TSINGHUA-PRINCETON-COMBUSTION INSTITUTE

2022 SUMMER SCHOOL ON COMBUSTION

FUNDAMENTAL OF FLAMES

Suk Ho Chung

King Abdullah University of Science and Technology

July 11-13, 2022

TSINGHUA-PRINCETON-COMBUSTION INSTITUTE

2022 SUMMER SCHOOL ON COMBUSTION

<table>
<tr><th colspan="6">Schedule</th></tr>
<tr><td>Beijing Time</td><td>July 11 (Mon.)</td><td>July 12 (Tue.)</td><td>July 13 (Wed.)</td><td>July 14 (Thu.)</td><td>July 15 (Fri.)</td></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="2">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 colspan="2">Current Status of Ammonia Combustion
William Roberts
VMN: 80506726244</td></tr>
<tr><td>19:00 ~ 22:00 Session I</td><td colspan="4">Combustion Chemistry and Kinetic Mechanism Development
Tiziano Faravelli
VMN: 35989357660</td></tr>
<tr><td>19:00 ~ 22:00 Session II</td><td colspan="3">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

2022 Tsinghua-Princeton Combustion Institute Summer School on Combustion

Fundamentals of Flames

Suk Ho Chung, Professor Emeritus

King Abdullah University of Science and Technology (KAUST)

Contents

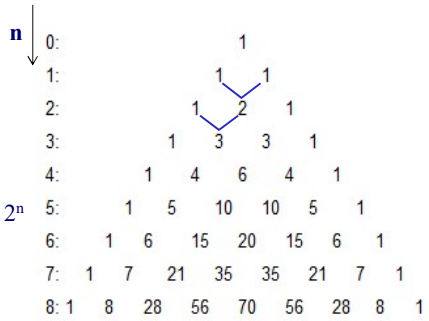
- Molecules, Reaction
- Transport Phenomena : Diffusion
- Governing Equations
- Chemical Kinetics
- Diffusion Flames
- Premixed Flames
- Flames in Partially-Premixed System
- Engine Fuels

Clean Combustion Research Center

Molecules, Diffusion, and Reaction

Random Walk

- **Drunkard's Walk**
  - Coin Toss Experiment
  - Number of cases
  - All the cases are equally probable
  - N-step: No of possible cases is 2^n



Pascal triangle

$(a+b)^n$

1

$a+b$

$a^2+2ab+b^2$

$a^3+3a^2b+3ab^2+b^3$

$a^4+4a^3b+6a^2b^2+4ab^3+b^4$

- **Binomial expansion**
  - As n large, approaches Gaussian

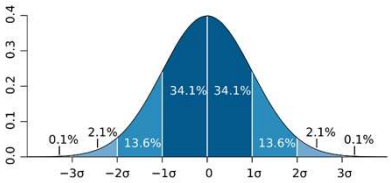
$$(a+b)^n = \sum_{k=0}^{n} \frac{n!}{k!(n-k)!} a^{n-k} b^k = \sum_{k=0}^{n} \binom{n}{k} a^{n-k} b^k$$

Random Walk

- For n → ∞
- Gaussian (Normal) distribution
  - Mean = $\bar{x}$, inflection point at σ
  - σ : Standard deviation (σ^2 : Variance)

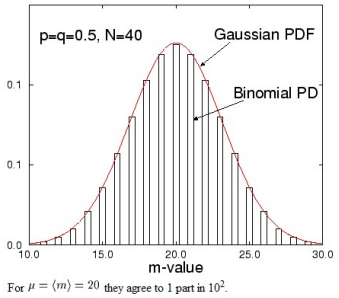
$$f^G(x;\bar{x},\sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{(x-\bar{x})^2}{2\sigma^2}\right\}$$

$$\int_{-\infty}^{\infty} (x-\bar{x})^2 f^G(x;\bar{x},\sigma)dx = \sigma^2$$



Pascal triangle

				1					→ k
0:				1					
1:				1	1				
2:				1	2	1			
n 3:				1	3	3	1		
4:			1	4	6	4	1		
5:			1	5	10	10	5	1	
2^n 6:		1	6	15	20	15	6	1	
7:	1	7	21	35	35	21	7	1	
8:	1	8	28	56	70	56	28	8	1



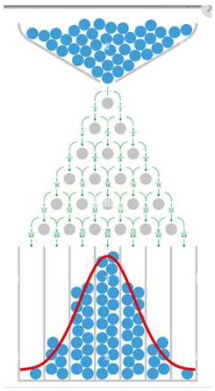
For $\mu = \langle m \rangle = 20$ they agree to 1 part in 10^2.

http://www2.ph.ed.ac.uk/~alastair/probstats/contents/fundamentaldists/gaussian/node1.html

Random Walk: Galton board

- Sir Francis Galton
- Galton box or bean machine

https://www.youtube.com/shorts/Kq7e6cj2nDw

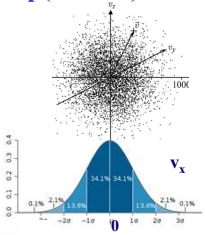


https://www.alamy.com/stock-photo-the-mathematics-of-the-galton-board-with-normal-distribution-and-gaussian-143514169.html?imageid=D8AEC041-DD5A-4D69-8669-5D5C403CDD7C&p=183153&pn=1&searchId=47b65cfbf7a865486dd5064719ec8c0a&searchtype=0

Maxwell-Boltzmann Velocity Distribution

- Probability for velocity in the range $v < \text{vel} < v+dv$: $f(v)dv$
  k^o : Boltzmann constant
- Molecular velocity : Random collision : Gaussian ~ $\exp(-v^2/2\sigma^2)$
  - Maxwell-Boltzmann velocity distribution function

$$f(v_x, v_y, v_z) = \frac{1}{\pi^{3/2}}\left(\frac{m}{2k^oT}\right)^{3/2} \exp\left\{-\frac{m(v_x^2+v_y^2+v_z^2)}{2k^oT}\right\} = \frac{1}{N}\frac{dN_{v_xv_yv_z}}{dv_xdv_ydv_z}$$

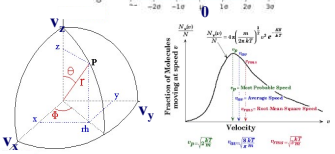


- Distribution of speed v : $v^2 = v_x^2 + v_y^2 + v_z^2$

$$f(v) = \frac{4}{\sqrt{\pi}}\left(\frac{m}{2k^oT}\right)^{3/2} v^2 \exp\left\{-\frac{mv^2}{2k^oT}\right\} = \frac{1}{N}\frac{dN_v}{dv}$$

$$v_m = \left(\frac{2kT}{m}\right)^{1/2} < \bar{v} = \left(\frac{8kT}{\pi m}\right)^{1/2} < v_{rms} = \left(\frac{3kT}{m}\right)^{1/2}$$

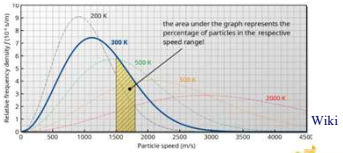
Most probable Mean speed Root mean square



- Distribution of energy $\varepsilon = \frac{1}{2}mv_i^2$

$$f(\varepsilon) = \frac{2}{\sqrt{\pi}}\left(\frac{1}{k^oT}\right)^{3/2} \exp\left(-\frac{\varepsilon}{k^oT}\right) = \frac{1}{N}\frac{dN_\varepsilon}{d\varepsilon}$$

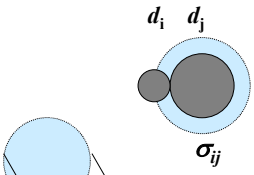
$$\varepsilon_m = \frac{1}{2}k^oT \qquad \bar{\varepsilon} = \frac{3}{2}k^oT$$



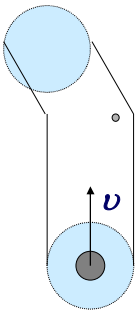
Wiki

Molecular Collision

- Consider 1D head-on collision
- Collision radius $R_{ij} = (d_i+d_j)/2$
- Collision cross-section: $\sigma_{ij} = \pi (d_i+d_i)^2/4$



- Sweep volume / time: $\sigma_{ij}\, \upsilon$
  - i-molecule w/ rel. vel. υ

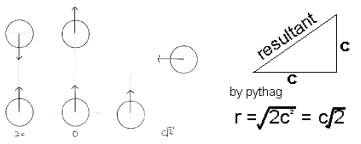


- Collision frequency of i-molecule wrt j :

$$n_j\, \sigma_{ij}\, \upsilon$$

  - n : # of molecule/vol
  - Mean free path $\lambda = \upsilon\, t/n\sigma\upsilon t = 1/n\sigma$
    - (consider υ is the mean vel)

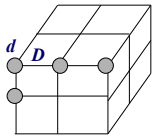
- Total collision frequency : $n_i\, n_j \sigma_{ij}\, \upsilon$



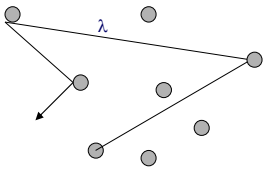
http://www.everyscience.com/Chemistry/Physical/Gases/c.1255.php

Distance between Molecules

- **Avogadro's Number :**
  - **6.022×10^{23} atoms per mol**



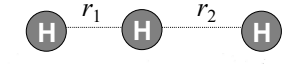
- **Titanium Metal**
  - **Body-centered cubic**
  - **density : 4.5 g/cm^3**
  - **Molecule diameter : d = 2.94 Å**
  - **Edge length D = 0.33 nm = 3.3 Å**

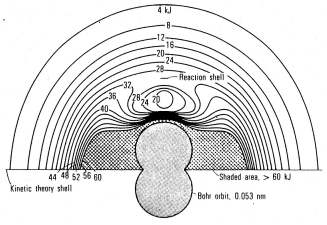


- **Gas : 1 mol at STP 22.4 liter**
  - **Assume cubic distribution**
  - **Molecule diameter : d = 3.1 Å**
  - **Molecular distance D = 3 nm = 30 Å**
  - **Mean free path $\lambda = 1/\sigma n$: 80 nm = 0.08 μm = 800 Å**

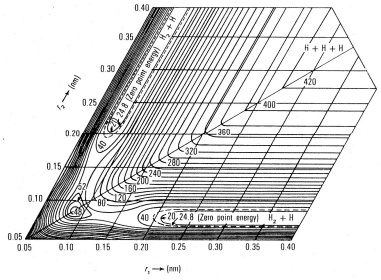
- **Continuum**
  - **Characteristic length of system L >> λ**

Potential Energy

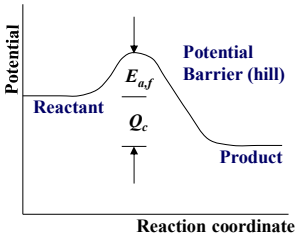


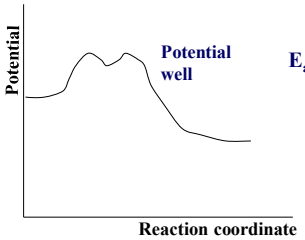


Coulomb force: electron-nucleus
electron-electron, proton-proton



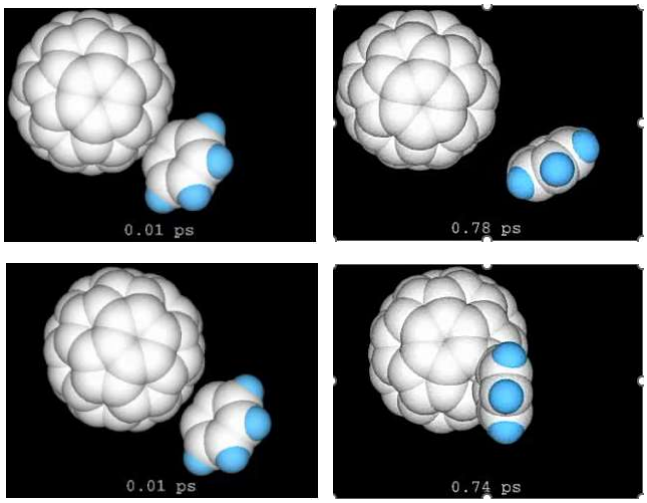
- **Reaction coordinate:**
  - **Steepest descent path / minimum energy path**





$E_{a,b} = E_{a,f} + Q_c$

C60 + C6H6 Reaction



www

Maxwell-Boltzmann Velocity Distribution

- Consider 1D head-on collision
- Probability for velocity in the range $\upsilon < \text{vel} < \upsilon + d\upsilon$: $f(\upsilon)d\upsilon$
- Molecular velocity : Random collision : Gaussian ~ $\exp(-x^2/2\sigma^2)$
  - Maxwell-Boltzmann velocity distribution function (in 1D)

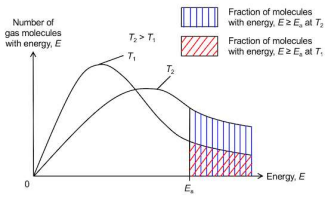
$$f(\upsilon)d\upsilon = c\left(\frac{m_{12}}{\pi k^o T}\right)^{1/2} \exp\left(-\frac{m_{12}\upsilon^2}{2k^o T}\right)d\upsilon$$

m_{12} : reduced mass $1/m_{12} = 1/m_1 + 1/m_2$
k^o : Boltzmann constant

- Average velocity & Collision frequency

$$\bar{V}_{ij} = \left(\frac{8k^o T}{\pi m_{ij}}\right)^{1/2} \qquad Z_{ij} = \pi\sigma_{ij}^2 n_i n_j \left(\frac{8k^o T}{\pi m_{ij}}\right)^{1/2}$$

- Define collision energy $\dfrac{E}{R^o} \equiv \dfrac{(1/2)m_{ij}\upsilon^2}{k^o}$



Reaction Rate : Collision Theory

- RR = total collision freq. × probability ($E > E_a$)

$$\int (\pi n_i n_j \sigma_{ij}^2 \upsilon) \times f(\upsilon) d\upsilon = \int (n_i n_j \sigma_{ij}^2) \times f(E) dE$$

$$\frac{n_i n_j A_{ij}}{R^o} c \left(\frac{k^o}{\pi m_{ij} T} \right)^{1/2} \int_{E_a}^{\infty} \exp\left(-\frac{E}{R^o T} \right) dE = \frac{n_i n_j A_{ij}}{R^o} c \left(\frac{k^o T}{\pi m_{ij}} \right)^{1/2} \exp\left(-\frac{E_a}{R^o T} \right)$$

$$\frac{dn_i}{dt} = -\frac{n_i n_j A_{ij}}{R^o} c \left(\frac{k^o T}{\pi m_{ij}} \right)^{1/2} \exp\left(-\frac{E_a}{R^o T} \right)$$

- Accounting geometric orientation : Steric factor ψ

$$\frac{dn_i}{dt} = -\psi \frac{n_i n_j A_{ij} c}{R^o} \left(\frac{k^o T}{\pi m_{ij}} \right)^{1/2} \exp\left(-\frac{E_a}{R^o T} \right)$$

- Phenomenological $\frac{dc_i}{dt} = -k c_i c_j$ $\quad c = n / A^\circ$ **Concentration [mol/vol]**

$$k(T) = A^\circ \psi A_{ij} \left(\frac{k^o T}{\pi m_{ij}} \right)^{1/2} \exp\left(-\frac{E_a}{R^o T} \right) = A(T) \exp\left(-\frac{E_a}{R^o T} \right) = B T^{1/2} \exp\left(-\frac{E_a}{R^o T} \right)$$

  - $k(T)$: specific reaction rate constant
  - A or B: collision frequency
  - $\exp(-E_a/R^oT)$: probability of $E > E_a$

$$k(T) = A^\circ P \sigma_{ij}^2 \left(\frac{8 k^o T}{\pi m_{ij}} \right)^{1/2} \exp\left(-\frac{E_a}{R^o T} \right)$$

- Steric factor ψ could be $O(1\text{-}10^{-8})$

Reaction Rate

- k-th step RR

$$\omega_k = k_k \prod_{j=1}^{N} c_j^{n_{j,k}} = k_k \prod_{j=1}^{N} \left(\frac{X_j p}{R^o T} \right)^{n_{j,k}}$$

