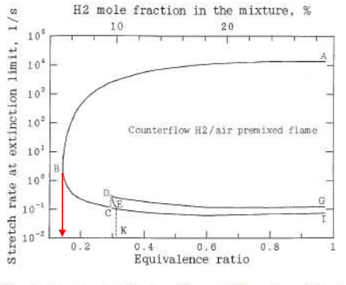
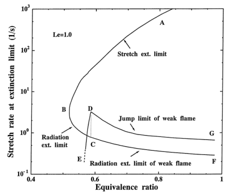


Figure 12. Flammable regions of H2–air counterflow premixed flames, where point K is the flammability limit of a one-dimensional premixed flame.

Guo et al., Combust. Theory Model. 4-4, 459 (2000).

Le = 1.0



Le = 1.82

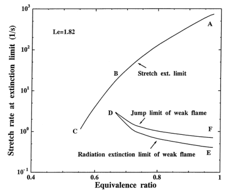


TABLE 1 Flammability Limits of Fuel Gases and Vapors in Air at 25°C and 1 atm

	Lean limit		Rich limit	
Fuel	Vol %	(Vol %)/(Vol %)$_{ST}$, [ϕ]	Vol %	(Vol %)/(Vol %)$_{ST}$, [ϕ]
Methane	5.0	0.53 [0.50]	15.0	1.6[1.7]
Propane	2.1	0.57 [0.56]	9.5	2.5 [2.7]
Hydrogen	4.0	0.14 [0.10]	75	2.54 [7.14]

Glassman, Combustion

Maruta, et al., Japanese Symp. Combust. 33, 137 (1995).
Maruta, Yoshida, Ju, Niioka, Symp. Int. Combust. 26, 1283 (1996).
Ju, Guo, Maruta, Niioka, Combust. Flame 113, 603 (1998).

Lean limits of radiative planar flame

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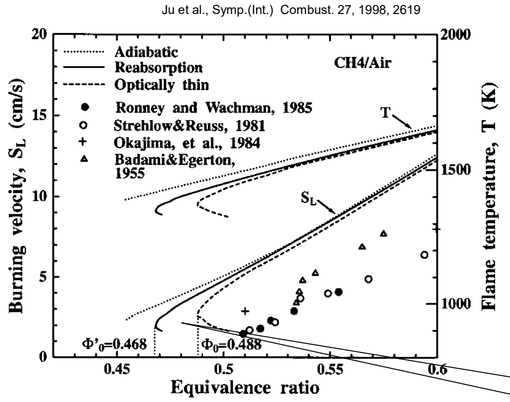
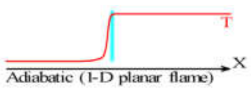
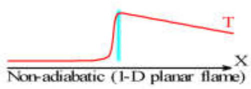
Ju et al., Symp.(Int.) Combust. 27, 1998, 2619



- Radiative heat transfer considered in energy equation
- Case of heat loss only (optically thin model)
- Case of heat reabsorption (Grey, SNB, etc.)





Mechanism of planar flame limit was clarified but for fire safety, Lewis number effect and reabsorption effect should be considered.

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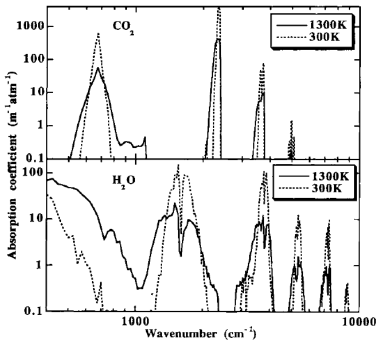
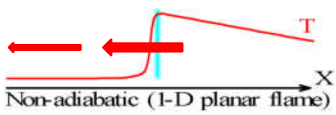
Lean limits of ideal planar flame

Ju et al., Symp.(Int.) Combust. 27, 1998, 2619





- Radiative heat from burned gas would be reabsorbed if optical thickness of cold mixture is large enough, e.g., large concentrations of CO_2, H_2O, etc.
- Absorption coefficients of radiative gases broadened at higher temperature. This leads to the limited degree of reabsorption.

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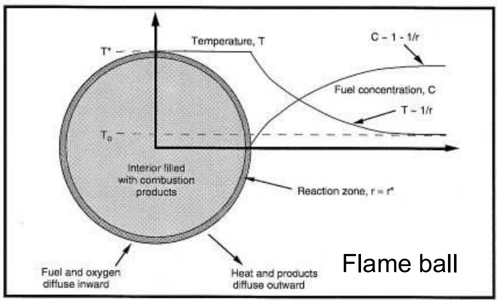
Microgravity combustion:

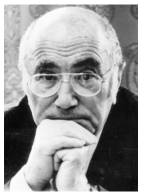
Flammability limit and near-limit flames

- History
- Counterflow flames
- Flame ball
- Near-limit flames with complicated combined effects

Peculiar flame in microgravity: Flame ball

Flame ball（Predicted theoretically at first in 1940’s）





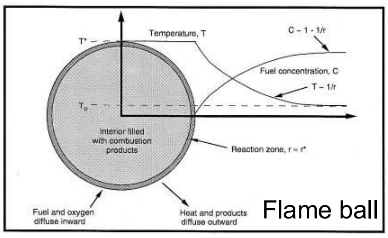
Zel’dovich

Zel’dovich predicted（1944）stationary spherical flame only sustained by heat and mass transports in molecular diffusions and reaction without any convective flows

Mathematical analysis indicated that it is unstable but radiative heat loss was not considered

Zeldovich, Y.B., *Theory of Combustion and Detonation, NN Semenov, 71, 1944.*

Flame ball solution, adiabatic



- Stationary spherical flame sustained by heat and mass diffusions
- Stable only if radiative heat loss exists

$$0 = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dT}{dr}\right) + B\exp(-\theta/2T_*)\,\delta(n) - \frac{1}{\theta}F$$

$$0 = \frac{1}{Le}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dY}{dr}\right) - B\exp(-\theta/2T_*)\,\delta(n)$$

$$F = \theta\frac{R_0^2 C_p f}{\lambda Q}, \quad \theta = \frac{EC_p}{RQ}$$

$$\frac{d}{dr}\left(r^2\frac{d}{dr}\right)\left(T + \frac{1}{Le}Y\right) = 0$$

$$T + \frac{1}{Le}Y = T_i + \frac{1}{Le}Y_i$$

$$T_b = T_i + \frac{1}{Le}(T_a - T_i) \qquad R_z = \frac{Y_i\lambda\exp(\theta/2T_b)}{Le\bar{B}C_p}$$

$$r < 1 \qquad T = T_b, \quad Y = 0$$

$$r > 1 \qquad T = T_i + \frac{Y_i}{Le}\frac{1}{r}, \quad Y = Y_i\left(1 - \frac{1}{r}\right)$$

Buckmaster, Weeratunga, Combust. Sci. Technol. 35, 287 (1983).
Deshaies, Joulin, Combust. Sci. Technol. 37, 99 (1984).
Zeldovich, Y.B., *Theory of Combustion and Detonation, NN Semenov, 71, 1944.*

Discovery of flame ball

Ronney (1990) Observation of spherical flames in microgravity experiments at 2.2 sec drop tower

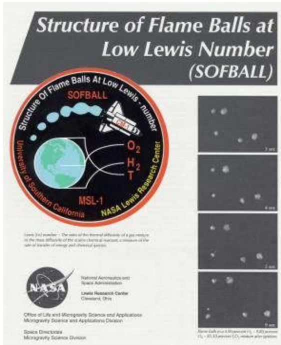
Ronney (1993) Observation of the flames in aircraft experiments, longer time microgravity duration but with severe gravity fluctuations

<u>Three essentials: microgravity, low Lewis number, vicinity of flammability limits</u>

Ronney (USC) + Tohoku (1996) collaboration at Japanese 10 sec drop tower (JAMIC) steady and stable flame balls observed

Space experiments in the Shuttle, 1997 STS-83/MSL-1, STS-94/MSL-1R, and 2003 STS-107

Ronney



Ronney, Combust. Flame 82, 1 (1990).
Buckmaster, Joulin, Ronney, Combust. Flame 79, 381 (1990).
Ronney, Symp. Int. Combust. 27, 2485 (1998).
Abid, M., et al., Combust. Flame 116, 348 (1999).

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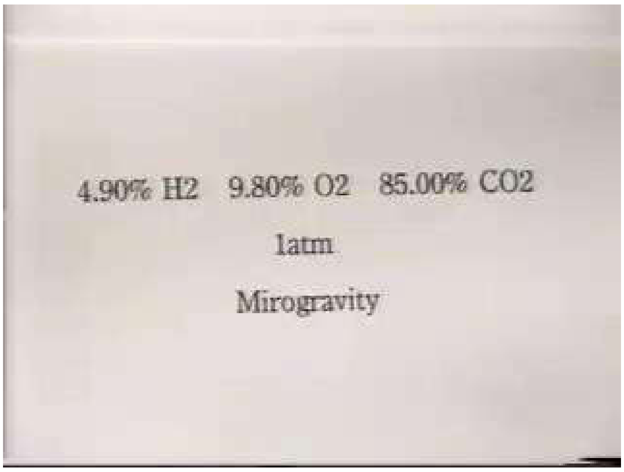
Flame ball in aircraft, KC-135

Ronney, early 90's

Flame ball, drop tower in Japan



Microgravity experiments at 10 sec drop tower（～10^{-4}G）

Late 90’s, USC + Tohoku, Combustion and Flame 116, 348 (1999).

Flame ball in Space Shuttle

Experiments in the Space Shuttle (STS-107, Ronney, 2003)

Regime of flame ball and planar flame

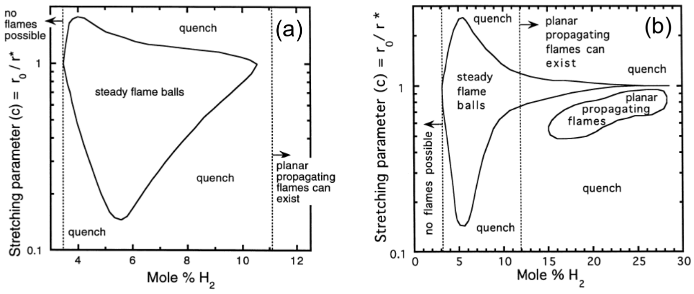
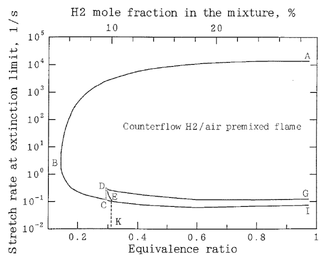


Fig. 8. (a) Eventual fate of flame balls as a function of r_o and X_{H2} for H_2–air mixtures. (b) Eventual fate of flame balls as a function of r_o and X_{H2} for H_2–O_2 mixtures.



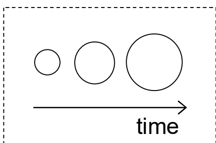
Flammable regions of H2-air counterflow premixed flame. Point K is the flammability limit of a planar premixed flame.

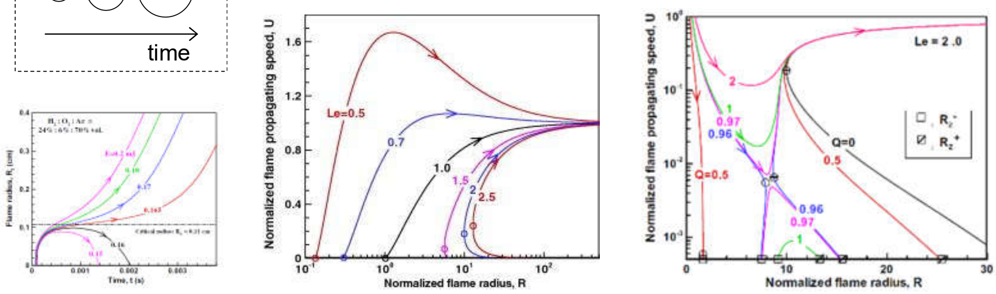
Wu, M.-S., et al., Combust. Flame 116(3) 387 (1999).

Guo et al., Combust. Theor. Model. 4, 459 (2000).

Critical flame radius for self-propagation at different Lewis numbers

- Q = 0 （Q: initial external energy deposition)





Le＝α/D Gasoline/air: Le ≈ 2.3

Chen, Burke, Ju, PCI 33 (2011).

Microgravity combustion:

Flammability limit and near-limit flames

- History
- Counterflow flames
- Flame ball
- Near-limit flames with complicated combined effects

Self Extinguishing Flames (SEFs) in microgravity

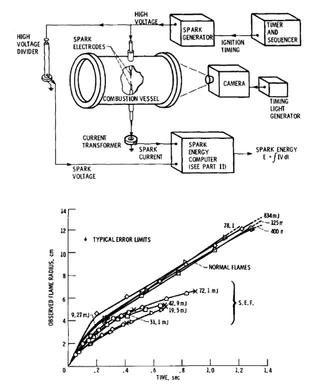


Fig. 5. Observed flame radius versus time for several values of initial spark energy. (a) 5.07% methane at 760 Torr.