  - $k_k(T)$: specific reaction rate constant for kth step
  - $n_{j,k}$: reaction order of jth species in kth step (overall reaction)

$$CH_4 + 2O_2 \leftrightarrow CO_2 + 2H_2O \qquad \omega = k X_{CH_4}^{n_{CH_4}} X_{O_2}^{n_{O_2}} (p / R^o T)^{n_{CH_4} + n_{O_2}}$$

  - n_j : not necessarily natural number

$$\sum_{j=1}^{N} n_{j,k} = n_{tot}$$ Overall reaction order

- Elementary Reaction
  - Reaction occurs in molecular level ($n_{tot} = 1,2,3$)
  - $n_{j,k}$ molecularity : # molecules involved in collision, natural number

Unimolecular reaction : 1st order
Bimolecular reaction : 2nd order $H + O_2 \rightarrow OH + O$
Termolecular reaction : 3rd order $H + H + M \rightarrow H_2 + M$ (recombination)

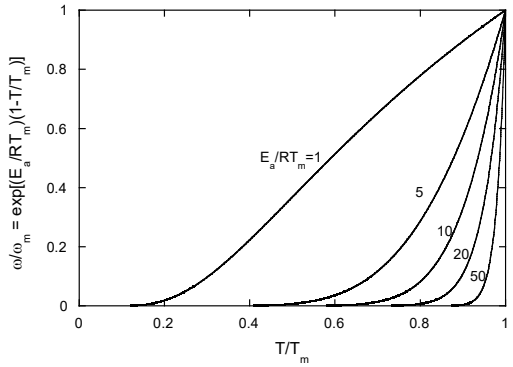
Arrhenius Law

- **Reaction** $k(T) = A(T)\exp\left(-\frac{E_a/R^o}{T}\right) = BT^{\alpha}\exp\left(-\frac{E_a/R^o}{T}\right)$
- **Empirical reaction rate constant**
  - E_a : **Activation energy [kcal/mol], [kJ/mol]**
  - R^o : **Universal gas constant 1.987 cal/mol-K, 8.3 J/mol-K**
  - $A(T)$: **Frequency factor, # of collision per unit time [s^{-1}]**
  - $A(T) = BT^a$, $0 \le a \le 1$: B **frequency factor**
  - $T_a \equiv E_a/R^o$: **Activation temperature**
- **Activation Energy**
  - **Potential hill for reactant to overcome for reaction to take place**
  - **exp($-E_a/R^oT$) : probability of reaction from collision**
  - **HC : overall activation energy $E_a \sim 40$ kcal/mol**
  - **$T_a \equiv E_a/R^o \sim 20{,}000$K :Activation temperature**

Activation Energy

- **RR ratio between T and T_m (max)**

$$\frac{\omega}{\omega_m} = \frac{\exp(-E_a/RT)}{\exp(-E_a/RT_m)} = \exp\left\{\left(\frac{E_a}{RT_m}\right)\left(1-\frac{T_m}{T}\right)\right\}$$



- E_a/R^oT_m = Ar : **Arrhenius number**
- **Ar $\rightarrow \infty$: Flame sheet limit (Large activation energy limit)**

Sample Calculations: Molecules

- O_2 molecules at 1 atm
  - Maxwell-Boltzmann : Avg. velocity
  - Avogadro number $N_A = 6.022 \times 10^{23}$ /mole
  - $d = 3.1 \times 10^{-10}$ m, $\sigma = 3.02 \times 10^{-19}$ m^2
  - $m = 5.32 \times 10^{-23}$ g $= 5.32 \times 10^{-26}$ kg

Temp [K]	300	1000	2000
n [particles/m^3]	2.69×10^{25} 2.7×10^{19}/cm^3	0.806×10^{25}	0.403×10^{25} 0.4×10^{19}/cm^3
Avg. v [m/s]	445	812	1150
z [coll/s]	3.62×10^{9} 3.6/ns	1.98×10^{9} 1.98/ns	1.40×10^{9} 1.4/ns
λ [m]	0.084×10^{-6} 0.084 µm 84 nm	0.26×10^{-6} 0.26 µm 260 nm	0.58×10^{-6} 0.58 µm 580 nm

$$\bar{v} = \left(\frac{8kT}{\pi m}\right)^{1/2}$$

$$z = n\sigma\bar{v}$$

$$\lambda = \frac{1}{\sqrt{2}\sigma n} = \frac{\bar{v}}{z}$$

$$\bar{v} = \left(\frac{8kT}{\pi m}\right)^{1/2} \propto T^{1/2}$$

$$z = n\sigma\bar{v} \propto PT^{-1/2}$$

$$\lambda = \frac{\bar{v}}{z} \propto \frac{T}{P}$$

Ions have larger σ by Coulomb field

Combustion Waves

- 1D Conservations

Mass
Momentum
Energy

$$\rho_o u_o = \rho_\infty u_\infty$$
$$\rho_o u_o^2 + p_o = \rho_\infty u_\infty^2 + p_\infty$$
$$h_o + u_o^2/2 = h_\infty + u_\infty^2/2$$

- Rayleigh Line

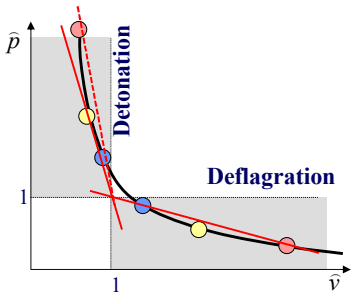
$$\hat{p} = p_\infty / p_o, \quad \hat{v} = v_\infty / v_o, \quad \hat{m} = m/\sqrt{p_o \rho_o}$$

$$(\hat{p} - 1) = -\hat{m}^2(\hat{v} - 1)$$

Crossing wave

$\hat{p}\uparrow \quad \hat{v}\downarrow \quad \hat{\rho}\uparrow$

$\hat{p}\downarrow \quad \hat{v}\uparrow \quad \hat{\rho}\downarrow$



Weak Deflagration $p\downarrow$ $v\uparrow$

CJ Detonation $p\uparrow$ $v\downarrow$

- Hugoniot Line

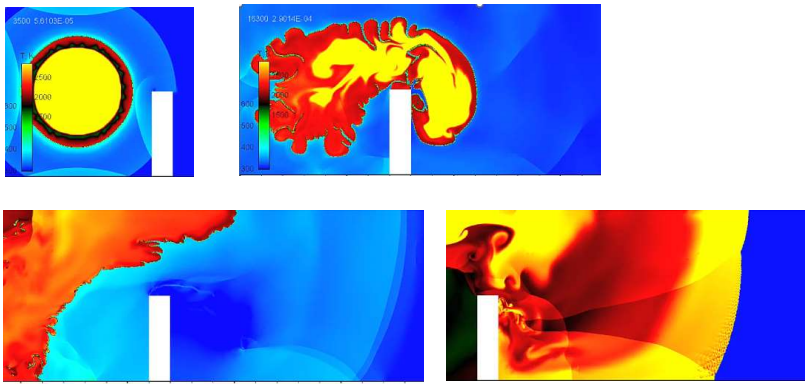
Thermodynamic eq.

Ideal Gas

$$(\hat{p} + \frac{\gamma-1}{\gamma+1})(\hat{v} - \frac{\gamma-1}{\gamma+1}) = \frac{4\gamma}{(\gamma+1)^2} + 2\hat{Q}\frac{\gamma-1}{\gamma+1}, \quad \hat{Q} = (\frac{\rho_o}{p_o})Q$$

Flame Propagation in Premixtures

- E. Oran : H_2 flame with obstacles
- Deflagration to Detonation Transition (DDT)



C-J Detonation Wave

Table 1. CJ-pressure and CJ-detonation velocity for some fuel-air mixtures. Initial conditions 25°C and 1.013 bar (Baker et al. 1983).

	Hydrogen	Ethylene	Propane	Methane
CJ-Pressure (bar)	15.8	18.6	18.6	17.4
CJ-Velocity (m/s)	1968	1822	1804	1802

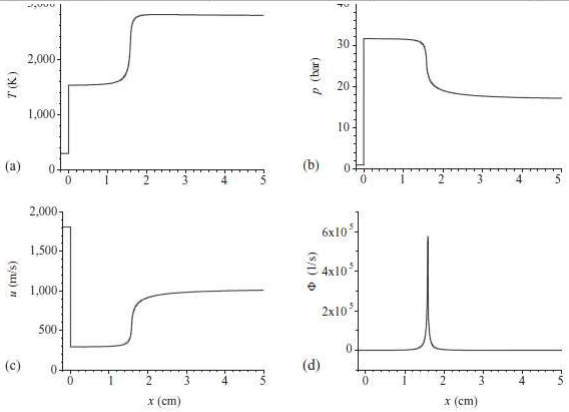
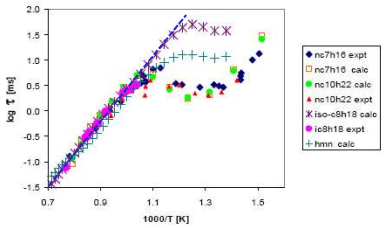


Figure 14.5.3. Calculated ZND structure of a CJ detonation in a stoichiometric methane–air mixture initially at atmospheric conditions: (a) temperature, (b) pressure, (c) gas velocity and (d) rate of energy release are plotted in terms of distance behind the leading shock.

Overall Activation Energy

- **Shock Tube Data**



Farooq

Global reaction rate constants for hydrocarbon fuels*

Fuel	A_0	E_a (kcal/mol)	a	b
CH_4	$1.3\cdot10^9$	48.4	-0.3	1.3
CH_4	$8.3\cdot10^5$	30	-0.3	1.3
C_2H_6	$1.1\cdot10^{12}$	30	0.1	1.65
C_3H_8	$8.6\cdot10^{11}$	30	0.1	1.65
C_4H_{10}	$7.4\cdot10^{11}$	30	0.15	1.6
C_5H_{12}	$6.4\cdot10^{11}$	30	0.25	1.5
C_6H_{14}	$5.7\cdot10^{11}$	30	0.25	1.5
C_7H_{16}	$5.1\cdot10^{11}$	30	0.25	1.5
C_8H_{18}	$4.6\cdot10^{11}$	30	0.25	1.5
C_9H_{20}	$4.2\cdot10^{11}$	30	0.25	1.5
$C_{10}H_{22}$	$3.8\cdot10^{11}$	30	0.25	1.5
CH_3OH	$3.2\cdot10^{11}$	30	0.25	1.5
C_2H_5OH	$1.5\cdot10^{12}$	30	0.15	1.6
C_6H_6	$2.0\cdot10^{11}$	30	-0.1	1.85
C_7H_8	$1.6\cdot10^{11}$	30	-0.1	1.85

* C.K. Westbrook, F. L. Dryer, "Chemical Kinetic Modeling of Hydrocarbon Combustion," Prog. Energy Comb. Sci. vol.10 pp 1-57, 1984. Units of A_0: $(mol/cc)^{1-a-b}/s$

Overall activation energy $E_a \approx 40$ kcal/mol

Overall activation temperature Ta = Ea/R ≈ 20,000 K

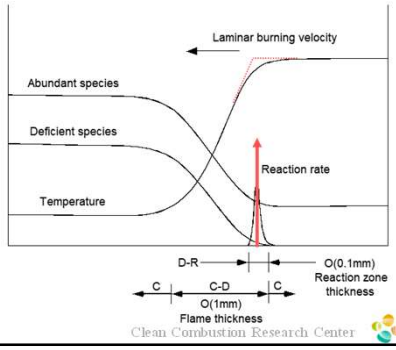
Collision Frequency and Probability

- **Premixed flame 2000K**

$$z = n\sigma\bar{v} \propto PT^{-1/2}$$

  - **Collision frequency 1/ns =10^9/s**
  - **Probability E > E_a** $\exp(-E_a/RT) = \exp(-20{,}000/2000) = 5\times10^{-5}$
  - **Time required for complete reaction (1/5)x10^{-4} s = 0.02 ms**
- **Detonation wave 30 bar 2000 K**
  - **collision frequency 1/ns =30x10^9/s**
  - **Probability E > E_a** $\exp(-E_a/RT) = \exp(-20{,}000/2000) = 5\times10^{-5}$
  - **Time required for complete reaction (1/5)x10^{-4} s /30= 0.02 ms/30 = 2 μs**

	Deflagration	Detonation
Flame Thickness	O(1mm)	O(2cm)
Reaction zone thickness	O(0.1 mm)	O(2 mm)
Flame speed (unburned)	O(40 cm/s)	O(2 km/s)
Flame speed (burnt)	O(250 cm/s)	
Residence time in reaction zone	0.04 ms	1 μs



Transport Phenomena

Diffusion Process

- **Transport by random molecular collision**
  - **Δt: characteristic collision time $\Delta t = (1/z)$**
  - **RMS translational distance : mean free path λ**
  - **RMS translational distance after n step:**
- **Central limit theorem: Walker's position: Variance**
  - **ε : Size of random walk step**
  - **Δt : time between successive step**

$$\sigma = \sqrt{t}\frac{\varepsilon}{\sqrt{\Delta t}}$$

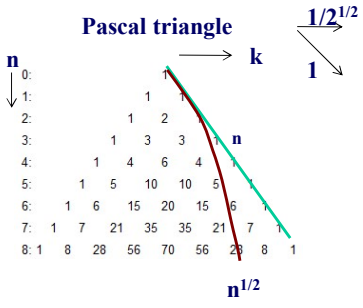
- **Molecular process : Diffusivity**

$$\varepsilon = \lambda/\sqrt{2} \quad \Delta t = 1/z\lambda = \bar{v}/z$$
$$D = \frac{1}{3}\lambda^2 z = \frac{1}{3}\bar{v}\lambda$$

- **Diffusion length ~ $t^{1/2}$**

Ref: Diffusion equation

$$\frac{\partial Y}{\partial t} = D\frac{\partial^2 Y}{\partial z^2} \qquad \eta = \frac{z}{\sqrt{2Dt}}$$



Diffusion Equations

- Governing equations: T=D+C+R

$$\frac{\partial Y}{\partial t} = A\frac{\partial^2 Y}{\partial z^2} + B\frac{\partial Y}{\partial z} + R$$

- Special cases
  - T=D : Diffusion equation

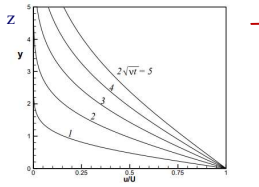
$$\frac{\partial u}{\partial t} = \nu\frac{\partial^2 u}{\partial z^2}$$

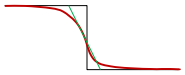
    - Rayleigh problem (Stokes first problem)
      - ✓ Impulsive motion infinite flat plate in semi-infinite fluids
      - ✓ Momentum diffusion
    - Thermal diffusion
    - Mass diffusion

$$\eta = \frac{z}{\sqrt{Dt}} \qquad u(x,t) = g(\eta)$$

$$\frac{d^2 g}{d\eta^2} + \frac{\eta}{2}\frac{dg}{d\eta} = 0$$

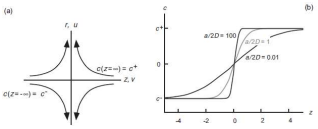
$$u(x,t) \sim \mathrm{erf}\left(\frac{z}{2\sqrt{Dt}}\right)$$





  - Counterflow: Diffusive convective (D=C)
    - $v = az$
    - a: strain rate (s^{-1})

$$D\frac{\partial^2 Y}{\partial z^2} + v\frac{\partial Y}{\partial z} = 0$$



Warnatz et al., Combustion

Momentum Transport

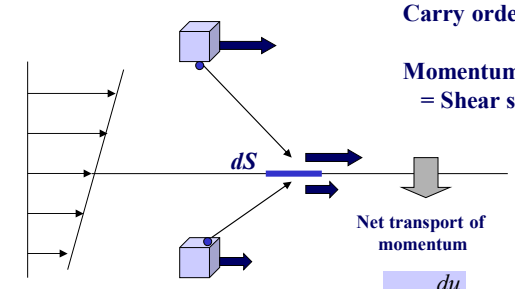
- Momentum Transport

Random momentum (related to T)
Ordered momentum (bulk velocity)

Collision frequency Z generates free path
Distribution of free path (dN~Ndx)
Survival equation
(Mean free path)
Solid angle heading toward dS
Molecular flux