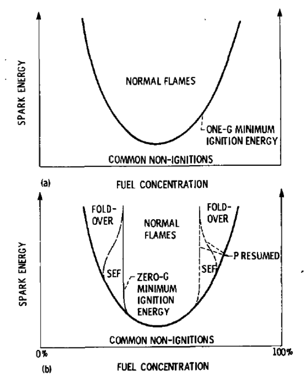


Fig. 4. Schematic diagram showing regions of flame ignition and extinction behavior: (a) one-g, (b) zero-g.

- Self extinguishing flames (SEFs) were observed in microgravity
- Effect of ignition energy, flame curvature and radiative loss were discussed
- SEFs could be interpreted through analogy with counterflow flames under microgravity

Ronney, P.D. and Wachman, H.Y., Combust. Flame 62(2) 107 (1985).
Ronney, P.D., Combust. Flame 62(2) 121 (1985).

Flame instability

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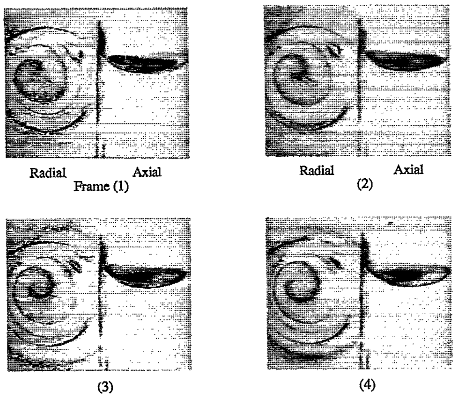
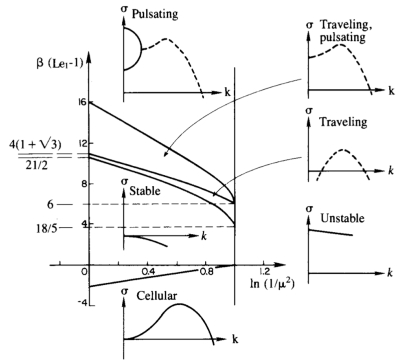


FIG. 2. A clockwise rotating spiral wave in 1.30% C_4H_{10}–21.0% O_2–He. The time between sequential frames is 1/500 s. Image intensities have been inverted, such that the blue flame appears dark and the back background appears light.

Pearlman, H.G., Ronney, P.D. 1994, *Physics of Fluids* 6 (12) , 4009.



Joulin, G. and Clavin, P., (1979) Combust. Flame 35: 139.
Williams, F. A., Combustion Theory., 1985

Related study, e.g., Kazakov, K. A. (2012). "Analytical study in the mechanism of flame movement in horizontal tubes." Physics of Fluids 24(2): 022108.

Flame spread along electric wire in microgravity

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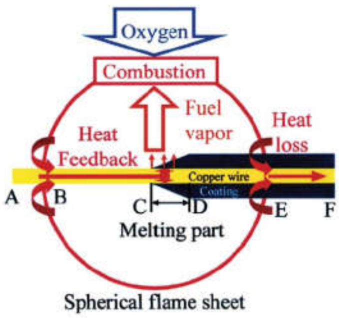

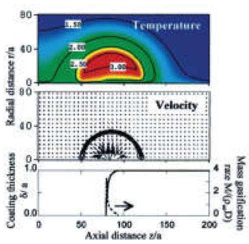

Umemura, A., et al. (2002). "Physical model analysis of flame spreading along an electrical wire in microgravity." Proceedings of the Combustion Institute 29(2): 2535-2543.

- Complicated combined effects of transport and reaction than gaseous combustion
- Phase change, pyrolysis, etc.. and difficulty in defining system boundary conditions
- Essential for space craft safety

Huang, X. and Y. Nakamura (2020). "A Review of Fundamental Combustion Phenomena in Wire Fires." Fire Technology 56(1): 315-360.

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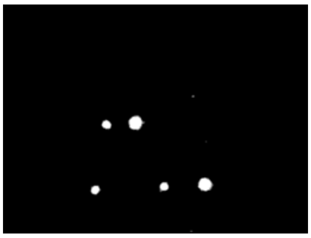
Low-speed counterflow flame experiments in microgravity for comprehensive combustion limit theory (2010-)

Counterflow flames



Flame ball

Constructing comprehensive combustion limit theory
which covers both conventional flames and flame ball
based on low speed counterflow flames under microgravity

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Microgravity experiments by aircrafts

DAS(2010~present)
https://www.das.co.jp/en/index.html

ZERO G (2019)
https://www.gozerog.com/

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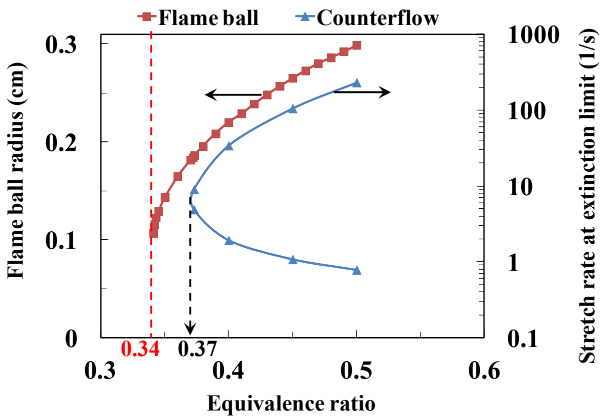
Counterflow flame and flame ball

CH_4/O_2/Xe mixture
OTM
T_0=300 K, 1.0 atm

$$Z = \frac{X_{O2}}{X_{Inert}} = 0.141$$



Possible experimental procedure can be made by the diagram

Takase, K., et al., Combust. Flame 160, 1235 (2013).

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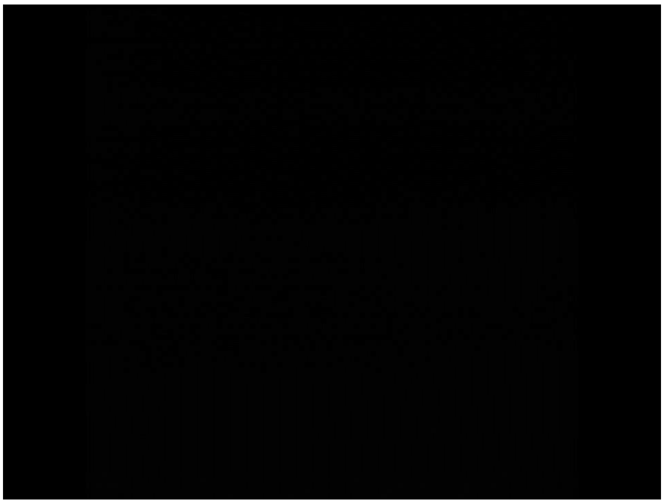
Result (Twin flames -> ball-like flame)

Equivalence ratio gradually decreased (Kr case)



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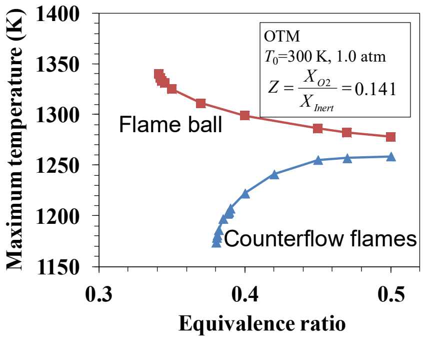
Flame transition: mechanism

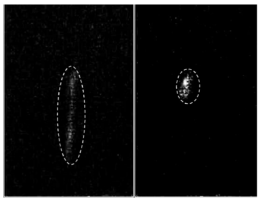
Computation (CH$_4$/O$_2$/Xe)

Stretch rate: 3.2 s^{-1}



Experiment

Stretch rate: 3.2 s^{-1}



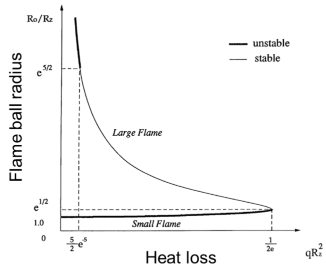
10.89 s Extinction of planar flame

10.93 s Formation of ball-like flame

(ER ~ 0.45)

Takase, K., et al., Combust. Flame 160, 1235 (2013).

Theory



Buckmaster et al. (1990) Combust. Flame 79: 381.

Buckmaster et al. (1991) Combust. Flame 84: 411.

Lee and Buckmaster (1991) Siam J. Applied Math. 51: 1315.

Maximum temperature:

Counterflow flames < Flame ball

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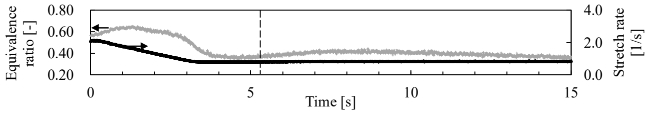
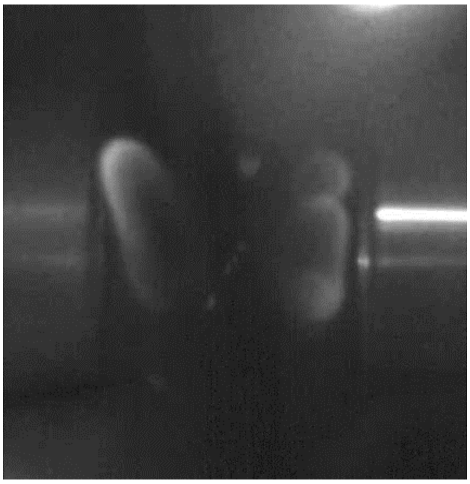
Result (Xe cellular flames)

Stretch rate 2.5 (1/s), ER : 0.58→0.3

Result (Xe sporadic flames -> extinction)

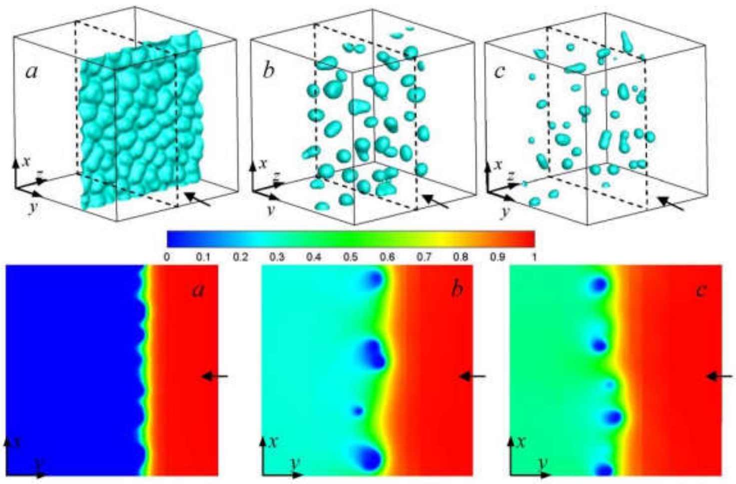




Extinction:
Stretch rate 0.802 s^{-1}
Equivalence ratio 0.372

Sporadic cellular flames by 3D computations

Contour of C=0.15 (top) and concentration distributions in z=0 (bottom) for Le=0.3;
(a) h=0, a=0.067, (b) h=0.6, a=0.033 (c) h=0.8, a=0.033.



Fursenko et al., Combust. Flame **162,** 1712 (2015).

Unified combustion limit theory?