Carry ordered momentum from origin

Momentum crossing/time-area
= Shear stress



$$\tau = \mu\frac{du}{dy}$$

$$\bar{v} = \sqrt{\frac{8}{\pi}\frac{kT}{m}}$$

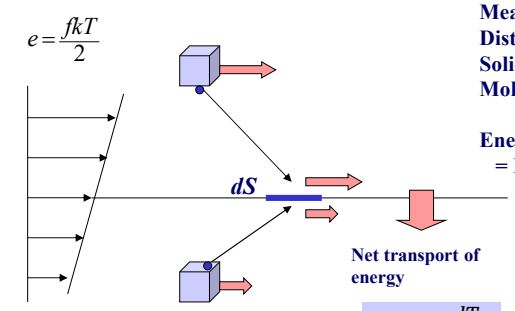
$$\mu = \frac{1}{3}nm\bar{v}\lambda = \frac{2}{3\sigma}\left(\frac{2mkT}{\pi}\right)^{1/2}$$

$$\mu = \frac{1}{3}nm\bar{v}\bar{l} = \frac{1}{3}\rho\bar{v}\lambda$$

$$\nu = \frac{1}{3}\bar{v}\lambda$$

Energy Transport

- **Energy Transport**



Collision frequency
Mean free path
Distribution of free path
Solid angle
Molecular flux

Energy crossing/time-area
= Heat flux

$$q = -\lambda \frac{dT}{dy}$$

$$\lambda = \frac{1}{6} n\bar{v}\lambda fk = \frac{1}{3}\frac{fk}{\sigma}\left(\frac{2kT}{\pi m}\right)^{1/2}$$

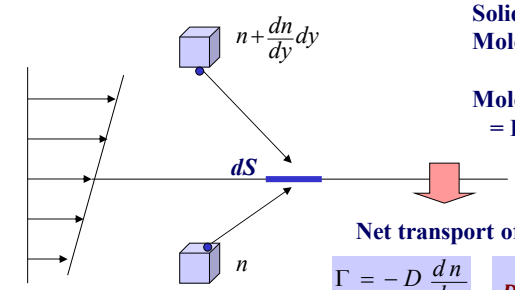
$$\lambda = \frac{1}{6} n\bar{v}\lambda fk = \frac{1}{3}\bar{v}\lambda n\frac{fk}{2} = \frac{1}{3}\bar{v}\lambda nm\frac{fk}{2m} = \frac{1}{3}\bar{v}\lambda\rho c_v$$

$$\alpha = \frac{\lambda}{\rho c_v} = \frac{1}{3}\bar{v}\lambda$$

Note based on c_v

Mass Transport

- **Mass Transport**



Collision frequency
Mean free path
Distribution of free path
Solid angle
Molecular flux

Molecule crossing/time-area
= Diffusion flux

Net transport of mass

$$\Gamma = -D\frac{dn}{dy}$$

$$D = \frac{1}{3}\bar{v}\lambda = \frac{2}{3}\frac{1}{n\sigma}\left(\frac{2kT}{\pi m}\right)^{1/2}$$

Mass Diffusivity

$$D = \frac{1}{3}\bar{v}\lambda$$

$$\bar{v} \sim T^{1/2} \quad l \sim T/P \quad D \sim T^{3/2}/P \quad \rho D \sim T^{1/2}$$

More complete theory

- So far we have

$$\mu = \frac{1}{3} nm\bar{v}\lambda = \frac{2}{3\sigma}\left(\frac{2mkT}{\pi}\right)^{1/2} \qquad \lambda = \frac{1}{6} n\bar{v}\lambda f_k = \frac{1}{3}\frac{f_k}{\sigma}\left(\frac{2kT}{\pi m}\right)^{1/2}$$

$$D = \frac{1}{3}\bar{v}\lambda = \frac{2}{3}\frac{1}{n\sigma}\left(\frac{2kT}{\pi m}\right)^{1/2}$$

- More complete theory provides

$$\mu = \frac{5}{16\sigma}(\pi mkT)^{1/2} \qquad \lambda = \frac{25}{64}\frac{f_k}{\sigma}\left(\frac{\pi kT}{m}\right)^{1/2} \qquad D = \frac{3}{8}\frac{1}{n\sigma}\left(\frac{\pi kT}{m}\right)^{1/2}$$

Nondimensional Numbers

Momentum	$\mu = \frac{1}{3} nm\bar{v}\bar{l} = \frac{2}{3\sigma}\left(\frac{2mkT}{\pi}\right)^{1/2}$	$\mu \sim T^{\alpha}$	
Energy	$\lambda = \frac{1}{6} n\bar{v}\bar{l}f_k = \frac{1}{3}\frac{f_k}{\sigma}\left(\frac{2kT}{\pi m}\right)^{1/2}$	$\lambda/C_p \sim T^{\alpha}$	α = 1/2 theoretically 0.75 experimentally
Mass	$D = \frac{1}{3}\bar{v}\bar{l} = \frac{2}{3}\frac{1}{n\sigma}\left(\frac{2kT}{\pi m}\right)^{1/2}$	$\rho D \sim T^{\alpha}$	*Independent of pressure*

Prandtl No $\mathrm{Pr} = \dfrac{\text{Rate of Momentum Diffusion}}{\text{Rate of Heat Diffusion}} = \dfrac{\mu}{\lambda/C_p} = \dfrac{\nu}{\alpha}$

Schmidt No $\mathrm{Sc} = \dfrac{\text{Rate of Momentum Diffusion}}{\text{Rate of Mass Diffusion}} = \dfrac{\mu}{\rho D} = \dfrac{\nu}{D}$

Lewis No $\mathrm{Le} = \dfrac{\text{Rate of Heat Diffusion}}{\text{Rate of Mass Diffusion}} = \dfrac{\lambda/C_p}{\rho D} = \dfrac{\alpha}{D}$

Insensitive to temp. & pressure variations

Primary Diffusion Process

- **Primary diffusion rate**
  - Characteristic spreading of area per unit time [L^2/T]

Process	Driving force	Transport coefficient	Diffusion rate [cm^2/s]
momentum	velocity gradient	viscosity μ	kinematic viscosity $\nu = \mu/\rho$
energy	temperature gradient	thermal conductivity λ	thermal diffusivity $\alpha = \lambda/\rho C_p$
mass	concentration gradient	binary diffusion coeff. D_{ij}	Mass diffusivity D_{ij}

- **Soret effect**
  - Mass diffusion arising from temp gradient
  - Thermal diffusion
  - Can be non-negligible for light molecule, e.g., hydrogen
- **Dufour effect**
  - Heat diffusion from concentration gradient
  - Generally negligible compared to primary diffusion

Diffusive Transport Coefficient: Mixture

Wilke's formula

$$\mu = \sum_{j=1}^{N} \mu_j \left(1 + \frac{\sqrt{2}}{4X_j} \sum_{k \neq j} X_k \phi_{jk} \right)^{-1} \qquad \phi_{jk} = \left[1 + \left(\frac{\mu_j}{\mu_k} \right)^{1/2} \left(\frac{W_k}{W_j} \right)^{1/4} \right]^2 \Big/ \left[1 + \left(\frac{W_k}{W_j} \right) \right]^{1/2}$$

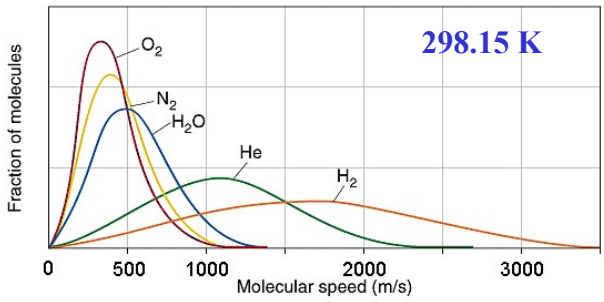
$$\lambda = \sum_{j=1}^{N} \lambda_j \left[1 + \frac{1}{2\sqrt{2}X_j} \sum_{k \neq j} X_k \phi_{jk} \right]^{-1}$$

Simple formula

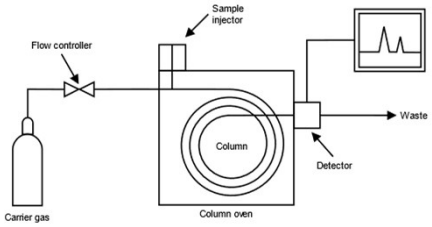
$$\mu = \frac{1}{2} \left(\sum_{j=1}^{N} X_j \mu_j + \frac{1}{\sum_{j=1}^{N} X_j / \mu_j} \right)$$

$$\lambda = \frac{1}{2} \left(\sum_{j=1}^{N} X_j \lambda_j + \frac{1}{\sum_{j=1}^{N} X_j / \lambda_j} \right)$$

Molecular speed distribution



https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Map%3A_Physical_Chemistry_(McQuarrie_and_Simon)/27%3A_The_Kinetic_Theory_of_Gases/27.3%3A_The_Distribution_of_Molecular_Speeds_is_Given_by_the_Maxwell-Boltzmann_Distribution



https://en.wikipedia.org/wiki/Gas_chromatography

Governing Equations

Momentum Equation

Compressible

$$\rho\left(\frac{\partial \vec{v}}{\partial t}+\vec{v}\cdot\nabla\vec{v}\right)=-\nabla p+\nabla\cdot\left[\mu\{(\nabla\vec{v})+(\nabla\vec{v})^T-\frac{2}{3}\mu(\nabla\cdot\vec{v})\|U\|\right]+\rho\vec{f}$$

$$\rho\left(\frac{\partial u_i}{\partial t}+u_k\frac{\partial u_i}{\partial x_k}\right)=-\frac{\partial p}{\partial x_i}+\frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}\mu\delta_{ij}\frac{\partial u_k}{\partial x_k}\right]+\rho f_j$$

$(\nabla\vec{v})=\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}$ Diadic

Navier-Stokes Equation

Williams

Incompressible ($\nabla\cdot v = 0$), const μ

$$\rho\left(\frac{\partial \vec{v}}{\partial t}+\vec{v}\cdot\nabla\vec{v}\right)=-\nabla p+\mu\nabla^2\vec{v}+\rho\vec{f}$$

Transient Convective Pressure Gradient Viscous Diffusion Body Force

Nonlinear

Mass averaged velocity

Species Conservation Equation

- **Molecular velocity : v_i**
- **Mass averaged velocity : v**
- **Diffusion velocity of species i : V_i**

$$\vec{v}_i=\vec{v}+\vec{V}_i$$
$$\vec{v}\equiv\Sigma Y_i\vec{v}_i=(\Sigma Y_i)\vec{v}+(\Sigma Y_i\vec{V}_i)$$
$$\Sigma Y_i\vec{V}_i=0$$

$$\rho\frac{\partial Y_i}{\partial t}+\rho\vec{v}\cdot\nabla Y_i=-\nabla\cdot(\rho Y_i\vec{V}_i)+\omega_i$$

Diffusion Velocity $\mathbf{V}_i$:

$$\nabla X_i=\sum_{j=1}^{N}\left(\frac{X_iX_j}{D_{i,j}}\right)(\mathbf{V}_j-\mathbf{V}_i)+(Y_i-X_i)\left(\frac{\nabla p}{p}\right)+\left(\frac{\rho}{p}\right)\sum_{j=1}^{N}Y_iY_j(\mathbf{f}_i-\mathbf{f}_j)$$

Molecular diffusion — Pressure gradient diffusion — Body force diffusion

$$+\sum_{j=1}^{N}\left[\left(\frac{X_iX_j}{\rho D_{i,j}}\right)\left(\frac{D_{T,j}}{Y_j}-\frac{D_{T,i}}{Y_i}\right)\right]\left(\frac{\nabla T}{T}\right),\quad i=1,\ldots,N\quad.\qquad(2.5)$$

Soret diffusion

Williams

Governing Equations: Summary

- **Energy** $\rho(\frac{\partial e}{\partial t}+\vec{v}\cdot\nabla e)=-\nabla\cdot\vec{q}-p(\nabla\cdot\vec{v})$
- **Species** $\rho\frac{\partial Y_i}{\partial t}+\rho\vec{v}\cdot\nabla Y_i=-\nabla\cdot(\rho Y_i\vec{V}_i)+\omega_i$
- **Constitutive Relations**
  - **Fick's Law** $\vec{V}_i=-D_i\nabla\ln Y_i$ $\rho\frac{\partial Y_i}{\partial t}+\rho\vec{v}\cdot\nabla Y_i=\nabla\cdot(\rho D_i\nabla Y_i)+\omega_i$
  - **Fourier's Law**

$$\vec{q}=-\lambda\nabla T+\rho\sum_{i=1}^{N}Y_i h_i\vec{V}_i$$

– **Enthalpy flow wrt mass-averaged motion**
–**Radiation neglected**

$$e=\sum_{i=1}^{N}Y_i h_i-p/\rho$$

$$h_i=h_i^o+h_i^s(T;T^o)=h_i^o+\int_{T^o}^{T}C_{p,i}dT$$

$$\omega_i=W_i\hat{\omega}_i \qquad \omega_i=W_i\sum_{k=1}^{N}(\nu''_{i,k}-\nu'_{i,k})B_k T^{\alpha_k}\exp(-E_k/R^oT)\prod_{j=1}^{N}c_j^{\nu'_{j,k}}$$

$$c_j=(X_j p/R^oT)$$

$$X_i=\frac{Y_i/W_i}{\sum Y_j/W_j}=\frac{Y_i/W_i}{1/\bar{W}}$$

Energy Equation

- **Time rate of change of energy + Energy convection = Heat flux + Work (pressure)**

$$\frac{\partial}{\partial t}(\rho e_t)=-\frac{\partial}{\partial x}(\rho u e_t)-\frac{\partial}{\partial y}(\rho v e_t)-(\frac{\partial q_x}{\partial x}+\frac{\partial q_y}{\partial y})-\{\frac{\partial}{\partial x}(pu)+\frac{\partial}{\partial y}(pv)\}$$

$$\frac{\partial}{\partial t}(\rho e_t)+\nabla\cdot(\rho\vec{v}e_t)=-\nabla\cdot\vec{q}-\nabla\cdot(p\vec{v})$$

- **Mechanical energy equation: Momentum eq (·v)**

$$\rho\frac{d}{dt}(\frac{v^2}{2})=-\vec{v}\cdot\nabla p+BFW+VFW$$

- **Energy Equation (combustion)**

$$\rho\frac{de}{dt}=\rho(\frac{\partial e}{\partial t}+\vec{v}\cdot\nabla e)=-\nabla\cdot\vec{q}-p(\nabla\cdot\vec{v})$$

Heat Flux Vector **q**:

$$\mathbf{q}=-\lambda\nabla T+\rho\sum_{i=1}^{N}h_i Y_i\mathbf{V}_i+R^oT\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{X_j D_{T,i}}{W_i D_{i,j}}\right)(\mathbf{V}_i-\mathbf{V}_j)+\mathbf{q}_R$$

Fourier Conduction — **Diffusion by** $\vec{v}_i-\vec{v}=\vec{V}_i$ — **Dufour effect** — **Radiation**

Governing Equations

- **Assume** $c_{p,i} = c_p$

$$h_i = h_i^o + h^s$$
$$e = \sum Y_i h_i^o + h^s - p/\rho$$
$$\vec{q} = -\lambda \nabla T + \rho \sum_{i=1}^{N} Y_i h_i^o \vec{V}_i \quad (\because \sum Y_i \vec{V}_i = 0)$$

- **Energy Eq.**

$$\rho \frac{\partial}{\partial t}(\sum Y_i h_i^o + h^s - p/\rho) + \rho \vec{v} \cdot \nabla (\sum Y_i h_i^o + h^s - p/\rho) = -\nabla \cdot \vec{q} - p(\nabla \cdot \vec{v})$$
$$\rho \frac{\partial h^s}{\partial t} + \rho \vec{v} \cdot \nabla h^s = \nabla \cdot (\lambda \nabla T) + \rho \frac{\partial (p/\rho)}{\partial t} + \rho \vec{v} \cdot \nabla (p/\rho) - p(\nabla \cdot \vec{v}) \quad (= \frac{dp}{dt})$$
$$- \{\rho \frac{\partial}{\partial t}(\sum Y_i h_i^o) + \rho \vec{v} \cdot \nabla (\sum Y_i h_i^o) + \nabla \cdot (\rho \sum Y_i h_i^o \vec{V}_i)\} \quad (= \sum h_i^o \omega_i)$$