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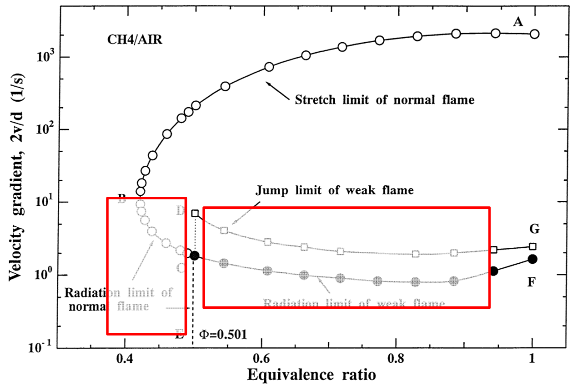

Regime diagram of flame transitions

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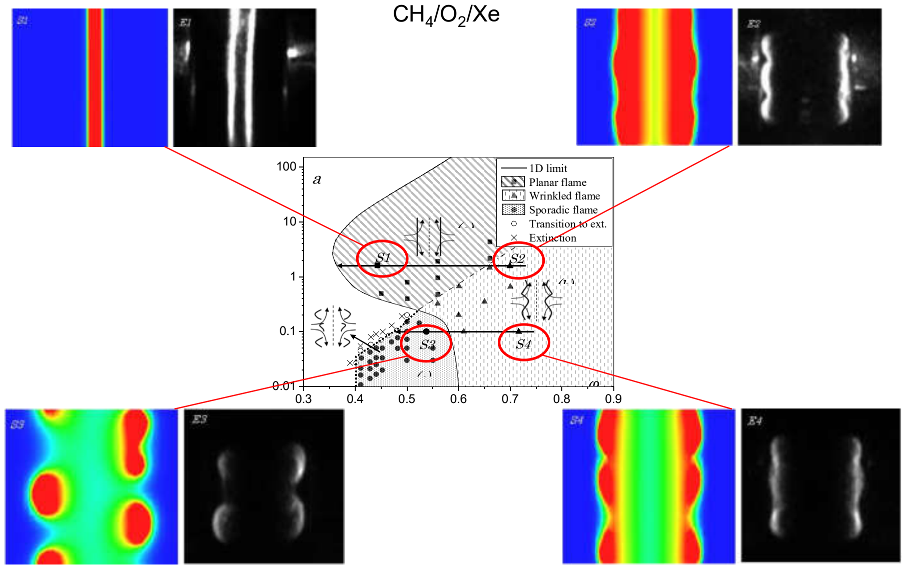
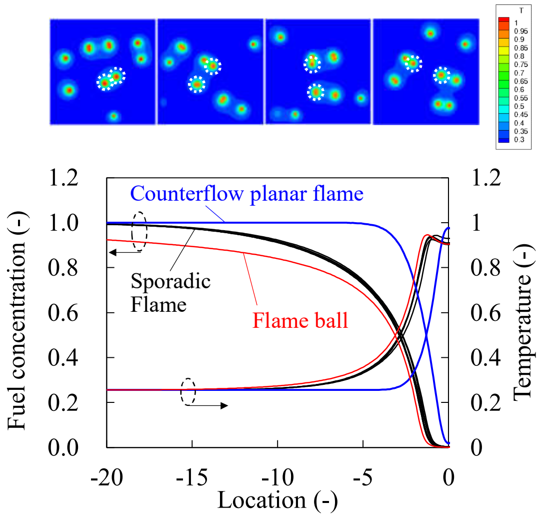
$CH_4/O_2/Xe$



Fursenko et al., Combust. Flame **162,** 1712 (2015).

Flame structures (ϕ = 0.42)

- Computations by 3D thermo-diffusive model
- Flame structure of counterflow flame, flame ball and sporadic flames are compared
- Temperature profiles showed sporadic flame is an intermediate mode of combustion between counterflow flame and flame ball



Okuno et al., Combust. Flame, accepted

Summary of part 2

We have surveyed the purpose, means, and projects of microgravity combustion, and selected the topics to be mainly discussed.

After a brief introduction of droplet combustion, flammability limits and near-limit flame behavior were discussed.

The low-speed counterflow flame method was introduced and radiative extinction, flame-bifurcation and limit mechanism were discussed.

Finally, flame ball was introduced and near-limit flames subject to multiple combined effects were discussed.

End of Part 2

Combustion in Microgravity and Microscale

Part 3: Microscale combustion

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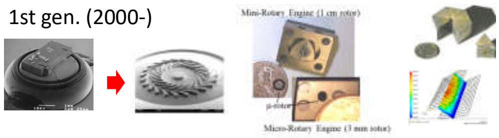
Institute of Fluid Science
Tohoku University

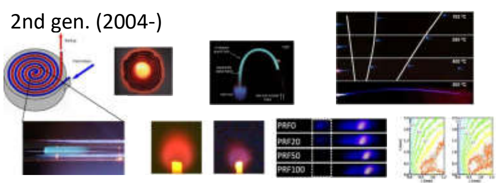
Introduction

Microscale combustion

1st gen. (2000-)

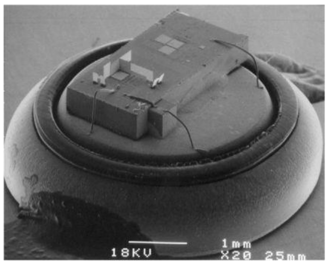


2nd gen. (2004-)



Not only for applications but also various combustion science studies in microscale platforms are conducted.

Initial motivation: to solve the problem of huge battery compared with small main device by employing liquid fuels.



Energy storage often too big…

Pister & Warneke

Numerous attempts have been made to aim for ultra-compact power generation and propulsion devices.

Reviews and book: Epstein et al. (1997) AIAA, Fernandez-Pello (2002) PROCI, Norton & Vlachos (2003) CES, Dunn-Rankin et al. (2005) PECS, Chigier & Gemci (2003) AIAA, Ju & Maruta (2011), Maruta (2011) PROCI, Norton & Vlachos (2012) PECS, Ju, Cadou, Maruta (2015).

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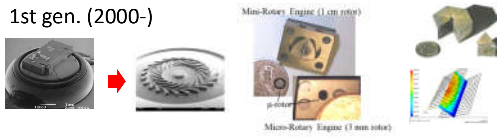
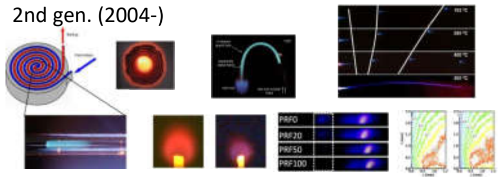
Microscale combustion

1st gen. (2000-)



2nd gen. (2004-)



Not only for applications but also various combustion science studies in microscale platforms are conducted.

In 2nd gen., novel combustion science is highlighted extensively in various micro- and mesoscale platforms.

Typical length and time scales in micro-scale combustion.

Length scales	Time scales
Combustor scales, d	Flow residence time, t_{res}
Combustor structure scale, d_s	Characteristic combustion time, t_c
Flame thickness, δ_f	Diffusion time scale of gas-phase, $t_\alpha = d^2/\alpha$
Quenching diameter, $d_0 = n\delta_f$	Diffusion time scale of solid phase, $t_s = d_s^2/\alpha_s$
Mass diffusion length, δ_D	Time scale of heat loss, t_h
Thermal diffusion length, δ_α	Time scale of acoustic wave, t_a
Mean free path, λ	Ignition time scale, t_{ig}

Ju and Maruta (2011) PECS 37.

flame stabilization, heat regeneration, novel catalysis utilization, new structures, thermal and chemical flame-wall interactions, nonlinear flame physics, cool-warm-hot flame interaction, chemical kinetics, etc.

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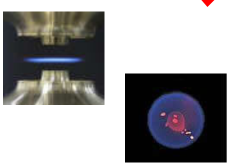
Characteristics of microscale combustion

Micro-combustion depends on many physical and chemical processes such as gas-phase and surface reactions, molecular transport, thermal and mass diffusion, convection, and radiation. The combustion process for micro-power generation involves many different length and time scales. [7)]

"Ideal" flames

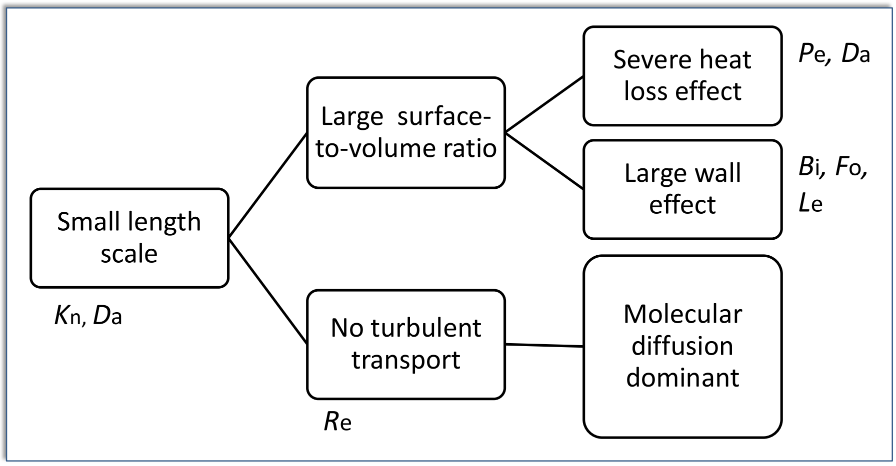


Non-ideal flames, flame-wall interaction, instability, non-linear physics, etc.

Flame quenching, wall thermal effect, wall chemical effect, Diffusion-controlled phenomena

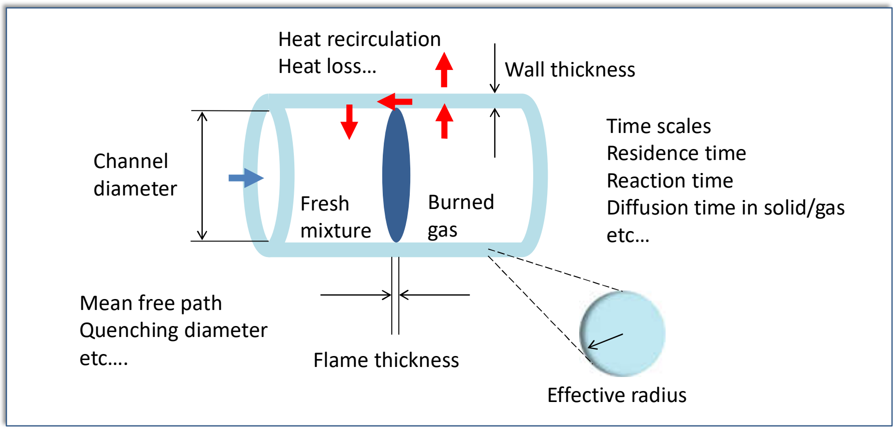
Selected early literatures on micro- and mesoscale combustion:
1) Fernandez-Pello, A. C. (2002) "Micropower generation using combustion: Issues and approaches." PROCI 29: 883-899.
2) Norton, D. G. and D. G. Vlachos (2003). "Combustion characteristics and flame stability at the microscale." Chem. Eng. Sci. 58(21): 4871-4882.
3) Ronney, P. D. (2003) "Analysis of non-adiabatic heat-recirculating combustors." Combust. Flame 135(4): 421-439.
4) Dunn-Rankin, D., et al. (2005) "Personal power systems." PECS 31(5-6): 422-465.
5) Miesse, C. M., et al. (2004) "Submillimeter-scale combustion." AIChE J. 50(12): 3206-3214.
6) Maruta, K. (2011) "Micro and mesoscale combustion." PROCI 33(1): 125-150.
7) Ju, Y. and K. Maruta (2011) "Microscale combustion: Technology development and fundamental research." PECS 37(6): 669-715.

Scaling of microscale combustion



Non-dimensional numbers
Length and time scales…

Scaling of microscale combustion



Length and time scales: $L=(DT)^{1/2}, T=L^2/D$
Non-dimensional numbers: Kn, Pe, Da, Bi, Fo, Le …

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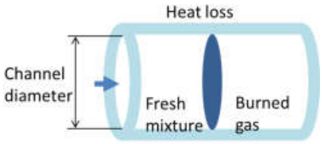
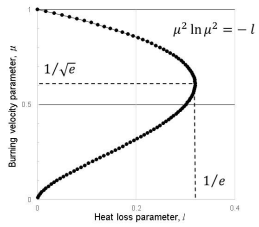
Quenching diameter



$$d_q = 2\sqrt{e\beta Nu}\,\delta_f$$

$$H = \frac{(Heat\,loss)}{(Heat\,generation)} = \frac{c_p(T_f - T_u)\omega(\pi d^2/4)\delta_f}{\pi d\delta_f h(T_f - T_u)} = 4Nu\delta_f^2/d^2$$

- Determined from the ratio of heat generation and heat loss
- Analogy with flammability limit
- What happen if heat loss is insulated, compensated by heat recirculation or high-temperature wall …



$$\lambda\frac{d^2T}{dx^2} - mc_p\frac{dT}{dx} = -\omega q^o + L$$

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Microscale combustion

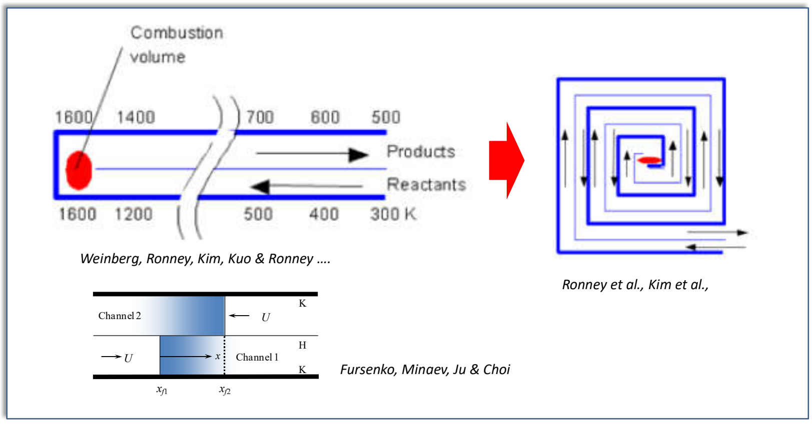
- Wall thermal effect and flame dynamics
- Wall chemical effect
- Microcombustors and microreactors (MFR)
- Industrial applications of the concepts

Wall thermal effect

Thermal stability managements

heat recirculation (excess enthalpy combustion)

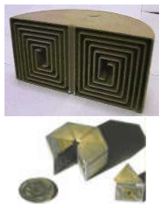
U-shape burner, counter current channel



Weinberg, Ronney, Kim, Kuo & Ronney ....