Multiply h_i^o and sum over i

$$\rho \frac{\partial h^s}{\partial t} + \rho \vec{v} \cdot \nabla h^s - \nabla \cdot (\lambda \nabla T) = -\sum h_i^o \omega_i + \frac{dp}{dt}$$

$$\rho \frac{\partial Y_i}{\partial t} + \rho \vec{v} \cdot \nabla Y_i - \nabla \cdot (\rho D_i \nabla Y_i) = \omega_i$$

Flow system w/ near const p

Shvab-Zel'dovich Formulation (1-step)

$$\rho \frac{\partial Y_i}{\partial t} + \rho \vec{v} \cdot \nabla Y_i - \nabla \cdot (\rho D_i \nabla Y_i) = \omega_i$$

$$\rho \frac{\partial (C_p T)}{\partial t} + \rho \vec{v} \cdot \nabla (C_p T) - \nabla \cdot \{\frac{\lambda}{C_p} \nabla (C_p T)\} = -\{\sum h_i^o W_i (\nu_i'' - \nu_i')\} \omega$$

- **Define**

$$\tilde{Y}_i = \frac{Y_i [W_F (\nu_F'' - \nu_F')]}{W_i (\nu_i'' - \nu_i')} \qquad \tilde{T} = \frac{C_p T [W_F (\nu_F'' - \nu_F')]}{\sum h_i^o W_i (\nu_i'' - \nu_i')} = \frac{C_p T}{Q}$$

$$\tilde{Y}_F = Y_F \qquad \tilde{Y}_O = Y_O / \sigma$$

σ: stoichiometric oxidizer to fuel mass ratio

Q : Heat of combustion per unit mass of fuel consumed

$$L_i(\tilde{Y}_i) = \omega [W_F (\nu_F'' - \nu_F')] = \omega_F$$
$$L_T(\tilde{T}) = -\omega [W_F (\nu_F'' - \nu_F')] = -\omega_F$$

If $\frac{\lambda/\rho C_p}{D_i} = \frac{\alpha}{D_i} = Le_i = 1$ **Lewis number**

$L_i = L_T = L$ $\quad L\{\tilde{Y}_i + \tilde{T}\} = 0$ **Shvab-Zel'dovich Formulation**

$\beta_i \equiv \tilde{Y}_i + \tilde{T}$ **Coupling Function**

Sigma & Q for HC

σ and Q

- **Stoichiometric oxidizer to fuel mass ratio σ**
  - $H_2 + (1/2)O_2 \rightarrow H_2O$: $32 \times (1/2)/2$ $\sigma = 8$
  - $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$: $32 \times 2/16$ $\sigma = 4$
  - $C_nH_{2n+2} + \{n+(n+1)/2\}\mathbf{O_2} \rightarrow nCO_2 + (n+1)H_2O$
    : $\{16 \times (3n+1)\} / (12n+2n+2)$ $\sigma = \mathbf{3.43}$ as $n \rightarrow \infty$
  - $C_nH_{2n+2} + \{n+(n+1)/2\}\{\mathbf{O_2 + 3.76N_2}\} \rightarrow nCO_2 + (n+1)H_2O + N_2$
    : $\{(16 + 3.76 \times 14)(3n+1)\} / (12n+2n+2) \rightarrow$ AF = **14.7** as $n \rightarrow \infty$

- **Heat of combustion per unit mass of fuel consumed Q**

$H_2(g)$	28,900 cal/g		
$CH_4(g)$	11,985		
$C_2H_6(g)$	11,375	C_2H_2	11,886
$C_3H_8(g)$	11,103	$C_6H_6(l)$	9,662
$C_4H_{10}(g)$	10,955	$C_2H_5OH(l)$	7,086

….

C_mH_{2m+2} ~ 10,000 (10 kcal/g)

TOE (ton of oil equivalent)

Damköhler Number

- **Energy & Species Equations**
  - **Heat & mass transport**
  - **Reaction**
  - **Convection + Diffusion = Reaction**

- **Characteristic times**
  - **Characteristic flow time: t_f**
    - **Convection $t_c = [L/U_o]$, Diffusion $t_d = [L^2/\alpha]$**
  - **Characteristic reaction time $t_r = [1/B]$**

- **Damköhler number**

$$Da \equiv \frac{\text{characteristic flow time } t_f}{\text{characteristic reaction time } t_r} = \begin{cases} \frac{B}{U_o/L} & \text{group I, III} \\ \frac{B}{\alpha/L^2} & \text{group II, IV} \end{cases}$$

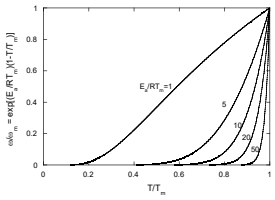
species, energy

Flame Sheet Limit

- **Nondimensional number**
  - **Limiting behavior (ignition/extinction)**
  - **Effect of large (small) parameter**
- **Convection + Diffusion = Da × Reaction**
- **Damköhler number limits :**

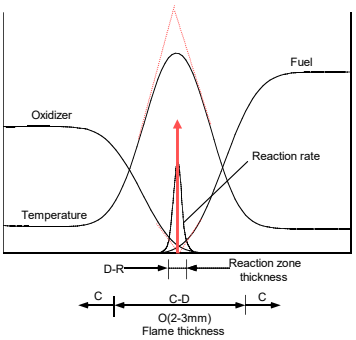
$$\mathrm{Da} \equiv \frac{\text{characteristic flow time } \ t_f}{\text{characteristic reaction time } \ t_r}$$

  - **Da → 0 : Frozen flow limit**
  - **Da → ∞ : Flame sheet limit (equilibrium flow)**
  - **Chemical reaction is confined at infinitesimally thin sheet**
- **Large Activation Energy** $E_a \to \infty$

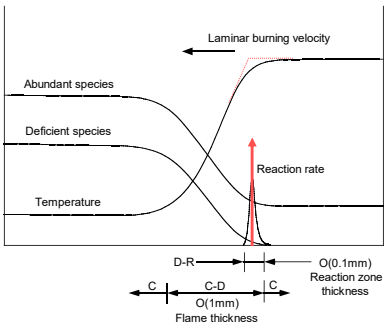


Typical Flame Structures

Diffusion Flame

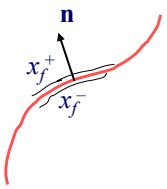


Premixed Flame



Flame Sheet Formulation

- **Background:**
  - **Continuity of T & Y_i**
  - **Jump for their gradients due to singularity (source of heat & sink of reactants)**
  - **Weak discontinuity**



- **Integrate direction normal to flame**

$$\frac{\partial(\rho\tilde{T})}{\partial t}+\frac{\partial}{\partial n}\{\rho u_n\tilde{T}-\frac{\lambda}{C_p}\frac{\partial\tilde{T}}{\partial n}\}=-\omega_F,\quad \frac{\partial(\rho\tilde{Y}_i)}{\partial t}+\frac{\partial}{\partial n}\{\rho u_n\tilde{Y}_i-\rho D_i\frac{\partial\tilde{Y}_i}{\partial n}\}=\omega_F$$

$$\frac{\partial}{\partial t}\{\rho(\tilde{T}+\tilde{Y}_i)\}+\frac{\partial}{\partial n}\{\rho u_n(\tilde{T}+\tilde{Y}_i)\}-\frac{\partial}{\partial n}(\frac{\lambda}{C_p}\frac{\partial\tilde{T}}{\partial n})-\frac{\partial}{\partial n}(\rho D_i\frac{\partial\tilde{Y}_i}{\partial n})=0$$

$$\int_{x_f^-}^{x_f^+}\frac{\partial}{\partial t}\{\rho(\tilde{T}+\tilde{Y}_i)\}dx+\int_{x_f^-}^{x_f^+}d\{\rho u_n(\tilde{T}+\tilde{Y}_i)\}-\int_{x_f^-}^{x_f^+}d\{\frac{\lambda}{C_p}\frac{\partial\tilde{T}}{\partial n}+\rho D_i\frac{\partial\tilde{Y}_i}{\partial n}\}=0$$

Jump Conditions

$$\left[\frac{\lambda}{C_p}\frac{\partial\tilde{T}}{\partial n}\right]_{x_f^-}^{x_f^+}=-\left[\rho D_i\frac{\partial\tilde{Y}_i}{\partial n}\right]_{x_f^-}^{x_f^+}$$

$$\left[\rho D_F\frac{\partial\tilde{Y}_F}{\partial n}\right]_{x_f^-}^{x_f^+}=\left[\rho D_O\frac{\partial\tilde{Y}_O}{\partial n}\right]_{x_f^-}^{x_f^+}$$

$$\left[\rho D_F\frac{\partial Y_F}{\partial n}\right]_{x_f^-}^{x_f^+}$$

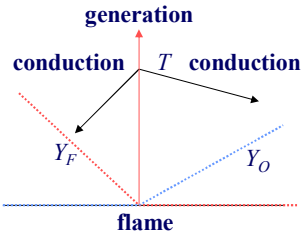
Fuel consumption
Net convection = 0
due to continuity of u & Y_i

$$\left[\lambda\frac{\partial T}{\partial n}\right]_{x_f^-}^{x_f^+}=-Q\left[\rho D_F\frac{\partial Y_F}{\partial n}\right]_{x_f^-}^{x_f^+}$$

Energy balance

$$\left[\rho D_F\frac{\partial Y_F}{\partial n}\right]_{x_f^-}^{x_f^+}=\frac{1}{\sigma}\left[\rho D_O\frac{\partial Y_O}{\partial n}\right]_{x_f^-}^{x_f^+}$$

Stoichiometric consumption



- **Complete consumption of deficient species for PF**
- **Complete consumption of fuel & oxidizer for DF**
  - **Maximum intensity**
- **Shvab-Zel'dovich formulation automatically satisfies the jump conditions**

Kinetic Mechanisms

Gas Research Institute

- **GRI-Mech Version 3.0 7/30/99 CHEMKIN-III format**
- **http://www.gri.org , under 'Basic Research',**

- **5 Elements, 53 Species**
- **ELEMENTS : O H C N AR**
- **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**

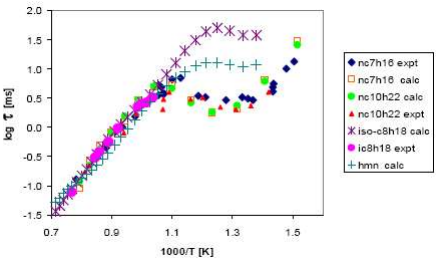
- $k_i = A_i T^{bi} \exp(-E_i/R^o T)$ **[mol-cm^3-s], [kJ/mol]**

```
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
```

Chaperon efficiency

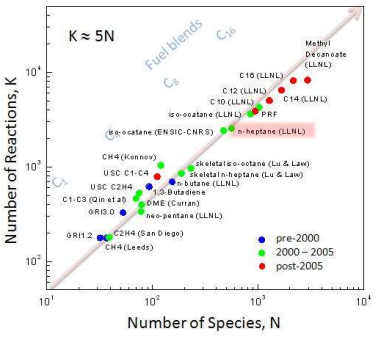
Kinetic Mechanisms

- **Kinetic Mechanisms of Large Molecules**
  - **n-decane: 950 species 3900 reactions**
  - **n-hexadecane : 2100 species 8000 reactions**
  - **Methyl decanoate : 3000 species 8600 reactions**
  - **Methyl stearate (C_{18} methyl ester) : 13000 reactions**



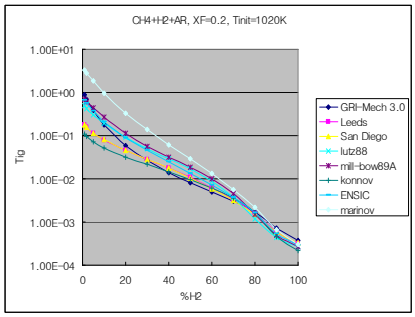
Farooq

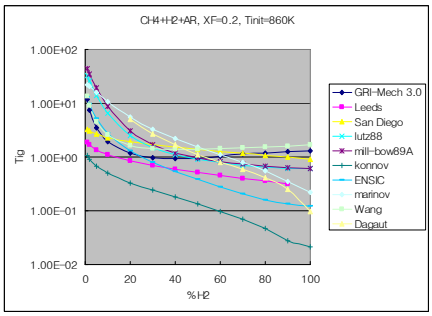
Lu-Law Diagram



Current Kinetic Mechanisms

- Developed based on
  - Shock tube ignition delay at high pressure (20-40 atm)
  - Laminar burning velocity at low pressure (1-10 atm)
  - τ_{ig} near 1 ms is consistent





Hydrogen Oxidation

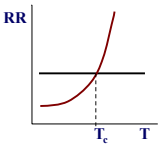
- Initiation
  - Initiation of H radical
  - $H_2 + O_2 \rightarrow HO_2 + H$
  - $H_2 + M \rightarrow H + H + M$
- Hydrogen-Oxygen Chain Reaction
  - Chain cycle of H, O, OH
- Hydroxyl Formation and Consumption : HO_2
- Hydroperoxyl Formation and Consumption : H_2O_2
- Recombination Reactions
  - Three-body recombination : Pressure sensitivity

Hydrogen Oxidation

- H radical formed through initiation
  - $H_2 + M \rightarrow H + H + M$ (E_a = 104.38 kcal/mol)
  - Only need initiation
- Subsequent chain mechanism (generating radical pool)
  - $H + O_2 \rightarrow OH + O$
  - $O + H_2 \rightarrow OH + H$
  - $OH + H_2 \rightarrow H_2O + H$
  - $OH + OH \rightarrow H_2O + O$

Straight chain mechanism
Branched chain mechanism

- Hydroxyl Formation and Consumption : HO_2
  - $H + O_2 + M \rightarrow HO_2 + M$ ($E_a = 0$)
  - Consumption HO_2 + H, O, OH
- Hydroperoxyl Formation and Consumption : H_2O_2
  - $HO_2 + HO_2 \rightarrow H_2O_2 + O2$
  - Consumption H_2O_2 + M, H, O, OH
- Recombination reactions (Three-body)
  - H+H+M→H2+M; O+O+M→O2+M; O+H+M→OH+M; H+OH+M→ H2O+M; $H + O_2 + M \rightarrow HO_2 + M$ ($E_a = 0$)
- Crossover temperature ≈ 1100K
  - $H + O_2 \rightarrow OH + O$ (E_a = 16.44 kcal/mol, relatively high E_a)



Chain Explosion of Hydrogen : Z-curve

1st Limit (Low pressure)
Wall termination dominate
Chain-branching becomes effective
$H + O_2 \rightarrow OH + O$

2nd Limit (Intermediate pressure)
Gas-phase termination
$H + O_2 + M \rightarrow HO_2 + M$

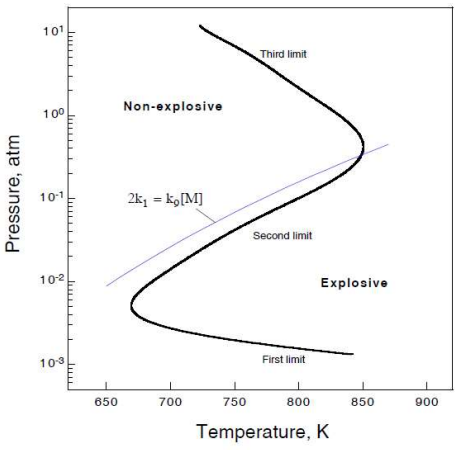
3rd Limit

$HO_2 + H_2 \rightarrow H_2O_2 + H$

$H_2O_2 + M \rightarrow 2OH + M$

High temp above 680°C

HO_2 can not be stable



Law

CO Oxidation Mechanism

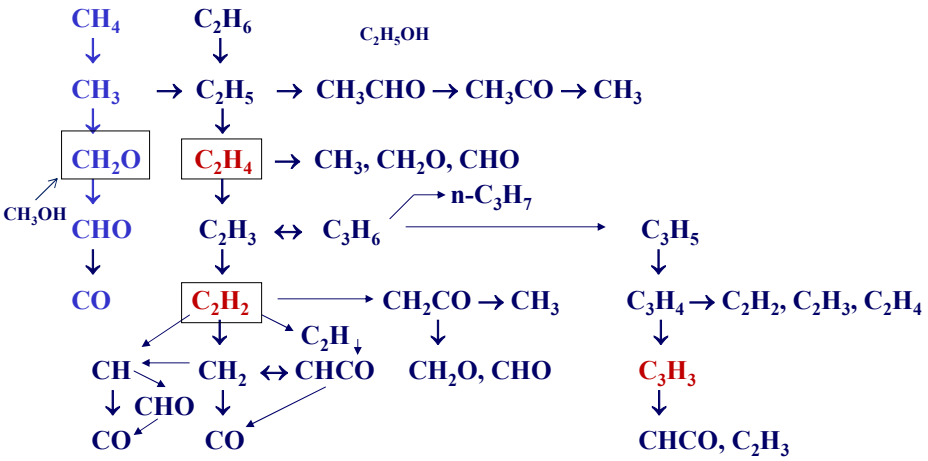
- Reaction with oxygen
  - $CO + O_2 \rightarrow CO_2 + O$
  - *E* very large and very slow (48 kcal/mol)
- If w/ H containing species (20 ppm) : exclusively
  - $CO + OH \rightarrow CO_2 + H$
- Moist air OH source
  - $O_2 + M \rightarrow O + O + M$
  - $O + H_2O \rightarrow OH + OH$
- High pressure
  - $CO + HO_2 \rightarrow CO_2 + OH$
- Overall reaction

$$CO + OH \rightarrow CO_2 + H$$
$$H_2O + H \rightarrow H_2 + OH \quad (PE)$$
$$CO + H_2O \rightarrow CO_2 + H_2$$

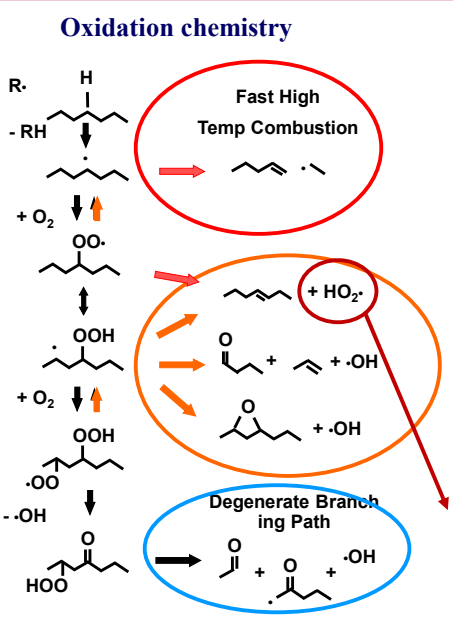
CO/CO_2 Mechanism				
18f	$CO + OH \rightarrow CO_2 + H$	4.400E+06	1.50	– 3.10
18b	$CO_2 + H \rightarrow CO + OH$	4.956E+08	1.50	89.76

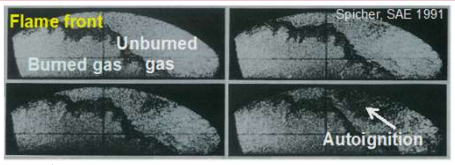
Water-gas shift reaction
OH acts as homogeneous catalyst

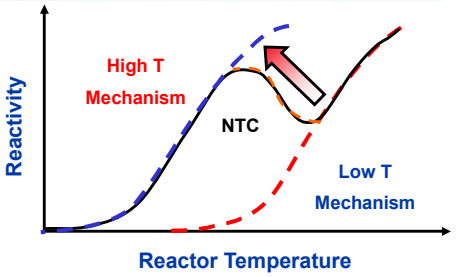
C_1-C_2 Hydrocarbon Oxidation



What causes knock?







HO_2 Radicals lead to the formation of H_2O_2, when the temperature increases $H_2O_2 \rightarrow 2OH$ triggering the transition to high temperature ignition

credit Marco Mehl, LLNL, 2014

Reaction Modeling

- **Arbitrary Approximation**
  - One-step overall reaction : global reaction
  - Thermal point of view: empirical constants
  - Semi-global reaction $\frac{dn_i}{dt} = Ap^a n_F^b n_O^c \exp\left(-E_a / R^o T\right)$
- **Detailed (Full) mechanism**
  - Based on kinetic data
  - Hierarchical : sub-mechanisms H_2, CO etc
  - Kinetic data comprehensive & accurate?
  - Numerical integration
- **Skeletal mechanism**
  - Sensitivity analysis
  - ∂lny/∂lnk (system response parameter/RR const)
- **Systematic reduction**
  - Computationally demanding/ stiff problem
  - Computational singular perturbation (CSP)
  - Quasi-Steady-State Assumption (QSSA)
  - Directed Relation Graph (DRG)

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

$$CH_4 + \tfrac{3}{2}O_2 \rightarrow CO + 2H_2O$$
$$CO + \tfrac{1}{2}O_2 \rightarrow CO_2$$

$$CH_4 + \tfrac{1}{2}O_2 \rightarrow CO + 2H_2$$
$$CO + \tfrac{1}{2}O_2 \rightarrow CO_2$$
$$H_2 + \tfrac{1}{2}O_2 \rightarrow H_2O$$

$$C_mH_{2m+2} \rightarrow \tfrac{m}{2}C_2H_4 + H_2$$
$$C_2H_4 + O_2 \rightarrow 2CO + 2H_2$$
$$CO + \tfrac{1}{2}O_2 \rightarrow CO_2$$
$$H_2 + \tfrac{1}{2}O_2 \rightarrow H_2O$$

Reduced Mechanism

$$3H_2 + O_2 \rightarrow 2H_2O + 2H$$
$$H + H + M \rightarrow H_2 + M$$

$$CH_4 + 2H + H_2O \rightarrow CO + 4H_2$$
$$CO + H_2O \leftrightarrow CO_2 + H_2$$
$$H + H + M \rightarrow H_2 + M$$
$$3H_2 + O_2 \rightarrow 2H_2O + 2H$$

Steady State Approximation

- **Reaction intermediates (Radical species)**
  - **If fast production and consumption : Net rate of production can be low**
  - **Maintained low concentration**

$$\hat{\omega}_i = \sum_{k=1}^{K} (\nu_i'' - \nu_i') \hat{\omega}_k \qquad \hat{\omega}_i = \hat{\omega}_i^+ - \hat{\omega}_i^-$$

when $\left| \dfrac{\omega_{i+} - \omega_{i-}}{\omega_{i+}} \right| \ll 1$

$\omega_{I+} \approx \omega_{i-}$ **Algebraic relation reducing 1 PDE**
Frequently implicit relation

Test required

$$|\hat{\omega}_i| \ll |\hat{\omega}_{i+}|, \quad \left| \frac{dc_i}{dt} \right| \ll |\hat{\omega}_{i+}|$$

- **Partial equilibrium assumption**
  - ***k*-step reaction** $\omega_k^+ \approx \omega_k^-$
  - **Simple algebraic relation**

$H_2 + OH \rightarrow H_2O + H$ $\qquad$ $H_2O + O \rightarrow OH + OH$

Reduced Oxidation Mechanisms

- **Hydrogen Oxidation**

$3H_2 + O_2 \rightarrow 2H_2O + 2H$
$H + H + M \rightarrow H_2 + M$

- **CO Oxidation**

$CO + H_2O \leftrightarrow CO_2 + H_2$

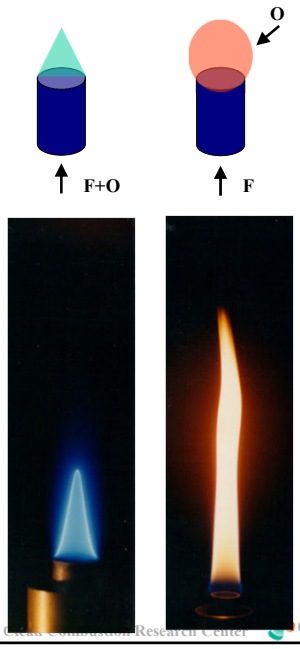
- **CH_4 Reduced Mechanism (4-step)**

$3H_2 + O_2 \rightarrow 2H_2O + 2H$
$H + H + M \rightarrow H_2 + M$
$CO + H_2O \leftrightarrow CO_2 + H_2$
$CH_4 + 2H + H_2O \rightarrow CO + 4H_2$

Flow Geometries for Fundamental Research

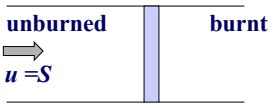
Classification : Mixing

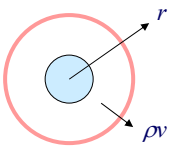
	Premixed Flame	Diffusion Flame
Fuel / Oxidizer	Mixed in molecular level initially	Initially separated Molecular mixing at flame through diffusion and convection
Controlling Mechanism	Reaction Diffusion	Diffusion
Flame Position	Wave propagation	Self-adjust to maximize flame intensity (Stoichiometry)
F/O Consumption at Flame	Complete consumption of lean component	Complete consumption of fuel/oxidizer
Analysis	Finite rate kinetics	Infinite rate kinetics

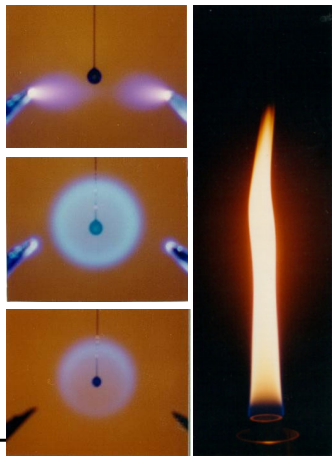


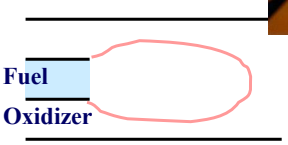
1D Flames & Coflow

- **1D Flames**
  - ρv = const
  - $\rho v r^2$ = const
  - Momentum eq. : pressure field
- **Coflow**
  - v = uniform
  - ρv = uniform
- **Jet**





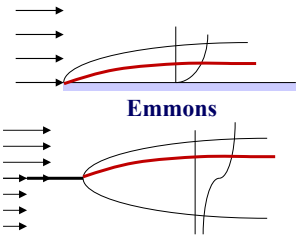




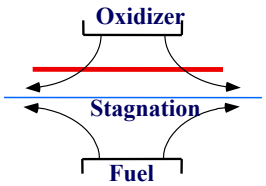
Flow Geometries

- **1D diffusion flame**

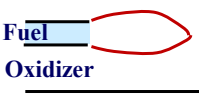
- **Mixing Layer: BL & Shear layer**



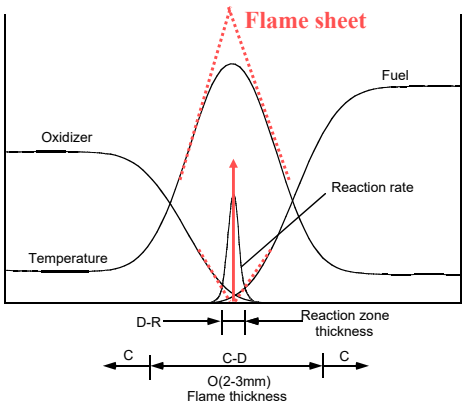
- **Counterflow flame**



- **Coflow / Jet**
  - v = uniform
  - ρv = uniform



Typical Structure of Diffusion Flame



- **Three Zone Structure**
  - **Fuel (Oxidizer) rich zone:**
    - **Relatively cold / negligible reaction**
    - **Transport dominant**
  - **Flame zone**
    - **F & O mix and react very fast**
    - **Source of heat / product**
    - **Sink of reactants**
    - **Flame position adjust to (stoichiometry)**
    - **Finite rate kinetics makes small amount of reactant leakage**

Characteristics of Diffusion Flames

- **Reaction thickness δ_R and diffusion thickness δ_T or δ_M**

$$\delta_R = O\left(\frac{RT_f}{E_a}\delta_T\right), \qquad \delta_R << \delta_T$$

  - **Diffusion $\alpha\partial^2(\bullet)/\partial x^2 \approx \alpha(\bullet)/\delta_R^2$ (Jump in the gradient of parameter)**
  - **Convection $u_o\partial(\bullet)/\partial x \approx u_o(\bullet)/\delta_R$ (Weak discontinuity)**
  - **Reaction zone : Diffusion >> Convection**

- **δ_R is infinitely thin as $E_a \to \infty$**
  - **Since E_a is large but finite, small amount of reactants leak**
  - **Reaction broadening**
  - **Chemical reaction could occur in much faster rate, however, reactants are supplied in slower rate by diffusion**
  - **Diffusion controlled**

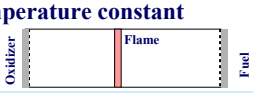
- **Infinite-rate Kinetics : Flame sheet limit**
  - **Most of flame characteristics can be determined**
  - **Flame location, temperature, burning rate**

1D Model Diffusion Flame

- 1D, constant cross-section, constant pressure, steady-state, pure diffusion
- Porous walls maintain concentration and temperature constant

$$\frac{\lambda}{C_p}\frac{d^2\tilde{T}}{dx^2}=\omega_F=[W_F(\nu_F''-\nu_F')]\omega$$

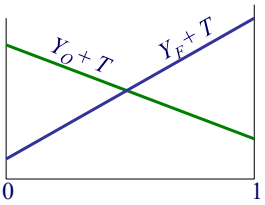
$$\rho D\frac{d^2\tilde{Y}_i}{dx^2}=-\omega_F$$



$x=0;\ \tilde{T}=\tilde{T}_0,\ \tilde{Y}_F=0,\ \tilde{Y}_O=\tilde{Y}_{O,0},\ \tilde{Y}_P=\tilde{Y}_{P,0}$
$x=l;\tilde{T}=\tilde{T}_l,\ \tilde{Y}_F=\tilde{Y}_{F,l}\ \tilde{Y}_O=0,\ \tilde{Y}_P=\tilde{Y}_{P,l}$

- For Le = $\lambda/\rho C_p D = 1$: Schvab-Zel'dovich Analysis

$$\frac{d^2}{dx^2}(\tilde{Y}_i+\tilde{T})=0 \qquad \tilde{Y}_i+\tilde{T}=a_i x+b_i$$



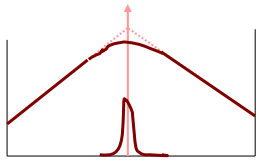
- Applying boundary conditions

$$\tilde{Y}_F+\tilde{T}=(\tilde{T}_l-\tilde{T}_0+\tilde{Y}_{F,l})(x/l)+\tilde{T}_0$$
$$\tilde{Y}_O+\tilde{T}=(\tilde{T}_l-\tilde{T}_0-\tilde{Y}_{O,0})(x/l)+(\tilde{Y}_{O,0}+\tilde{T}_0)$$
$$\tilde{Y}_F-\tilde{Y}_O=(\tilde{Y}_{F,l}+\tilde{Y}_{O,0})(x/l)-\tilde{Y}_{O,0}$$

- Using $Y_i = -T + a_i x + b_i$: $\omega = \omega(T,x)$, substitute to energy equation

$$\frac{\lambda}{C_p}\frac{d^2\tilde{T}}{dx^2}=\omega_F=[W_F(\nu_F''-\nu_F')]\omega=f(T,x)$$

$x=0;\tilde{T}=\tilde{T}_0 : x=l;\tilde{T}=\tilde{T}_l$



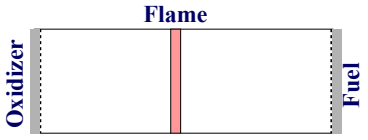
- Nonlinear 2nd order ODE
  - The solution provides flame structure

1D Model : Flame Sheet Solution

- In the flame sheet limit at $x = x_f$

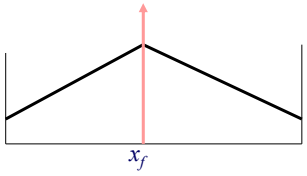
$$\tilde{T}=\tilde{T}_f \ \ \&\ \ \tilde{Y}_{F,f}=\tilde{Y}_{O,f}=0$$

$$\frac{x_f}{l}=\frac{\tilde{Y}_{O,0}}{\tilde{Y}_{F,l}+\tilde{Y}_{O,0}} \qquad \tilde{T}_f=\tilde{T}_0+(\tilde{T}_l-\tilde{T}_0+\tilde{Y}_{F,l})\frac{\tilde{Y}_{O,0}}{\tilde{Y}_{F,l}+\tilde{Y}_{O,0}}$$