Fursenko, Minaev, Ju & Choi

Ronney et al., Kim et al.,



Ronney, 3D Swiss roll (2001).

Excess enthalpy combustion

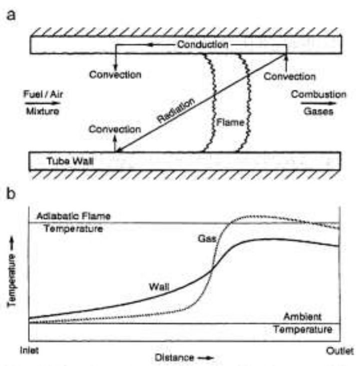
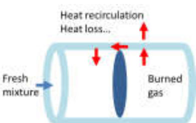
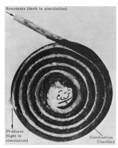


Fig. 3. (a) Schematic representation of heat recirculation in a porous medium idealised as an insulated refractory tube and (b) the corresponding variation in gas and tube wall temperature with distance [14].

Wood, S. and Harris, A.T., *Porous burners for lean-burn applications*, PECS 34, 667 (2008).



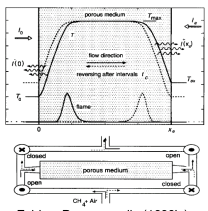
- Essential heat transfer condition for excess enthalpy combustion could be attained not only in Swiss roll geometry but also in radiant emitter and receiver, porous media, small channel, etc.
- Fundamental studies of EEC have been conducted in various platforms.
- Super-adiabatic and super-lean combustion available



Weinberg (1972).

Ronney, 3D Swiss roll (2001).

Maruta, Microcombustor (2005).



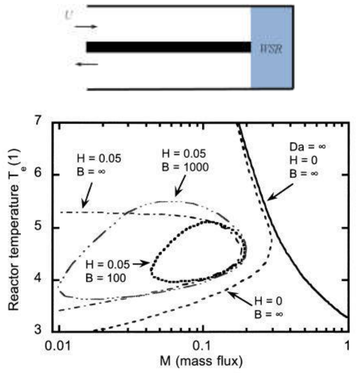
Echigo, Porous media (1990's).

Takeno, Sato, Combust. Sci. Technol. 20, 73 (1979).
Hanamura, Echigo & Zhdanok, Int. JHMT **36,** 3201 (1993).
Hoffmann et al., Combust. Flame 111, 32 (1997).

Ju, Choi, Combust. Flame 133, 483 (2003).
Ronney, P.D., Combust. Flame 135, 421 (2003).
Kim, N.I., et al., Combust. Flame 141, 229 (2005).

Excess enthalpy combustion revisited

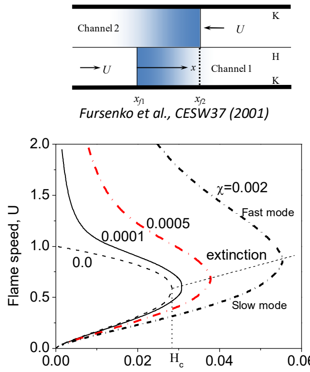
U-shaped channel



Effect of Mass flux on WSR temp.

Ronney, CNF135 (2003)

Opposite flows



Effect of Heat loss on Flame speed

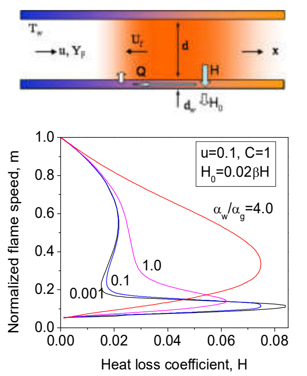
Ju & Choi, CNF133 (2003)

Excess enthalpy combustion: *Weinberg (1975), Takeno, Echigo, Babkin et al.,*
Microcombustion: *Kuo & Ronney, Leach & Cadou, Jackson et al, Ju & Xu, Kim et al., Pizza et al., & others.*

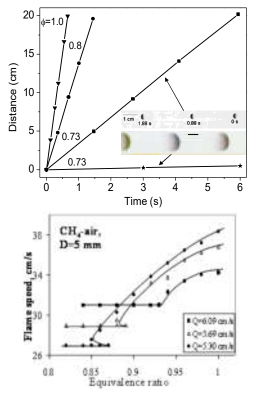
Flame bifurcation

Premixed flame in a meso-scale tube
→ flame bifurcation … weak flames

as particle laden flames and microgravity counterflow flames



Theory



Experiment

Ju & Xu, PCI30 (2005), CST178 (2006)

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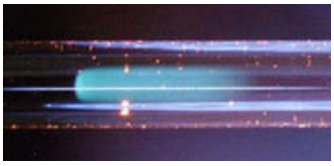
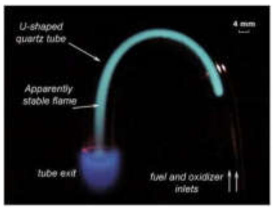
Repetitive extinction and ignition instability (FREI)

Broadened (?) reaction zone
at intermediate flow velocity



Flame with Repetitive Extinction and Ignition, FREI
Maruta et al., PCI30 (2005)



Richecoeur & Kyritsis, PCI30 (2005)

LIF, Fan, Suzuki, Kasagi, PCI32, 33 (2009, 2010)

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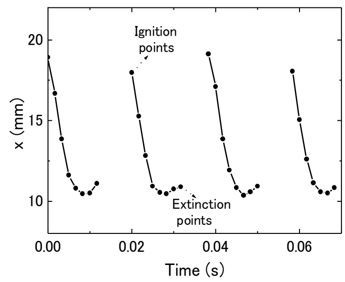
Repetitive extinction and ignition instability (FREI)

High-speed OH movies show:
- auto-ignition at high temperature zone →
- flame propagation toward upstream →
- extinction → charging fresh mixture → auto-ignition

Repetition with frequency 10-100 Hz



Maruta et al., PCI30 (2005),

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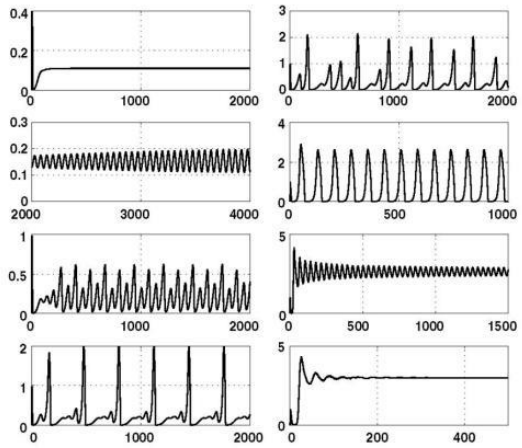
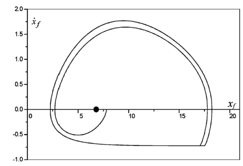
Dynamic flame behaviors, chaotic



Temporal fluctuation of maximum reaction rate

Jackson, Buckmaster, et al., PCI31 (2007)

Experimental results reproduced Chaotic behavior predicted by computations and theories



Phase diagram of flame movement

Minaev et al., CTM11 (2007),

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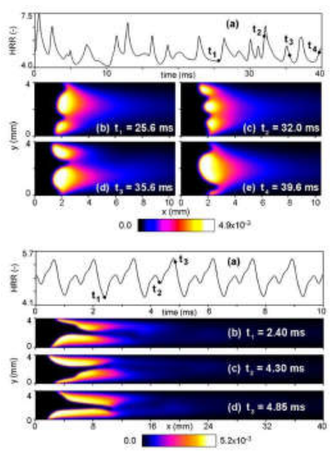
Complex flame dynamics



(a) temporal variation of the integral heat release rate, and (b) maps of Y_{OH}
h = 4 mm, Vin = 100, 300 cm/s

Mantzaras et al., CNF155 (2008)

Broken flame appears at higher velocity
DNS with full hydrogen chemistry

Mechanism?
Interpretations of DNS is generally difficult

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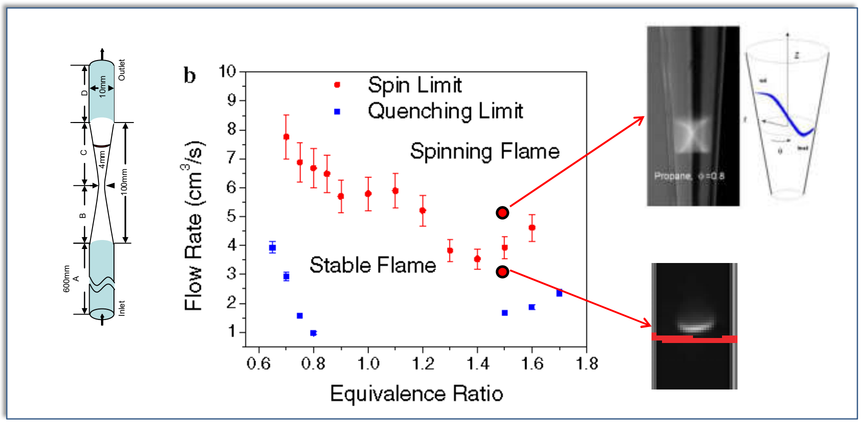
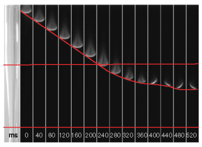
Spinning flames 1 of 3





Spinning/non-spinning flame regimes appear at different flow rates

Xu & Ju, PCI31 (2007)

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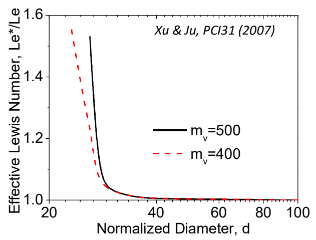
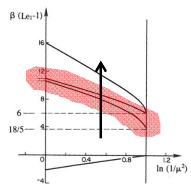
Spinning flames 2 of 3





Effective Lewis number exceeds critical value for the onset of DT instability

Effective Lewis number which includes solid phase heat conduction

Conventional theory on diffusive-thermal instability is valid when effective Lewis number is introduced

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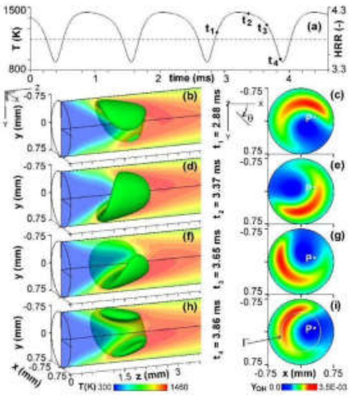
Spinning flames 3 of 3



Pizza, Frouzakis, Mantzaras et al., JFM (2010)

H_2/air spinning flames in heated duct

Spinning flames also predicted by 3D-DNS with hydrogen full chemistry

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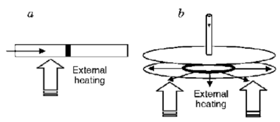
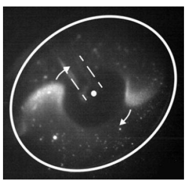
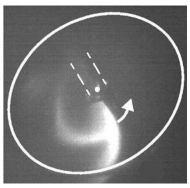
Flame pattern formation

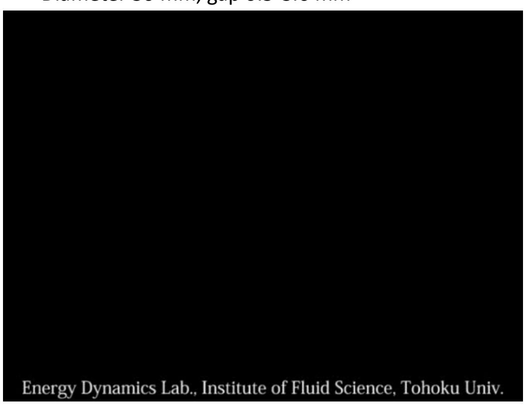


Rich varieties of flame patterns observed in radial micro channel

Diameter 50 mm, gap 0.5-3.0 mm







Kumar et al., PRE, Phys. Fluid, JMM (2007-2008), Fan et al., CNF, PCI, JMM (2007-2010)

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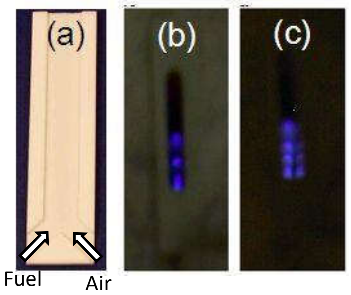
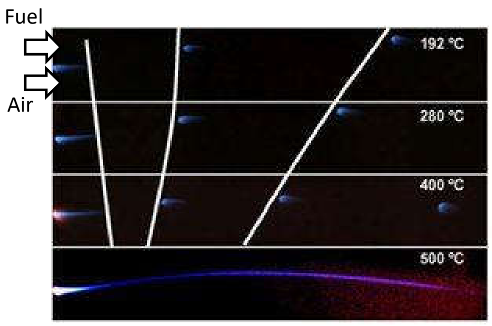
Flame streets

Novel cellular-type diffusion-flame instability observed in 30x5x0.75mm Y-shaped channel
Scale-up experiment clarifies flame streets in the mixing layer   Flow rate, wall temperature, fuel diffusivity...