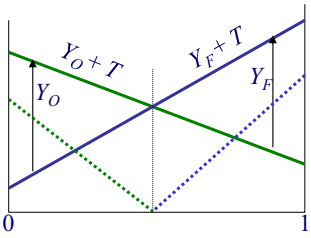


- Temperature profiles

$$0<x<x_f\ ;\ \tilde{Y}_F=0:\ \ \tilde{T}=(\tilde{T}_f-\tilde{T}_0)(x/x_f)+\tilde{T}_0$$
$$x_f<x<l\ ;\ \tilde{Y}_O=0:\ \ \tilde{T}=\tilde{T}_f+(\tilde{T}_l-\tilde{T}_f)(x-x_f)/(l-x_f)$$



- Concentration profiles determined from S-Z function
- Inert profile from diffusion equation
- Product from $\Sigma Y_i = 1$



1D Model : Flame Location

- **Flame Location**
  - As $Y_{F,l}$ increases, x_f decreases
  - Stoichiometric consumption
  - Same angle at cross-section

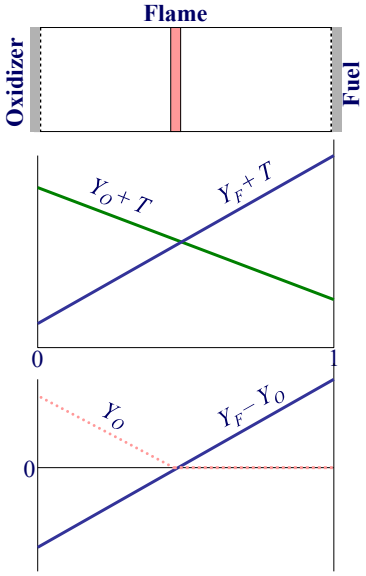
$$\frac{x_f}{l}=\frac{\tilde{Y}_{O,0}}{\tilde{Y}_{F,l}+\tilde{Y}_{O,0}}=\frac{1}{1+(\tilde{Y}_{F,l}/\tilde{Y}_{O,0})}$$

- **Mass flux of fuel : Burning rate**

$$\tilde{Y}_F-\tilde{Y}_O=(\tilde{Y}_{F,l}+\tilde{Y}_{O,0})(x/l)-\tilde{Y}_{O,0}$$

$$\rho D\frac{dY_F}{dx}=\frac{\rho D}{l}(Y_{F,l}+Y_{O,0}/\sigma)=-\frac{1}{\sigma}\rho D\frac{dY_O}{dx}$$

Maximum burning rate when $Y_{F,l}=Y_{O,0}=1$



1D Model : Flame Temperature

- **Flame Temperature**

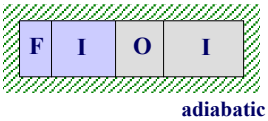
$$\frac{\tilde{T}_f-\tilde{T}_l}{\tilde{Y}_{F,l}}+\frac{\tilde{T}_f-\tilde{T}_0}{\tilde{Y}_{O,0}}=1 \qquad \frac{C_p(T_f-T_l)}{Y_{F,l}}+\frac{C_p(T_f-T_0)}{Y_{O,0}/\sigma}=Q$$

- **Rearrange**

$$\left\{C_p(T_f-T_l)+(\frac{1}{Y_{F,l}}-1)C_p(T_f-T_l)\right\}+\sigma\left\{C_p(T_f-T_0)+(\frac{1}{Y_{O,0}}-1)C_p(T_f-T_0)\right\}=Q$$

1kg fuel Enthalpy change	Inert corresponding to fuel side	σ kg oxidizer	Inert corresponding to oxidizer side	Heat of combustion for 1 kg fuel

- **Implication**

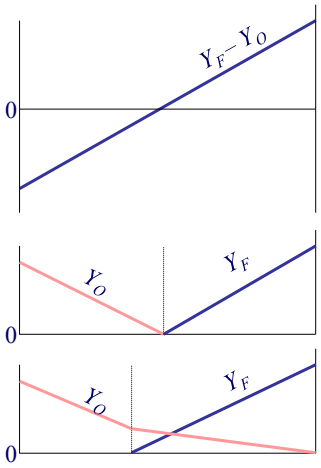


adiabatic

Adiabatic Flame Temperature

1D Model : Flame Intensity

- **Stoichiometric consumption should be satisfied all the time**
- **Coupling function is independent to reaction model**
- **If flame is disturbed from x_f**
  - **Only one reactant can be completely consumed because of stoichiometric consumption**
  - **Burning intensity decreases**
  - **That side becomes premixed**
- **Flame will travel in premixed side toward the flame sheet resulting in maximum intensity (complete consumption of F and O)**



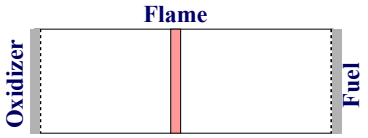
1D Model : Le ≠ 1 w/ Pure Diffusion

$$\frac{\lambda}{C_p}\frac{d^2\tilde{T}}{dx^2} = -\omega_F = -[W_F(\nu_F'' - \nu_F')]$$

$$\rho D \frac{d^2\tilde{Y}_i}{dx^2} = \omega_F$$

$$x = 0;\quad \tilde{T} = \tilde{T}_0,\ \tilde{Y}_F = 0,\quad \tilde{Y}_O = \tilde{Y}_{O,0},\ \tilde{Y}_P = \tilde{Y}_{P,0}$$

$$x = l;\quad \tilde{T} = \tilde{T}_l,\ \tilde{Y}_F = \tilde{Y}_{F,l},\ \tilde{Y}_O = 0,\quad \tilde{Y}_P = \tilde{Y}_{P,l}$$

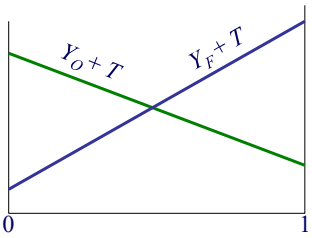


- **Non-convective system : Define effective concentration** $\bar{Y}_i = \tilde{Y}_i / \mathrm{Le}_i$
- **Shvab-Zel'dovich coupling function exists**

$$\frac{d^2}{dx^2}(\bar{Y}_i + \tilde{T}) = 0 \qquad \bar{Y}_i + \tilde{T} = a_i x + b_i$$

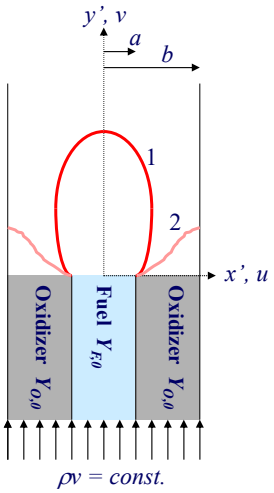
- **Non-unity Le effectively changes boundary concentration**
- **With convection**

CK Law, SH Chung, "Steady State Diffusion Flame Structure with Lewis Number Variations," Combust. Sci. Technol. 29 (1982) 129-145.



Burke-Schumann Flame

- **Burke & Schumann 1928**
  - **Steady-state**
  - **Coaxial flow of fuel and oxidizer**
  - **Parameters : a, b, ρv, concentration**
- **Two-types of flames are possible**
  - **Over-ventilated flame (1)**
    - **Excess oxidizer supply**
    - **Normal diffusion flame**
  - **Under-ventilated flame (2)**
    - **Deficient oxidizer supply**
    - **Inverse diffusion flame**
- **Practical Interest**
  - **Flame height**

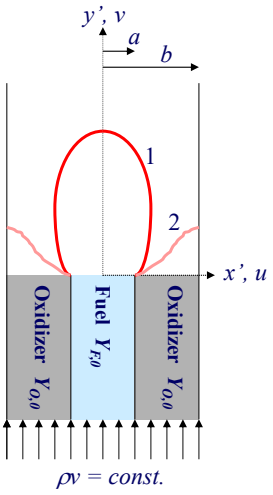


Burke-Schumann Flame

- **Assumptions**
  - **Only streamwise velocity component $u \equiv 0$**
  - **Supported by symmetry & wall**
  - **Continuity dictates that ρv = const.**
  - No mixing layer effect
- **Boundary layer formulation**
  - Transverse diffusion >> streamwise diffusion
  - Only valid for large jet velocity

$$\frac{\partial^2}{\partial y'^2} << \frac{\partial^2}{\partial x'^2} \approx v\frac{\partial}{\partial y'}$$

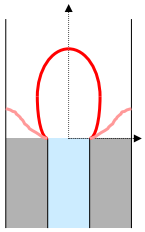
- **Practical limitations**
  - **Jet mixing**
  - **High velocity leads to turbulence**
  - **Buoyancy will play a role for small velocity**



Burke-Schumann Formulation

- **Governing Equations**

$$\rho v\frac{\partial \tilde{T}}{\partial y'}-\frac{\lambda}{C_p}\frac{\partial^2 \tilde{T}}{\partial x'^2}=-\omega_F\ ,\quad \rho v\frac{\partial \tilde{Y}_i}{\partial y'}-\rho D_i\frac{\partial^2 \tilde{Y}_i}{\partial x'^2}=\omega_F$$



- **Let** $\rho v = m$, $x = x'/b$, $y = y'/(b\mathrm{Pe})$, $c = a/b$, $\mathrm{Le}_i = 1$
  - **Pe : Peclet number**

$$\mathrm{Pe}=\frac{\rho v b}{\lambda/C_p}=\frac{v b}{\lambda/\rho C_p}=\frac{v b}{\alpha}=\frac{\text{convection}}{\text{diffusion}}$$

- **Coupling function formulation**

$$\frac{\partial \beta_i}{\partial y}-\frac{\partial^2 \beta_i}{\partial x^2}=0 \qquad \beta_i=\tilde{T}+\tilde{Y}_i\ :\ \tilde{T}=C_pT/QY_{F,o}\quad \tilde{Y}_F=Y_F/Y_{F,o}\quad \tilde{Y}_O=Y_O/\sigma Y_{F,o}$$

- **Boundary Conditions**

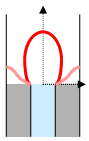
$y = 0$: $0 < x < c$; $\tilde{Y}_F = 1$, $\tilde{T} = \tilde{T}_o$
$c < x < 1$; $\tilde{Y}_O = \tilde{Y}_{O,o} \equiv \nu$, $\tilde{T} = \tilde{T}_o$
$y \to \infty$: bounded
$x = 0$: $\partial/\partial x = 0$ (symmetry)
$x = 1$: $\partial/\partial x = 0$ (adiabaticity & impermeability)

- **Can be solved with Separation of Variables** $\beta_i = X(x)Y(y)$

Burke-Schumann Flame

- **Separation of Variables**

$$\frac{\partial \beta_i}{\partial y}-\frac{\partial^2 \beta_i}{\partial x^2}=0$$



$$\beta_i=X(x)Y(y) \qquad \frac{Y'}{Y}=\frac{X''}{X}=-k^2$$

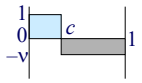
$$Y'+k^2Y=0 \quad ;\ Y=\exp(-k^2y)$$

$$X''+k^2X=0\ ;\ X=\sin kx+\cos kx$$

symmetry

- **BC at** $x = 1$

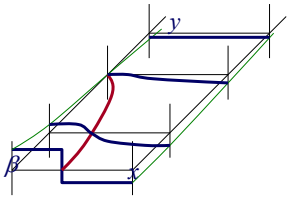
$$\partial X/\partial x=0\ ;\ -\sin k=0\ ,\quad k=n\pi$$



$$\beta_i=C_0+\sum_{n=1}^{\infty}C_n\cos n\pi x\exp(-n^2\pi^2y)$$

- **Apply BC at** $y = 0$ **& use orthogonality for**

$$\beta_i(y=0)=C_0+\sum_{n=1}^{\infty}C_n\cos n\pi x \qquad \beta=\tilde{Y}_F-\tilde{Y}_O$$



$$C_0=\int_0^1\beta_i(y=0)dx=\int_0^c 1dx+\int_c^1(-\nu)dx=c-(1-c)\nu$$

$$C_n=\int_0^1\beta_i(y=0)\cos n\pi x dx=2\frac{(1+\nu)}{n\pi}\sin n\pi c$$

- **Soution**

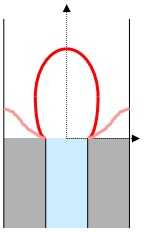
$$\beta=\{c-(1-c)\nu\}+2(1+\nu)\sum_{n=1}^{\infty}\frac{\sin n\pi c}{n\pi}\cos n\pi x\exp(-n^2\pi^2y)$$

- **Flame location :** $\beta = 0$ **at** (x_f, y_f)

$$-\frac{\{c(1+\nu)-\nu\}}{(1+\nu)}=2\sum_{n=1}^{\infty}\frac{\sin n\pi c}{n\pi}\cos n\pi x_f\exp(-n^2\pi^2y_f)$$

Burke-Schumann Flame

- **Apply BC at $y = 0$ & use orthogonality for β_T**



$$\beta_T = \tilde{T} + \tilde{Y}_F = (c + \tilde{T}_0) + 2\sum_{n=1}^{\infty} \frac{\sin n\pi c}{n\pi} \cos n\pi x \exp(-n^2\pi^2 y)$$

- **Flame Temperature**

$$(x_f, y_f): \beta_T = \tilde{T}_f = (c + \tilde{T}_0) - \{c - \frac{\nu}{1+\nu}\} = \tilde{T}_0 + \frac{\nu}{1+\nu}$$

$$\frac{C_p(T_f - T_0)}{Y_{F,0}} + \frac{C_p(T_f - T_0)}{Y_{O,0}/\sigma} = Q \qquad \frac{\tilde{T}_f - \tilde{T}_0}{\nu} + (\tilde{T}_f - \tilde{T}_0) = 1$$

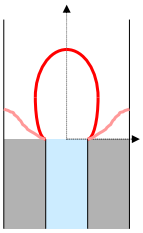
$$C_p(T_f - T_0) + (\frac{1}{Y_{F,0}} - 1)C_p(T_f - T_0) + \sigma\{C_p(T_f - T_0) + (\frac{1}{Y_{O,0}} - 1)C_p(T_f - T_0)\} = Q$$

1kg fuel Enthalpy change	Inert corresponding to fuel side	σ kg oxidizer	Inert corresponding to oxidizer side	Heat of combustion for 1 kg fuel

- **Adiabatic Flame temperature**

Burke-Schumann Flame

- **Over-ventilated flame (β(∞)<0)**
- **Under-ventilated flame (β(∞)>0** $\beta = \tilde{Y}_F - \tilde{Y}_O$



$$\beta(y \to \infty) = \{c - (1+c)\nu\} = \frac{1}{Y_{F,o}}\{cY_{F,o} - (1-c)Y_{O,o}/\sigma)$$

- **Flame height H_f**

$$\beta(x_f = 0 \text{ or } 1, H_f) = \{c - (1-c)\nu\} + 2(1+\nu)\sum_{n=1}^{\infty} \frac{\sin n\pi c}{n\pi} \exp(-n^2\pi^2 H_f) = 0$$

$$H_f = \frac{H_f'}{b}\frac{1}{\mathrm{Pe}} = f(c,\nu)$$

$$\frac{H_f'}{b} \propto \mathrm{Pe} = \frac{\upsilon b}{\alpha} \qquad H_f' \propto \upsilon b^2$$

$$n = 1: H_f = \frac{1}{\pi^2}\ln\left\{\frac{\sin\pi c}{\pi}\frac{2(1+\nu)}{(1-c)\nu - c}\right\}$$

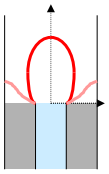
Burke-Schumann Flame

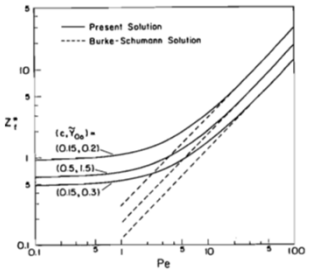
- **Streamwise diffusion / Preferential diffusion**
- **Governing Equations**

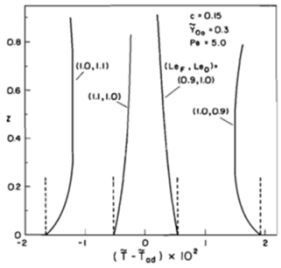
$$\rho v = m$$

$$\rho v \frac{\partial \tilde{T}}{\partial y'} - \frac{\lambda}{C_p}\left\{\frac{\partial^2 \tilde{T}}{\partial x'^2} + \frac{\partial^2 \tilde{T}}{\partial y'^2}\right\} = -\omega_F$$

$$\rho v \frac{\partial \tilde{Y}_i}{\partial y'} - \rho D_i \left\{\frac{\partial^2 \tilde{Y}_i}{\partial x'^2} + \frac{\partial^2 \tilde{Y}_i}{\partial y'^2}\right\} = \omega_F$$





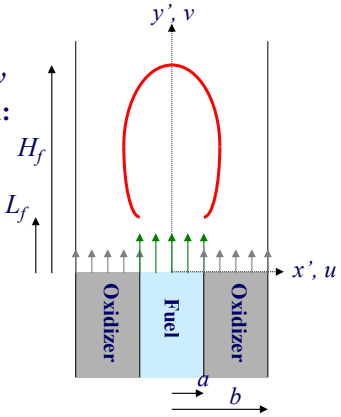


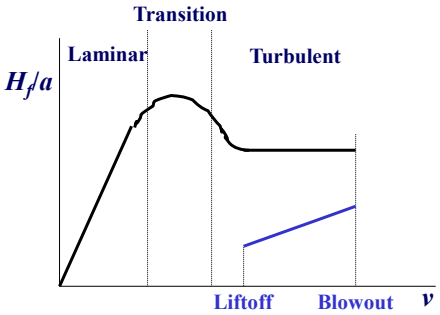
- **Green's function theory**

SH Chung, CK Law, "Burke-Schumann Flame with streamwise and preferential diffusion," Combust. Sci. Tech. 37 (1984) 21-46.