Miesse et al., PCI30 (2005)



Xu & Ju PCI32 (2009)

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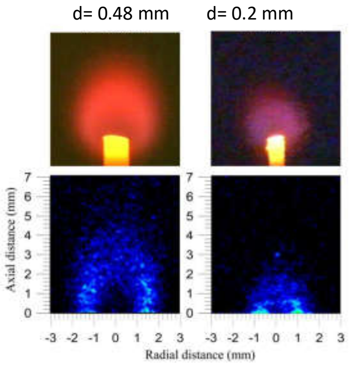
Micro jet flames

Lighter radicals disappeared from the nozzle exit close to the limit, diffusive loss?



Direct photographs and LIPF-OH images of microscale hydrogen diffusion flames

Cheng, Chao, Nakamura et al., PCI30 (2005)

Extinction mechanism probably important for establishing the weakest self-stabilizing flame

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Microscale combustion

- Wall thermal effect and flame dynamics
- Wall chemical effect
- Microcombustors and microreactors (MFR)
- Wide applications of the concepts

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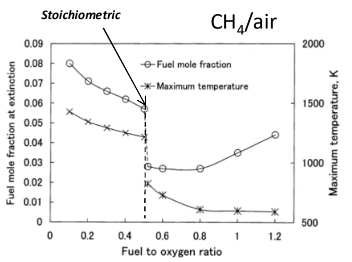
Wall chemical effect
Self-sustained low temperature reaction

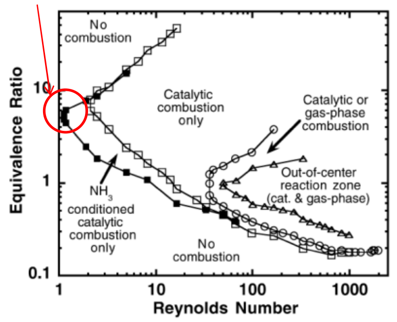
Low temperature catalytic reaction based on different surface coverage in lean & rich mixtures → plastic combustor, etc…



Lowest self-sustaining temperature lower due to less O(s) effect in fuel-rich condition

Maruta et al., PCI29 (2002)

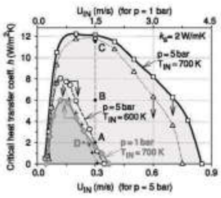
Lowest peak temperature 75 deg. C at *Re* =1.2



Ahn, Ronney et al., PCI30 (2005)

Gas-phase & surface reaction interaction

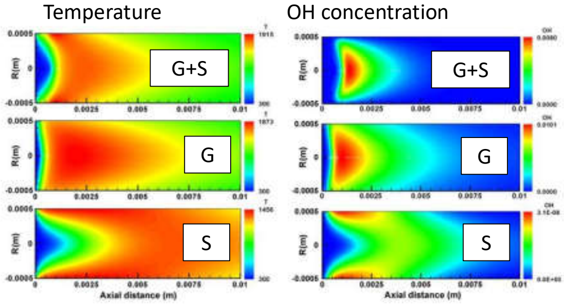
Blow-off limits extended if gas-phase reaction is considered (CH_4/air, ϕ = 0.4)
Surface reaction inhibits gas-phase reaction…



CH_4/air mixture of ϕ = 0.4 in 1mm-channel

Karagiannidis, Mantzaras et al., PCI31 (2007)

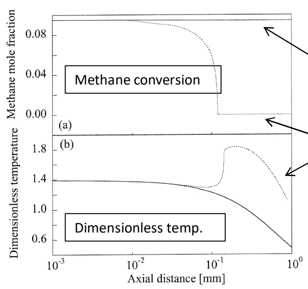
Temperature   OH concentration



Stoichiometric H_2/air mixture in 1 mm channel

Chao et al., Applied Catalysis A 332 (2007)

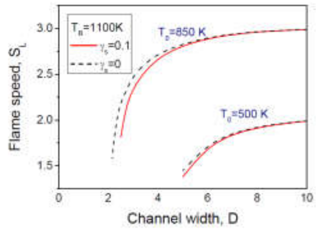
Radical quenching, computational



Raimondeau et al., PCI29 (2002)

100μm channel with inlet temp 1782K
Radical quenching results in no methane conversion

w/o radical quenching



Ju & Xu, AIAA (2006)

Effect of channel width & inlet temperature
Radical quenching plays significant role at smaller channel widths & higher inlet temp.

Experimental studies by Miesse et al, Kim et al.

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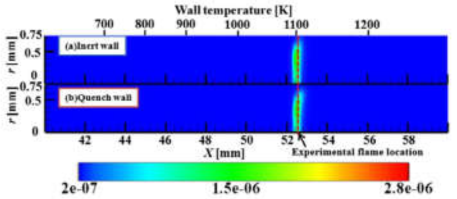
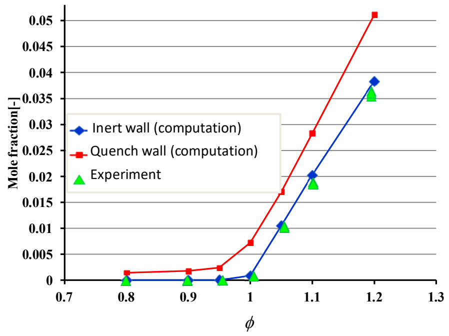
Radical quenching,
experiment & computation

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., PCI 35 (2015).

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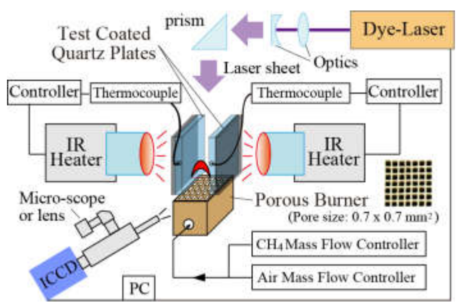
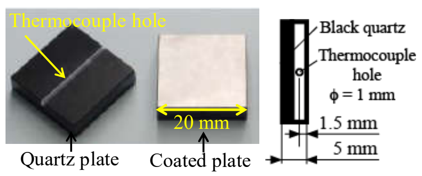
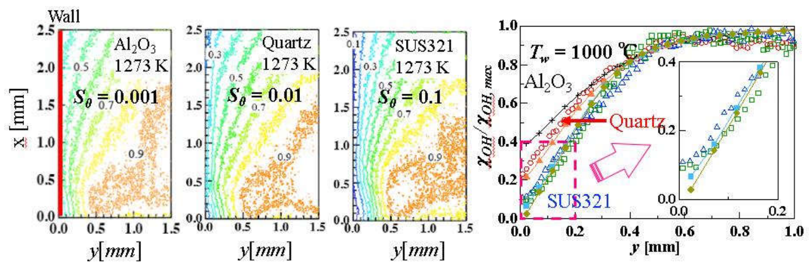
Quantitative measurement of wall chemical effect





- 100 nm-thick thin films on quartz plate
  Metal: Sputtering/Arc plasma gun
  Al_2O_3: Atomic Layer Deposition



Saiki, Fan & Suzuki, Combust. Flame (2015).

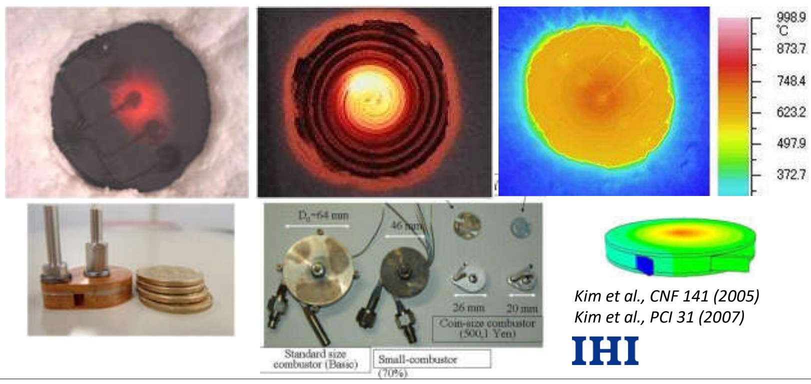
Further study:
Cool flame-wall interaction:
Wan et al., PROCI 37, 5565 (2019).

Microscale combustion

- Wall thermal effect and flame dynamics
- Wall chemical effect
- Microcombustors and microreactors (MFR)
- Industrial applications of the concepts

Swiss roll microcombustor as heat sources

Disk-type heaters: D = 64, 46, 26, 20 mm
Surface temperature: 650 - 1250K
Temperature controllability: within 1 K at 1173K
Thermal efficiency as a heater: up to 85%
100W-1kW for various industrial heating, heat source for TE, TPV…..



Kim et al., CNF 141 (2005)
Kim et al., PCI 31 (2007)
IHI

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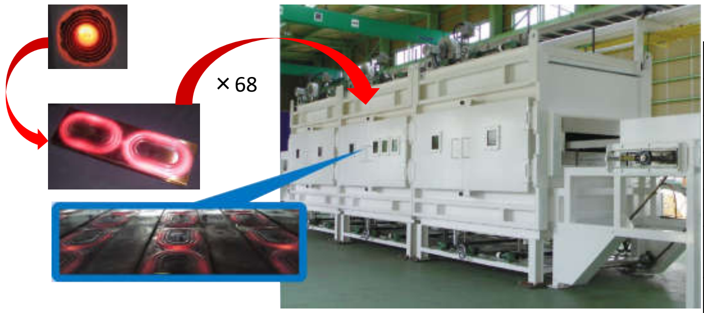
Possible application of microcombustors

(Proto-type industrial heating furnace)



IHI

Specification	
Length	7 m
Width	0.9 m
Temperature	Max 400°C
Control	3 zone
Number of heaters	68
Bed speed	0.6m～12m/min

70 % reduction of fuel consumption

- Baking and drying food
- Drying for painting
- Thermal treatment of glass panel, polymer film and material with low melting point

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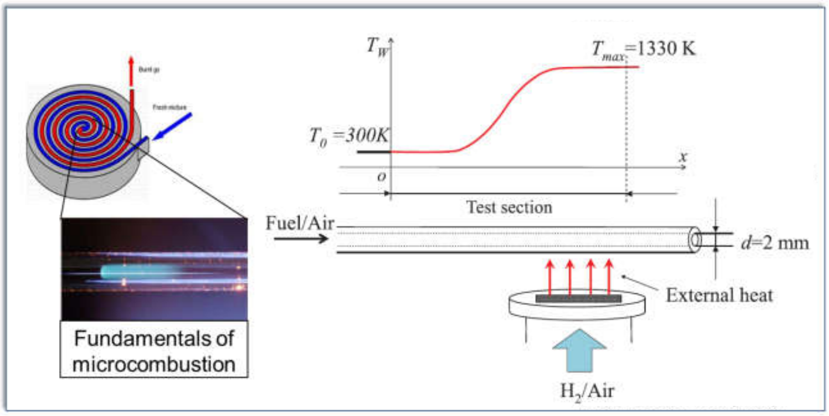
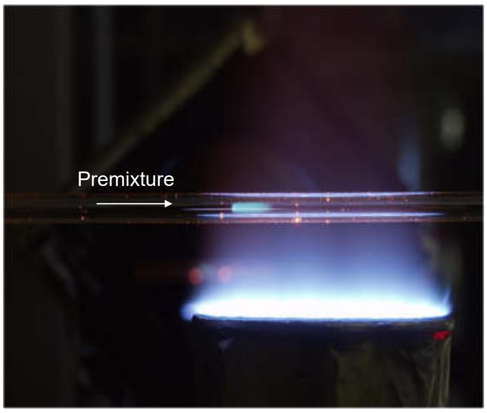
Micro flow reactor with a controlled temperature profile (MFR)

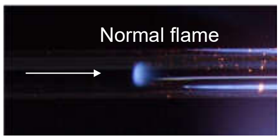


Maruta et al., PCI 30 (2005).

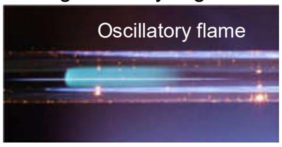
Stationary wall-temperature profile
Tube diameter < conventional quenching diameter
Gas phase temperature dominated by wall temperature profile
Laminar and constant pressure

Flame behaviors in a meso-scale channel with a prescribed temperature profile

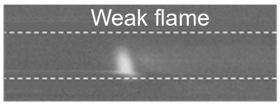




High velocity region



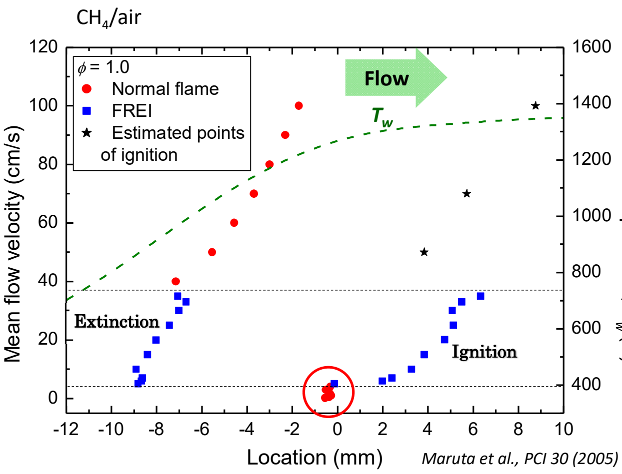
Intermediate velocity region



Low velocity region

Maruta et al., PCI 30 (2005).

Three kinds of flame responses



Maruta et al., PCI 30 (2005)

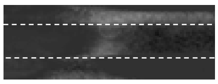
(1) Normal flame

V=50cm/s

(2) Oscillatory flame

V=20cm/s

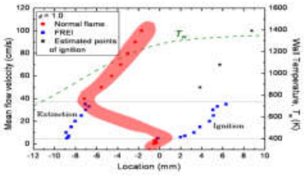
(3) Weak flame

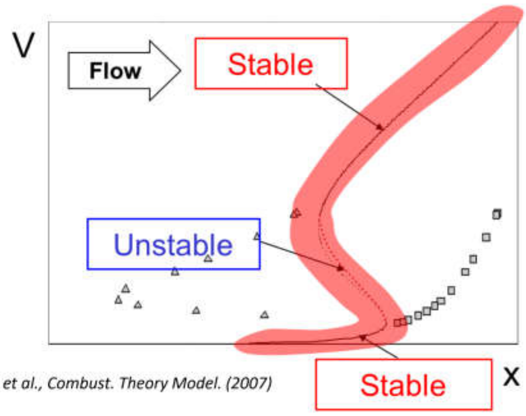


V=0.2cm/s

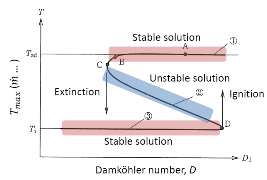
Normal flame, oscillatory flame, weak flame

Theoretical S-shaped response for MFR



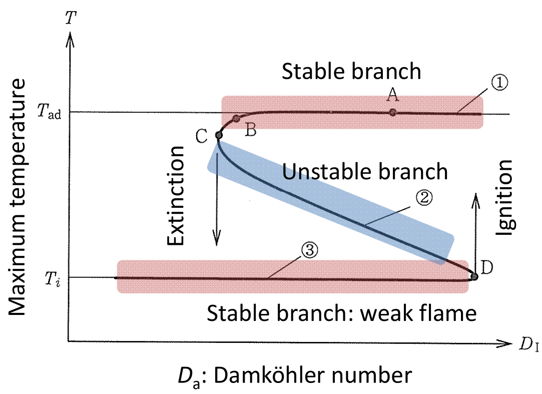


Minaev et al., Combust. Theory Model. (2007)



Two stable and one unstable solutions were predicted theoretically

Analogy between MFR S-curve and conventional Fendell-curve



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

- 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:

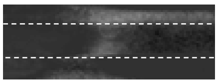
(1) Normal flame

Measurements of laminar burning velocity of highly preheated mixtures

(2) Oscillatory flame

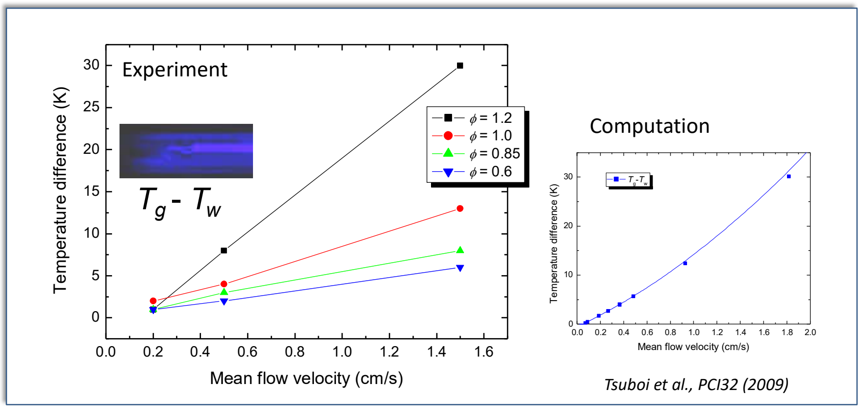
Investigations of non-linear dynamics of given fuels

(3) Weak flame



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

Lower limit of weak flames identified



At V = 0.2 cm/s, T_w = 1225 K, T_g-T_w< 2 K
Extremely small temperature increase
Flame position close to the ignition point
Lowest flame temperature → ignition temperature?

Limit mechanism

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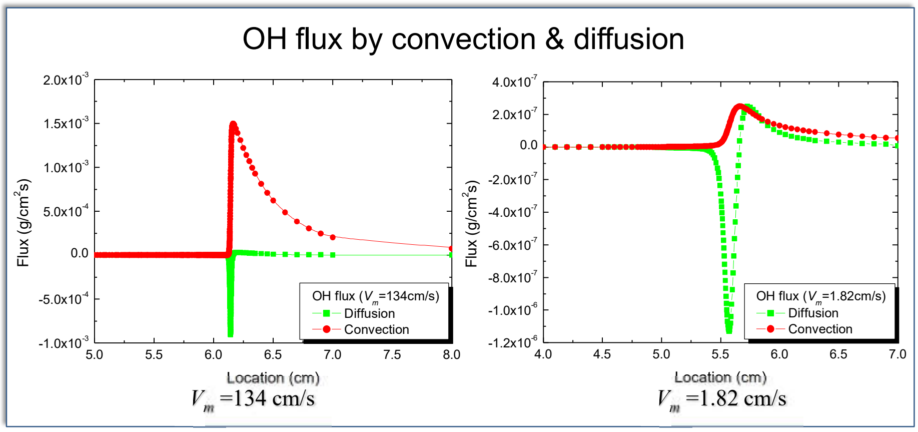

Mass dissipation at low velocity region significantly larger than that at higher velocity region
Lower limit of weak flame by diffusive dissipation?

Tsuboi et al., PCI32 (2009)

Triple weak flames, n-heptane

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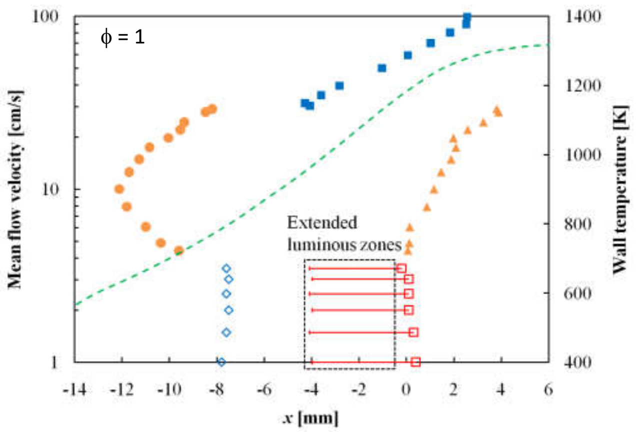

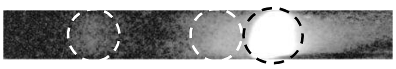

U = 3 cm/s

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

Yamamoto et al., PCI 33

Computation (one-dimensional)

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One-dimensional reactive flow w/o boundary layer

Gas-phase energy equation

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

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

CanteraMFR code will be open for public in WiPP in 39th Symp.

Triple weak flames, n-heptane

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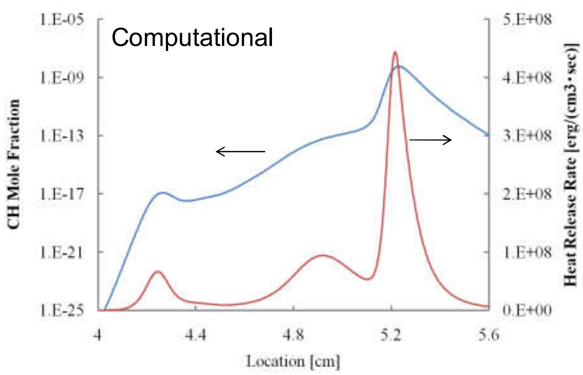
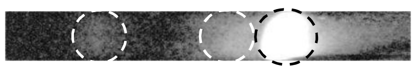


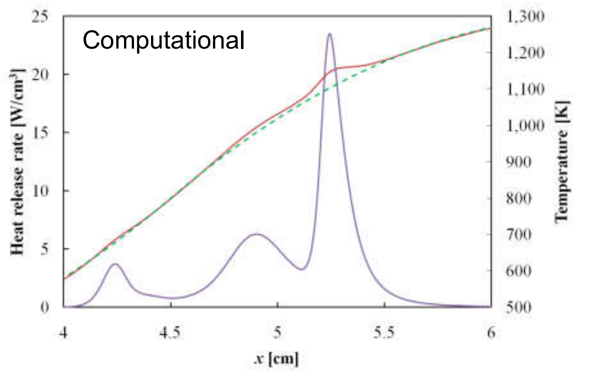


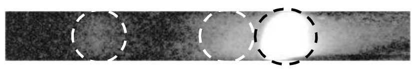
U = 3 cm/s

Three-stage heat releases

Yamamoto et al., PCI 33

Triple weak flames, n-heptane

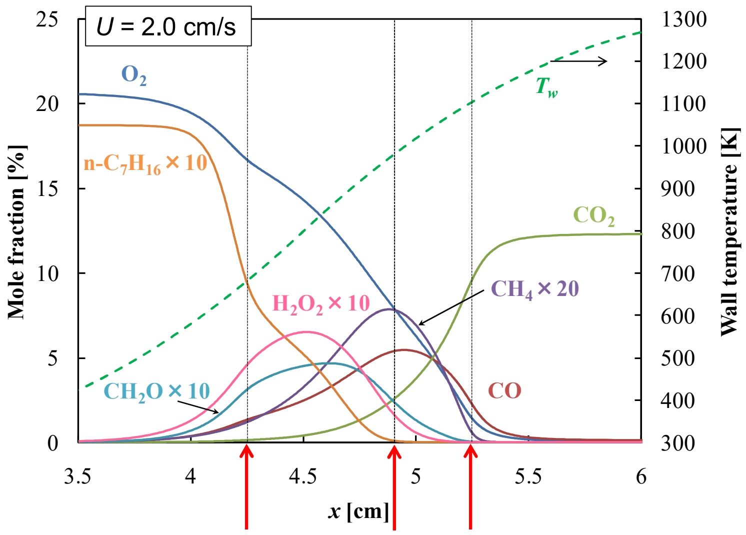




Three-stage heat releases

Yamamoto et al., PCI 33

Computational species profiles



Three peaks of heat release rate

Yamamoto et al., PCI 33

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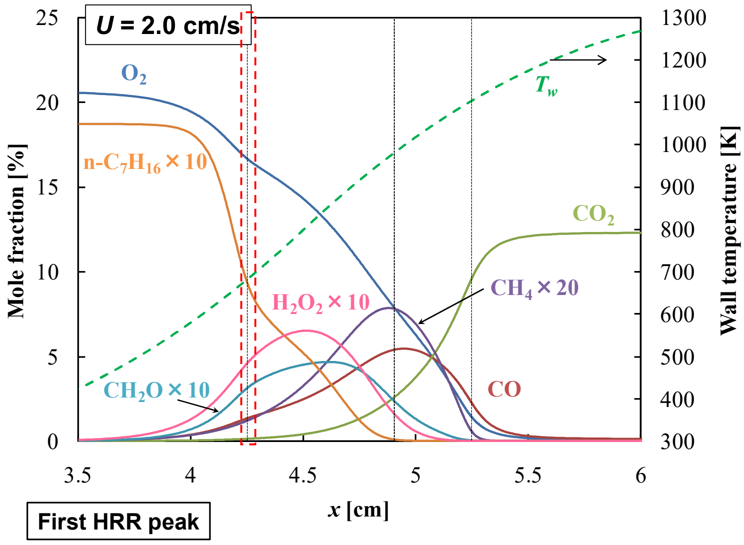
Computational species profiles