Coflow Diffusion Flames

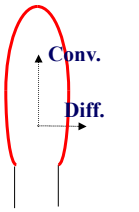
- **Flame Height H_f**
- **Liftoff Height L_f : Flame Stabilization**
- **Burke-Schumann flame velocities : $v_F = v_O = v$**
- **Fuel jet into infinite stagnant oxidizer stream:**
  - **$v_F = v$, $v_O = 0$, $b \to \infty$**

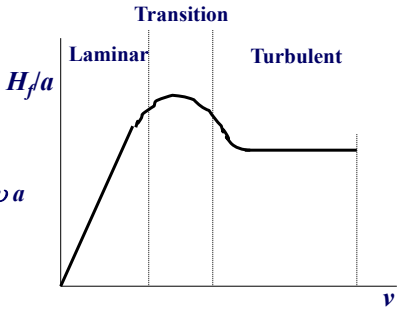




Jet Diffusion Flames : B-S View

- For $b \rightarrow \infty$: Jet Flame
  - Parameter a, υ, D
  - D/υ [L]
  - Dimensional analysis $H_f = \frac{D}{\upsilon} f(\frac{D}{a\upsilon})$
- Boundary Layer Approximation
  - Vertical convection time $t_c = H_f/\upsilon$
  - Horizontal diffusion time $t_d = a^2/D$
  - Thus $\frac{H_f}{\upsilon} = \frac{a^2}{D} : \quad \frac{H_f}{a} = \frac{\upsilon a}{D}$
- Diffusivity
  - Laminar regime: Mass diffusivity
  - Turbulent regime :
    Turbulent diffusion coefficient $D_T \sim \upsilon\, a$





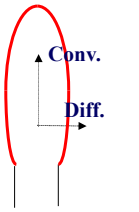
Laminar regime : $H_f/a \sim \upsilon\, a$
Turbulent regime : $H_f/a \sim$ constant

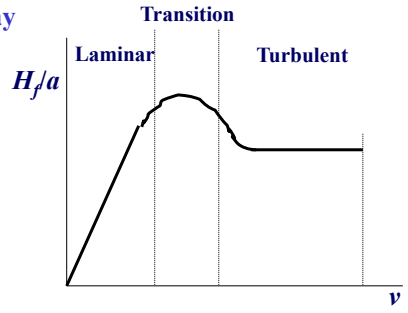
Buoyancy Effect : Jet Diffusion Flames

- Buoyancy : First glance
  - Vertical convection time $t_c = \sqrt{H_f / g}$
  - Horizontal diffusion time $t_d = a^2 / D$

$$\therefore H_f \sim \frac{g a^4}{D^2}$$

- May conclude that flame height may not be controlled by buoyancy

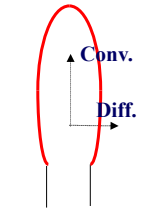


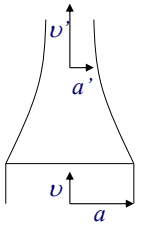


Jet Diffusion Flames : Roper's View

- There are strong inward flow due to buoyancy
- Mass conservation dictates that $\rho a'^2 \upsilon' = \rho_o a^2 \upsilon$
- Buoyant velocity $\upsilon' = \sqrt{gH_f}$
- Neglecting density variation $a'^2 = \dfrac{a^2 \upsilon}{\sqrt{gH_f}}$
- Balance of vertical convection and horizontal diffusion

$$t_d = \frac{a'^2}{D} = \frac{a^2 \upsilon / \sqrt{gH_f}}{D} : \quad t_c = \sqrt{\frac{H_f}{g}} \qquad \boxed{\frac{H_f}{a} \sim \frac{\upsilon a}{D}}$$





- 2D slot burner - mass conservation $\rho a' \upsilon' = \rho_o a \upsilon$

$$a' = \frac{a\upsilon}{\sqrt{gH_f}} \qquad \boxed{H_f \sim a^{4/3} \upsilon^{4/3}}$$

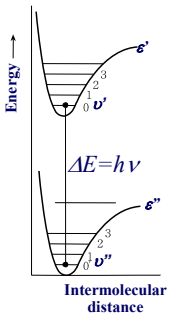
Experimentally substantiated

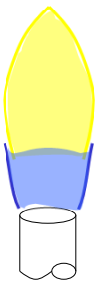
Note: B-S predicts $\boxed{H_f \sim a^2 \upsilon}$

Linear dependence in laminar regime is due to buoyancy control

Flame Height

- Theory : Maximum temperature along centerline
- Experiment : photography or by eye
  - Flame luminosity
  - Usually yellow height
  - Difference bet Yellow & Blue heights is 10 – 20%





Yellow: Blackbody radiation

Blue: Chemiluminescence

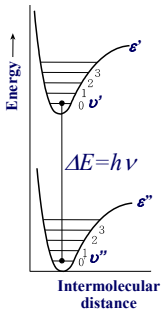
C_2 greenish blue
CH blue-violet
OH UV

- Chemiluminescence
- Chemical reaction leads an atom or a molecule in an electronically excited state, from which radiation may occur
- C_2 Swan band : 516.5 nm (Greenish blue)
- CH band : 431.2 nm (Blue violet)
- OH band : 309.0 nm (UV)

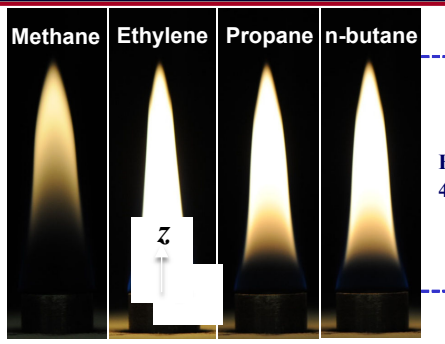
Chemiluminescence

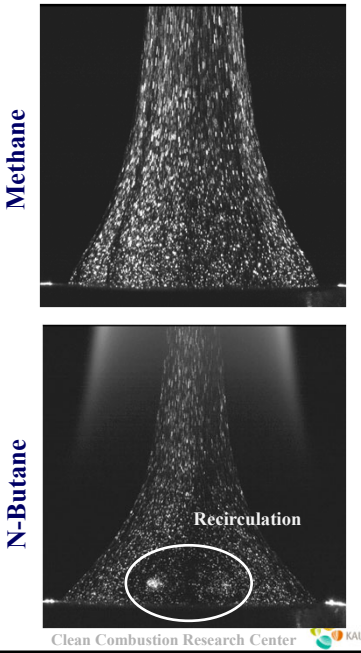
- Chemical reaction leads an atom or a molecule in an electronically excited state, from which radiation may occur

- C_2 Swan band : 516.5 nm (Greenish blue)
- CH band : 431.2 nm (Blue violet)
- OH band : 309.0 nm (UV)
- CO Fourth Positive band below 240.0 nm (UV)
  - $CH + O_2 = CO + OH^*$
  - $O + H = OH(^4\Sigma^-) = OH(A^2\Sigma^+)$
  - $H + OH + OH = H_2O + OH^*$
  - $C_2 + OH = CO + CH^*$
  - $CH_2 + C = C_2^* + H_2$



Coflow Diffusion Flame : Fuel Density Effect

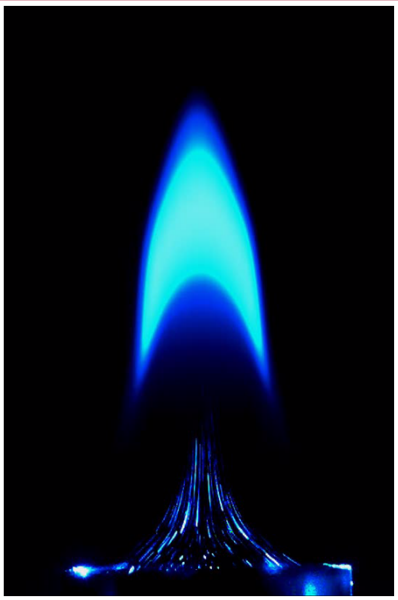




Y Xiong, MS Cha, SH Chung, "Fuel density effect on near nozzle flow field in small laminar coflow diffusion flames," *Proc. Combust. Inst.* 35 (2015) 873–880

Reynolds number effect

- Vortex structure as Re increase
  - Blow away?
- Increasing flow velocity?
  - Kelvin-Helmholtz instability
  - Flame flicker
- Fuel
  - n-butane
- Jet Reynolds number
  - 20 ~ 300



Buoyant Jet Diffusion Flame

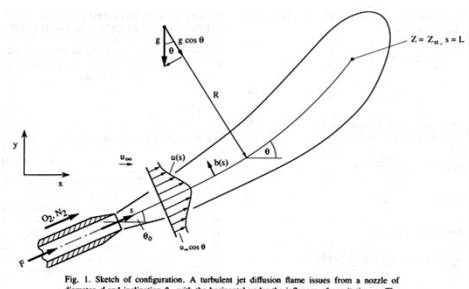


Fig. 1. Sketch of configuration. A turbulent jet diffusion flame issues from a nozzle of diameter d and inclination θ_0 with the horizontal under the influence of gravitation g. The present model also takes the effects of a uniform cross-wind u_∞ into account.

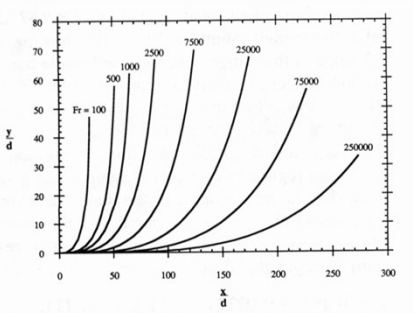


Fig. 3. Flame axis for various Froude numbers with $u_\infty = 0$ and $\theta_0 = 0°$ (propane).

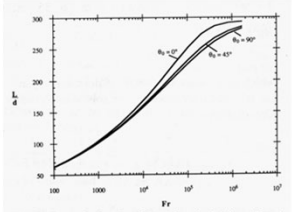


Fig. 5. Dimensionless chord flame length, L/d, vs. Froude number, Fr, for $u_\infty = 0$ and $\theta_0 = 0°$, 45°, and 90° (propane).

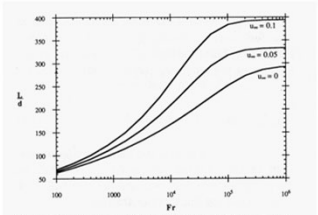


Fig. 6. Dimensionless chord flame length, L/d, vs. Froude number, Fr, for $u_\infty = 0$, 0.05, 0.1, and $\theta_0 = 0°$ (propane).

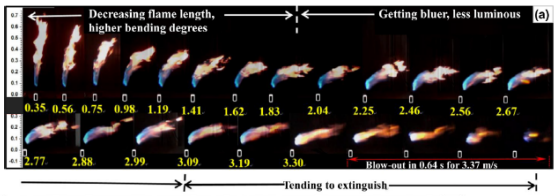
Peters 1991 CNF 85:206

Jet Flame in Crossflow

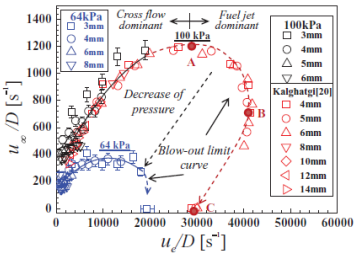
Tsue et al., Proc. Combust. Inst 28:295-302 (2000)

Ogawa, Katoda, DTD 2002, pp. 169-173.

Q Wang, L Hu, SH Yoon, S Lu, M Delichatsios, SH Chung, "Blow-out limits of nonpremixed turbulent jet flames in a cross flow at atmospheric and sub-atmospheric pressures," *Combustion and Flame* 162 (2015) 3562-3568



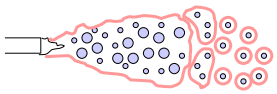
Crossflow dominant regime
Jet dominant regime



Droplet Combustion

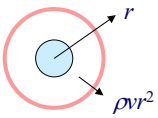
Droplet Combustion : Introduction

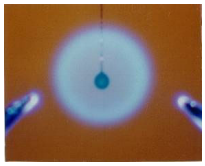
- **Fuel Supply**
  - **Spray : Ensemble of non-uniformly distributed droplets**
  - **Element : Droplet w/ 10 ~ 100 μm**



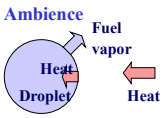
Group combustion mode : Envelope flame (Chiu)

Single droplet combustion mode

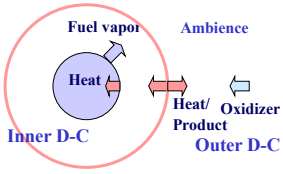




- **Idealized Model**
  - **Stagnant environment, Buoyancy absent**
  - **Free of forced & natural convection**
  - **Spherical symmetry**



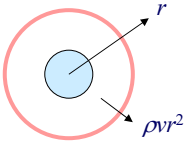
Pure vaporization



Combustion

Characteristic Rates

- **Liquid-vapor Phase Change** α_p (very fast)
- **Gas-phase Heat/Mass Diffusion** $\alpha_g \sim 10^0$ cm^2/s
- **Surface Regression** $\alpha_s \sim (\rho_g/\rho_l)\ \alpha_g \sim 10^{-3}$ cm^2/s
- **Liquid-phase Heat Conduction** $\alpha_{l,t} \sim 10^{-3}$ cm^2/s

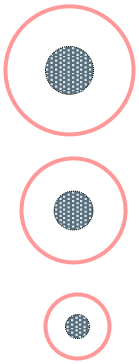


- **$\alpha_p >> \alpha_g$: Equilibrium vaporization at surface (saturated vapor pressure)**
- **$\alpha_g >> \alpha_s$: Gas-phase Quasi-steadiness**
- **$\alpha_g >> \alpha_{l,t}$: Surface temp. constant during characteristic time of gas-phase transport**

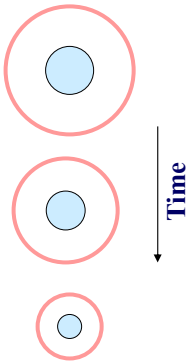
- **Limitations**
  - **Near critical pressure** $\rho_g \sim \rho_l$
  - **Far-field** $\rho v r^2 =$ const: for $r > (\rho_l/\rho_g)^{1/2}$ then $v_g \sim v_s$

Gas-phase Quasi-steadiness

- Porous sphere
  Steady-state

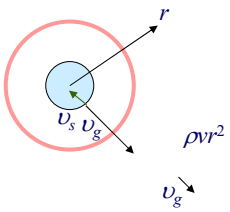


- Droplet
  Combustion



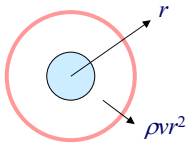
Size variation from
mass conservation

- Far-field



Droplet Model : Spalding

- Assumptions
  - Spherically symmetric
  - Isobaric
  - Single-component, constant properties
  - Uniform droplet temperature (T_B boiling temp.)
  - Unity Lewis number ($Le_i = 1$)
  - Gas-phase quasi-steadiness
  - Diffusion controlled (flame sheet limit)