First HRR peak

LTO: CH_2O, H_2O_2, CO, CH_4 produced

Yamamoto et al., PCI 33

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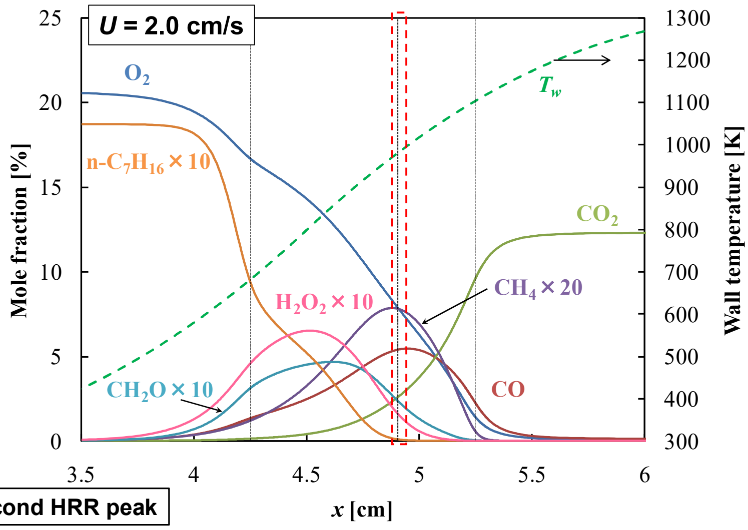
Computational species profiles



Second HRR peak

Partial oxidations:

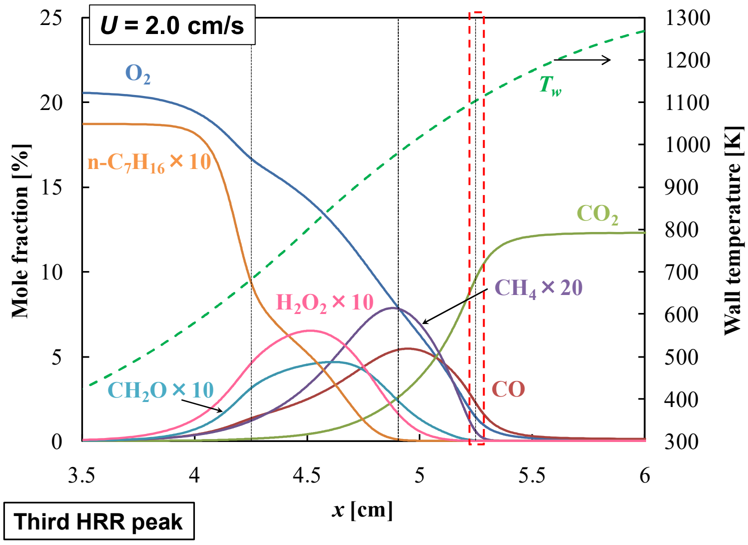
$\mathbf{H_2O_2}$ (+M) ⇒ 2OH (+M)

$\mathbf{CH_2O}$ + OH ⇒ <u>HCO</u> + H_2O

<u>HCO</u> + O_2 ⇒ **CO** + HO_2

Yamamoto et al., PCI 33

Computational species profiles

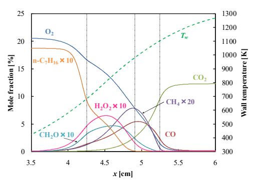


Full oxidations: $CO + OH \Rightarrow CO_2 + H$

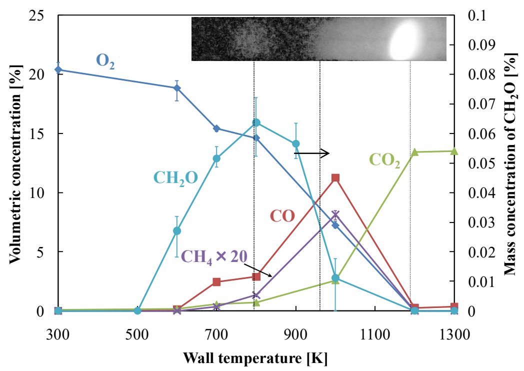
Measurements and computations

(U = 2.0 cm/s)

Computations



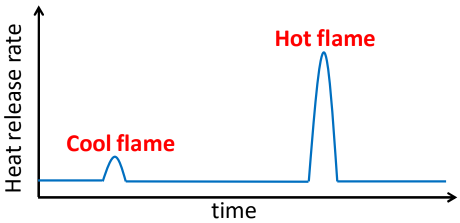
Measurement by GC

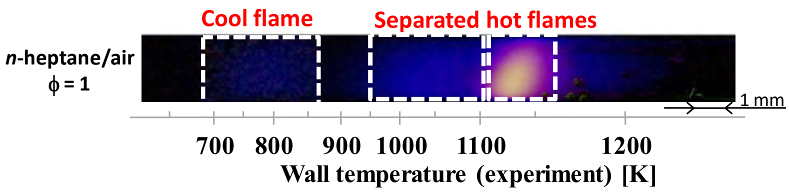


Three-stage oxidation process was
confirmed by gas sampling experiment

Interpretation of triple weak flames

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

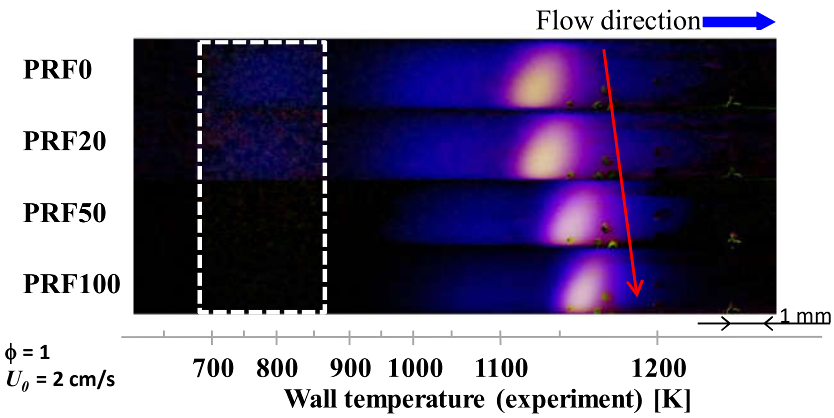




Conventional two-stage ignition converted into steady, three-stage, spatially-separated weak flames in MFR

MFR applied for gasoline PRF

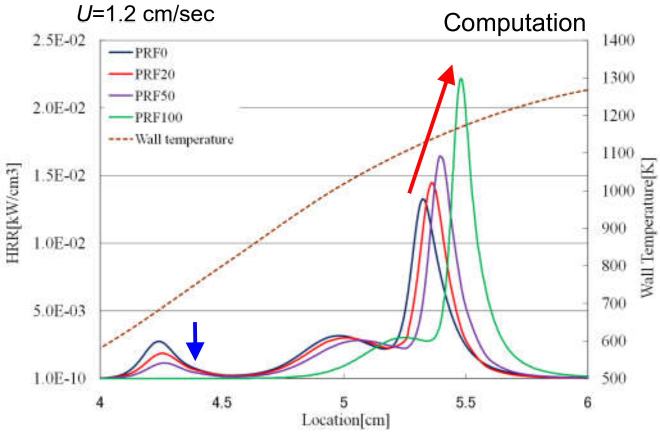
n-heptane + *iso*-octane (PRF)



Appearances of multiple weak flames represent Research Octane Number

Hori, et al., CNF 2012

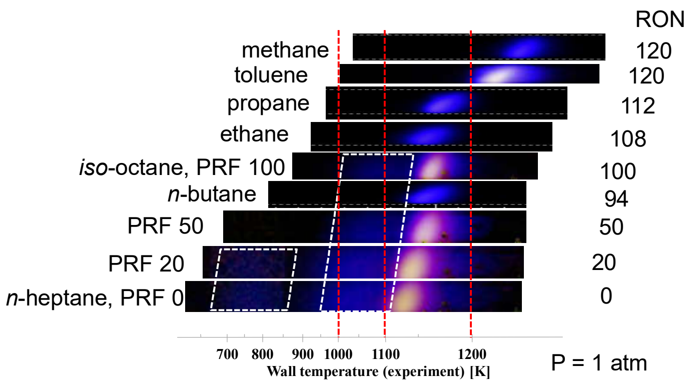
Weak flames at different RON



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

Data from:
Hori et al., CNF 159, 2012.
Hori et al., PCI 34, 2013.
Kamada et al., CNF 161, 2014.
Presented:
1st flame chemistry WS, 2012
Grajetzki et al., Fuel 245, 2019.

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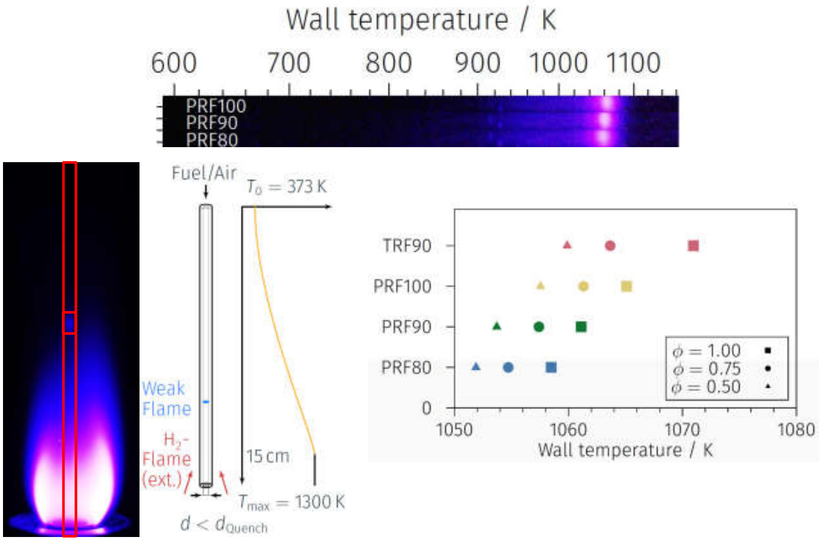
PRFs, ultra lean, higher resolution



Vertical-type reactor

Grajetzki, et al., 36 Symp, WIPP. 2016.
Grajetzki, et al., COMODIA, 2017.

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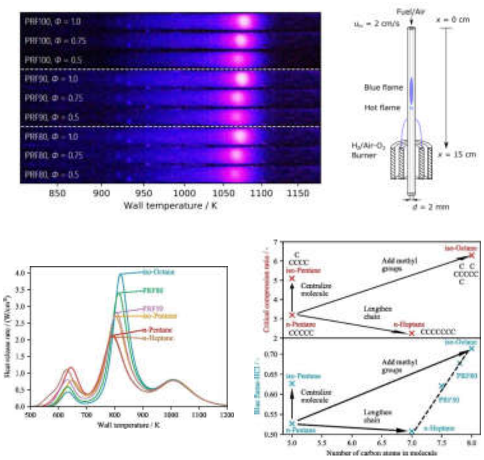
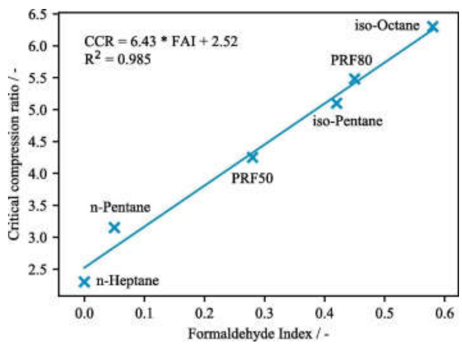
Alternative fuel index based on CH2O among cool, warm(blue) and hot weak flames

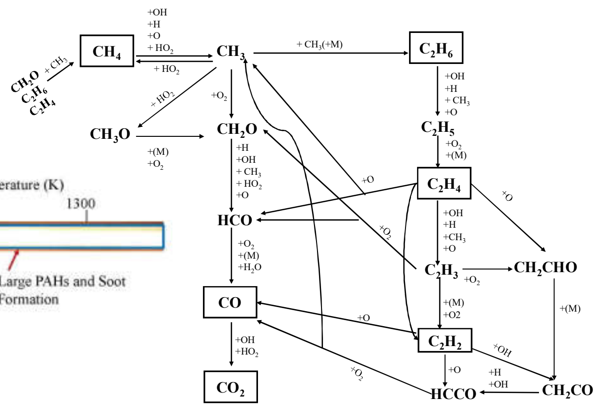


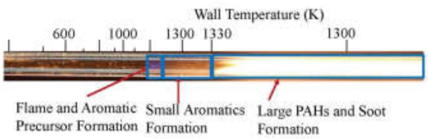


Vertical high resolution MFR + trade-off between cool and blue flames
=> General ignition property

Grajetzki et al., CST 190, 1950 (2018).
Grajetzki et al., Fuel 245, 429 (2019).

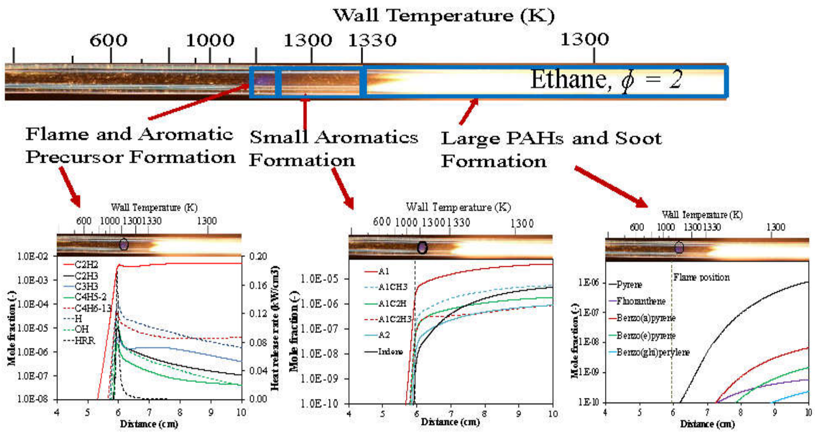
Soot and PAH formations at temperature below 1400 K





Dubey et al., CNF 174, 2017.

Soot and PAH formations at temperature below 1400 K



Dubey et al., CNF 174, 2017.

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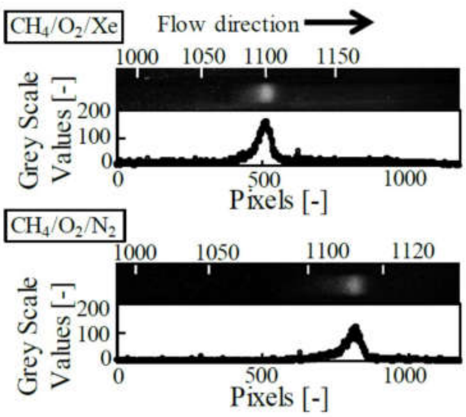
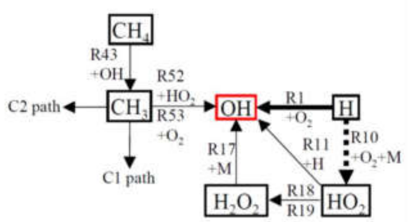
CH_4, ultra lean and Xe dilution

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.

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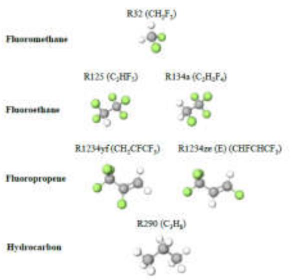
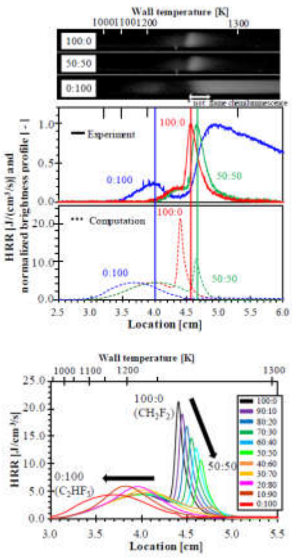
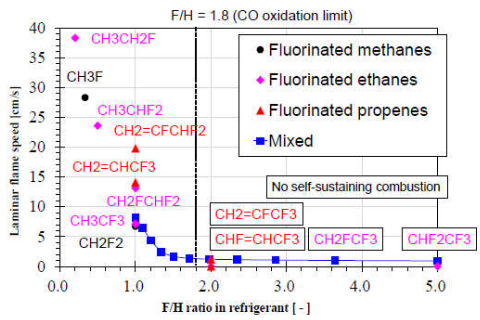
Reactivity of weakly flammable hydrofluorocarbon refrigerants, R32(CH2F2), R125(C2HF5), R410A(R32+R125), R1234yf(C3H2F4)

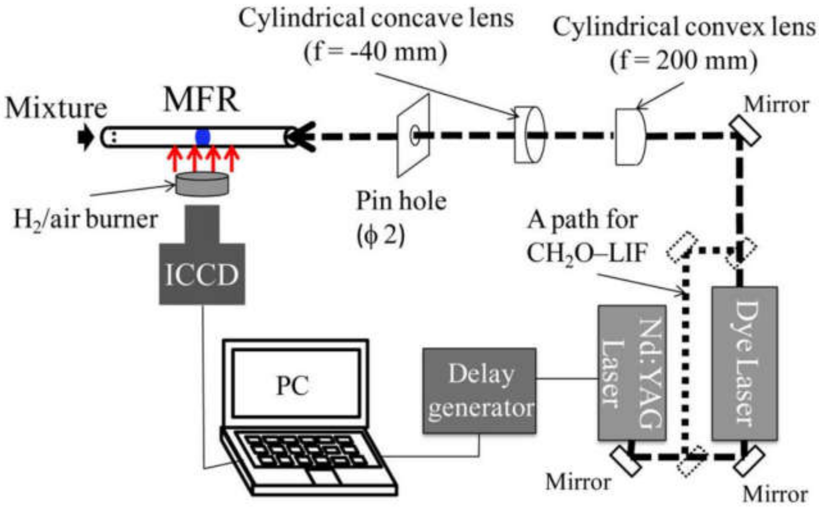






Takahashi, S., et al. (2021) PROCI 38: 2487.
Takahashi, S., Thesis, 2022.

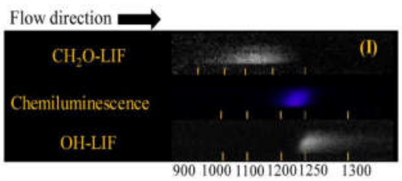
LIF for CH2O and OH applied

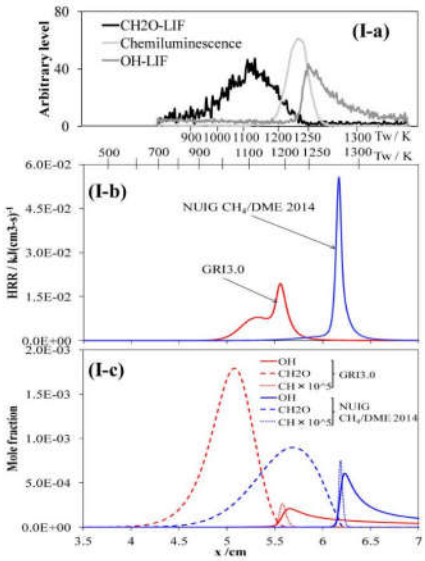


Shimizu et al., Energ. & Fuels 31, 2017.

LIF of CH2O & OH and Chemiluminescence

methane/air





Shimizu et al., Energ. & Fuels 31, 2017.

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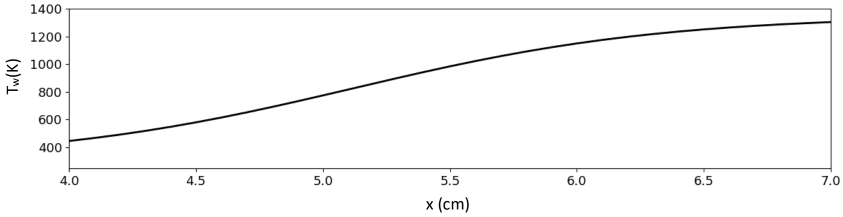
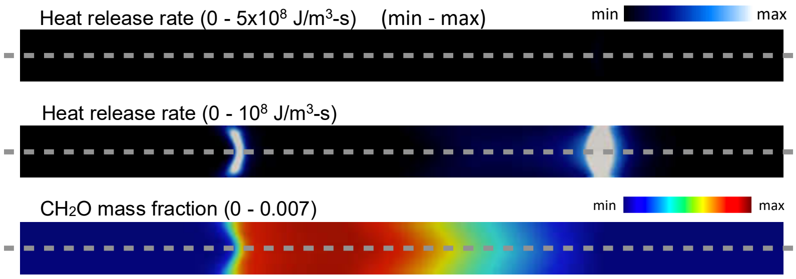
FREI of n-heptane/air mixture

nC_7H_{16}/air, u=15 cm/s, φ=1.0, p=1 atm, $T_{w,max}$=1350 K, Lu-mech





Akita et al., PROCI 38.

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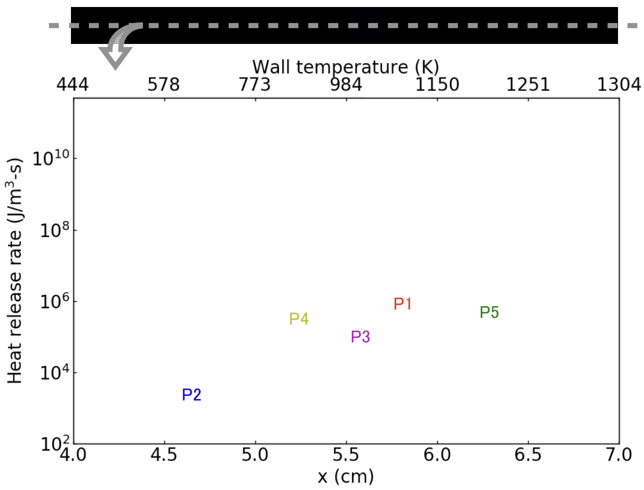
Time history of HRR peaks

nC_7H_{16}/air, u=15 cm/s, φ=1.0, p=1 atm, $T_{w,max}$=1350 K, Lu-mech



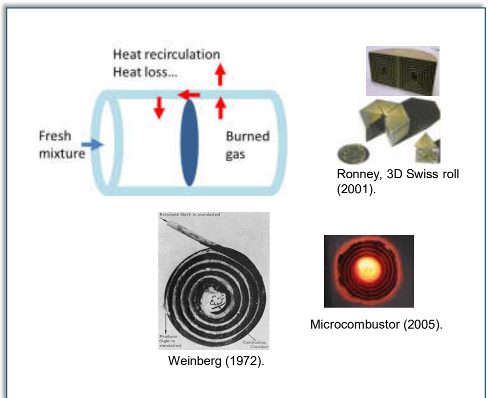
Extract five HRR peaks P1 to P5

Akita et al., PROCI 38.

Microscale combustion

- Wall thermal effect and flame dynamics
- Wall chemical effect
- Microcombustors and microreactors (MFR)
- Industrial applications of the concepts

Excess enthalpy combustion revisited again!



HiCOT, HiTAC,
MILD combustion

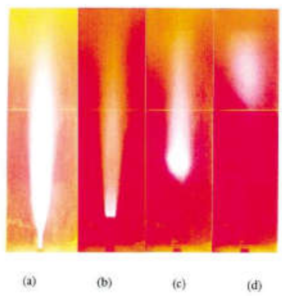


FIG. 2. Photographs of turbulent methane jet flames. Methane flow rate is 3 Nl/min. Coflowing air temperature is (a) 1470 K, (b) 1383 K, (c) 1303 K, and (d) 1223 K.

Fujimori et al., PCI 27, 1998

- Fundamental concept of excess enthalpy combustion that attained in various microcombustion platforms could be also applied to wider applications, such as industrial furnace.
- Super-adiabatic combustion and super-lean combustion are available and of use for better thermal efficiency.

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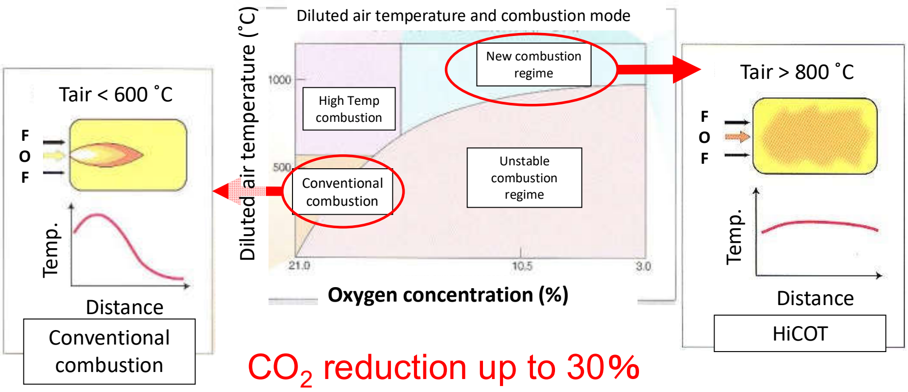
High temperature air combustion technology
(Concept and technical merits)



CO_2 reduction up to 30%
Extremely low NO_x
emissions No combustion
noise Downsizing

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Summary of part 3

The scope of microcombustion research has expanded from power generation (first generation) to combustion science (second generation).

After touching the scaling analysis, wall thermal effects, including excess enthalpy combustion, flame bifurcation, instability, and pattern formation, were introduced.

For the wall chemical effects, radical quenching and its quantification were introduced.

Finally, microcombustors and microreactors (MFR) were introduced. Applications of MFR to kinetics study, fuel indexing, weakly-flammable mixtures and recent computations on FREI with cool flame were presented.

End of Part 3