- Governing Equations
  - Continuity

$$\frac{d}{dr}(\rho u r^2) = 0$$

  - Coupling function

$$\frac{d}{dr}\{\rho u r^2 \beta_i - (\lambda / C_p) r^2 \frac{d\beta_i}{dr}\} = 0, \quad i = O, F$$

Droplet Model : Spalding

- **Instantaneous mass flow rate : Evaporation rate**

$$m = 4\pi r^2 \rho u = const.$$

- **Nondimensionalization** $\quad \tilde{r} = r/r_s, \;\; \tilde{m} = \dfrac{m}{4\pi(\lambda/C_p)r_s}$

$$\frac{d}{d\tilde{r}}\left(\tilde{m}\beta_i - \tilde{r}^2 \frac{d\beta_i}{d\tilde{r}}\right) = 0, \;\; i = O, F \qquad \therefore \;\; \beta_i = C_{i,1} + C_{i,2}\exp\left(-\frac{\tilde{m}}{\tilde{r}}\right)$$

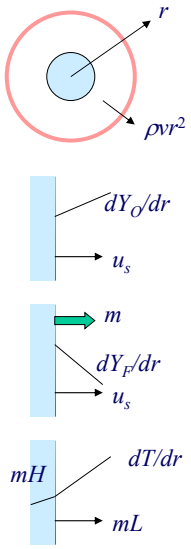
- **Boundary Conditions at droplet surface (r = 1)**
  - **Convection + Diffusion = Source**

$$\rho u r^2 Y_O - \rho D r^2 \frac{dY_O}{dr} = 0$$ **No penetration of oxidizer**

$$\rho u r^2 Y_F - \rho D r^2 \frac{dY_F}{dr} = \rho u r^2$$ **Evaporation**

$$\lambda r^2 \frac{dT}{dr} = \rho u r^2 \left(L + H\right)$$

H **: Heating up liquid fuel**
L **: Latent heat of vaporization**



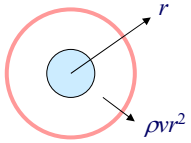
Droplet Model : Spalding

- **Nondimensional BC's**

$$\tilde{r} \to \infty: \;\; \tilde{Y}_o = \tilde{Y}_{o,\infty}, \;\; \tilde{Y}_F = 0, \;\; \tilde{T} = \tilde{T}_\infty$$

$$\tilde{r} = 1: \;\; \tilde{m}\tilde{Y}_O - \frac{d\tilde{Y}_O}{d\tilde{r}} = 0, \;\; \tilde{m}\tilde{Y}_F - \frac{d\tilde{Y}_F}{d\tilde{r}} = \tilde{m}, \;\; \frac{d\tilde{T}}{d\tilde{r}} = \tilde{m}\left(\tilde{L} + \tilde{H}\right)$$

$$\tilde{T} = \tilde{T}_s$$



- **Applying BC's**

$$\beta_O = \tilde{T} + \tilde{Y}_O = \{\tilde{T}_s - (\tilde{L} + \tilde{H})\} + \{(\tilde{T}_\infty - \tilde{T}_s) + (\tilde{L} + \tilde{H}) + \tilde{Y}_{O\infty}\}\exp\left\{-\tilde{m}/\tilde{r}\right\}$$

$$\beta_F = \tilde{T} + \tilde{Y}_F = \{1 + \tilde{T}_s - (\tilde{L} + \tilde{H})\} + \{(\tilde{T}_\infty - \tilde{T}_s) + (\tilde{L} + \tilde{H}) - 1\}\exp\left\{-\tilde{m}/\tilde{r}\right\}$$

- **Extra BC to determine** m
- **Flame sheet :** $Y_F(r_f) = Y_O(r_f) = 0$

$$\tilde{m} = \ln\left(1 + B\right) \qquad B = \frac{(\tilde{T}_\infty - \tilde{T}_s) + \tilde{Y}_{o\infty}}{\tilde{L} + \tilde{H}} = \frac{C_p(T_\infty - T_s) + (Y_{o\infty}/\sigma)Q}{L + H}$$ **Transfer number**

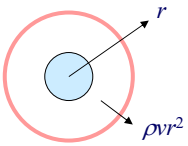
$$\tilde{r}_f = \frac{\tilde{m}}{\ln(1 + \tilde{Y}_{o\infty})}$$ **Flame front standoff ratio**

$$\tilde{T}_f = \frac{\tilde{T}_\infty + \tilde{Y}_{o\infty}\{1 + \tilde{T}_s - (\tilde{L} + \tilde{H})\}}{1 + \tilde{Y}_{o\infty}}$$ **Flame Temperature**

- **Clausius-Clapeyron Relation**
  - **Equilibrium vaporization at droplet surface**

D^2 - Law

- **Constant droplet temperature**
  - **Temp. limited by boiling temp.** T_B
  - **Approaches** T_B **fairly rapidly O(0.1**t_L**)**
  - **Accurate enough in determining evaporation rate**
  - $T_s = T_B$, $H = 0$



- **Transfer number** $B = \dfrac{C_p(T_\infty - T_s) + (Y_{o\infty}/\sigma)Q}{L} = \dfrac{\text{Driving force for vaporization}}{\text{Resistence to vaporization}}$

$$\tilde{m} = \ln(1+B) \qquad \textbf{B: O(1~10)}$$

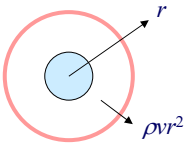
- **Flame front standoff ratio** $\tilde{r}_f = 1 + \dfrac{\ln\{1+(\tilde{T}_f - \tilde{T}_s)/\tilde{L}\}}{\ln(1+\tilde{Y}_{o\infty})}$

- **Flame temperature** $\{C_p(T_f - T_s) + L\} + \sigma\{1 + \dfrac{1-Y_{o\infty}}{Y_{o\infty}}\}C_p(T_f - T_\infty) = Q$

Adiabatic Flame Temperature

D^2 - Law

- **Definition :** $m = 4\pi r^2 \rho u$



$$m = -\frac{d}{dt}\left(\frac{1}{6}\pi d_s^3 \rho_l\right) = -\frac{\pi}{4}\rho_l d_s \frac{d}{dt}(d_s^2)$$

$$\tilde{m} = \frac{m}{4\pi(\lambda/C_p)r_s} = const.\ (given\ T_\infty, T_s, Y_{o_\infty}, L)$$

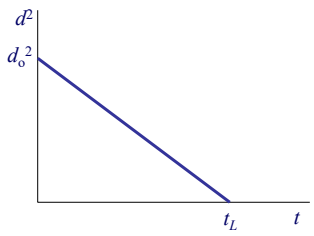
$$-\frac{d}{dt}\left(d_s^2\right) = \frac{8(\lambda/C_p)}{\rho_l}\tilde{m} = K$$ **Evaporation rate constant**

$$\boxed{d_s^2 = d_{s_o}^2 - Kt}$$ **d^2-Law**

- **Droplet Lifetime** $\boxed{t_L = d_{s_o}^2/K}$

$d_{s_o} \rightarrow 1/10$; $t_L \rightarrow 1/100$

Fine atomization accelerates vaporization

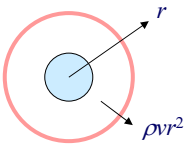


Droplet Combustion : Results

- **Evaporation Rate Constant** $K \equiv -\frac{d}{dt}\left(d_s^2\right)$

$$K = \frac{8(\lambda/C_p)}{\rho_l}\ln\left\{1+\frac{C_p(T_\infty - T_s)+(Y_{O\infty}/\sigma)Q}{L}\right\}$$

$\lambda/C_p \propto T^{0.75}$: $Y_{O\infty}\uparrow$, $T_f\uparrow$, $\lambda/C_p\uparrow$



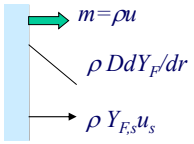
$$\frac{K}{(\lambda/\rho_g C_p)} \sim \frac{\rho_g}{\rho_l} \sim 10^{-3}$$

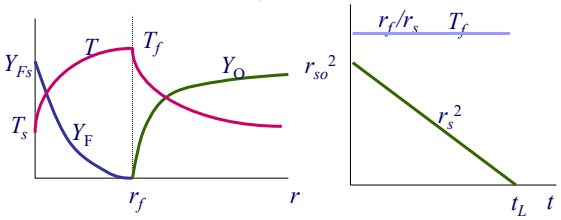
Surface regression is much slower than gas-phase diffusion

- **Surface Concentration of Fuel**

$$\tilde{Y}_{F,s} = (1-\tilde{L}) + \{\tilde{T}_\infty - \tilde{T}_s + \tilde{L} - 1\}\exp(-\tilde{m})$$

  - Even under boiling condition, it is not maintained unity, due to diffusion.
  - If no diffusion, $Y_{F,s} = 1$

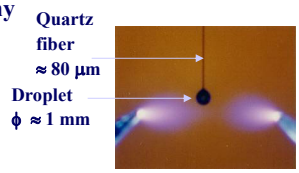




- r_f/r_s constant ~ 40
- T_f constant
- d^2 - Law

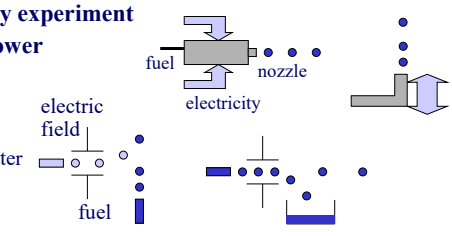
Single-Droplet Experiment

- **Suspended Droplet**
  - Easy to setup, stationary, cine-microphotography
  - Minimum 1 mm, spherocity due to buoyancy
  - Heat transfer through fiber (minimal)
  - Limited to non-volatile fuel

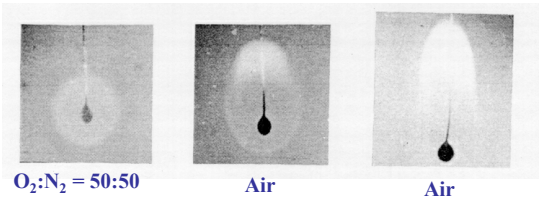


- **Porous Sphere**
  - Steady-state, various measurement
  - 2 mm smallest, no transient effect

- **Free Droplet**
  - No interference w/ fiber, small droplet
  - Complex, data recording, convection changes
- **Drop Tower : Free-Fall Chamber**
  - Buoyancy free micro-gravity experiment
  - Largest : 10 s 900 m drop tower
- **Free droplet experiment**
  - Mechanical chopper
  - Electro-mechanical squirting (Piezo-electric material)
  - Vibrating bed ($\phi \approx 2D$) (too dense)



Buoyancy Effect



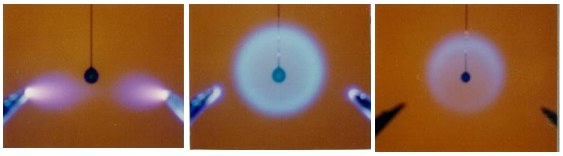
O_2:N_2 = 50:50
0.1 atm

Air
0.5 atm

Air
1.0 atm

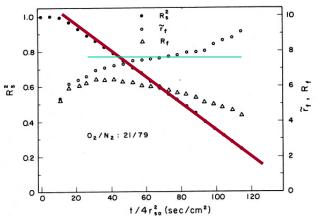
CK Law, SH Chung, N. Srinivasan, "Gas-phase quasi-steadiness and fuel vapor accumulation effects in droplet burning," *Combust. Flame* 38 (1980) 173-198.

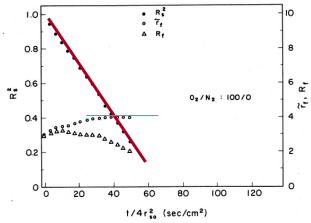
- **Buoyancy : density difference → pressure dependent**
- **Droplet combustion is diffusion controlled, thus pressure insensitive**



SH Chung, CK Law, "An experimental study of droplet extinction in the absence of external convection," *Combust. Flame* 64 (1986) 237-241.

Droplet Experiment





0.15 atm, Air, D_o = 1.02 mm

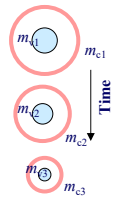
0.10 atm, Pure oxygen, D_o = 1.24 mm

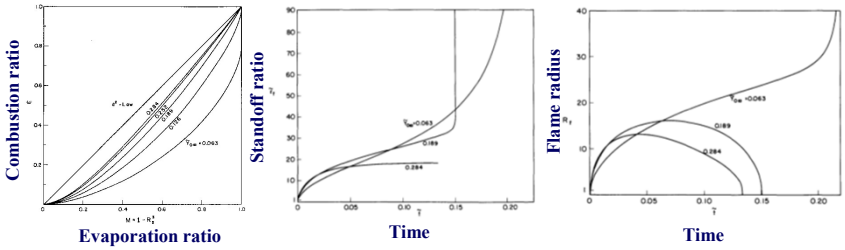
- **Experiment**
  - **d^2 – Law reasonable**
  - **Initially, m small : Droplet heating (~ 0.1 t_L)**
  - **r_f/r_s < 10 : Variable property, $D_{fuel} < D_{oxygen}$**
  - **r_f/r_s not constant :**

- **Prediction**
  - **d^2 – Law**
  - **m constant**
  - **r_f/r_s constant ~ 40**
  - **T_f constant - too high**

Variation in Flame Size

- Gas-phase unsteadiness (far-field) negligible
- Fuel-vapor accumulation effect
  - Delay in vaporization and combustion
  - Accumulation or depletion





CK Law, SH Chung, N. Srinivasan, "Gas-phase quasi-steadiness and fuel vapor accumulation effects in droplet burning," *Combust. Flame* 38 (1980) 173-198.

Droplet Lifetime

- Evaporation rate
  - Insensitive to pressure
  - Rule of thumb : $t_L \sim 1$ s for $D = 1$mm droplet
- Diesel Engine
  - 3000 rpm = 50 rps, 20 ms for 1 rev.
  - Combustion duration 40° CA = 1/9 rev.
  - 2 ms available : 1/500 s ~ 1/(20)^2 s
  - Thus, 1/20 mm = D 50 μm size droplet
  - High pressure injection required (200 ~ 1500 atm)
- Gasoline Engine
  - Port injection, 1 rev. 20 ms = 1/50 s available
  - Much larger droplet could be OK even considering vaporization
  - GDI P_{inj} = 5-20 MPa into pressure of -50 kPa to 2-3 MPa depending on injection timing

Forced & Natural Convection

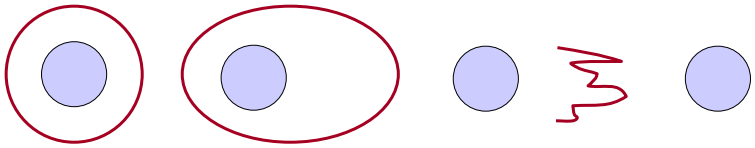
- **Forced Convection**
  - **For both pure vaporization and combustion up to Re = 1800**
  - **Faeth, 1977** $\frac{K}{K_0} = 1 + \frac{0.276\,\mathrm{Re}^{1/2}\,\mathrm{Pr}^{1/3}}{(1+1.232/\mathrm{RePr}^{4/3})^{1/2}}$
- **Natural Convection**

$$\frac{K}{K_0} = 1 + 0.533\,\mathrm{Gr}^{0.52} \approx 1 + 13.0(d_{so}^3 p^2)^{0.52} \qquad \mathrm{Gr} \equiv \left(\frac{\rho g d^3}{\mu^2}\right)\left(\frac{\Delta T}{T}\right)$$

atm

cm

- **Rel. vel. bet droplet and gas-phase due to droplet inertia at spraying**



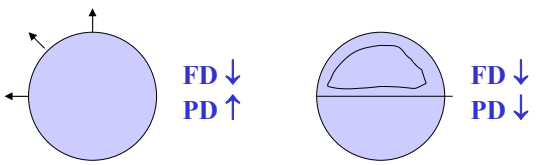
Spherical symmetric **Wake flame** **Blowoff (vaporization)**

Drag Dynamics

- **Outward mass flux : friction drag ↓, pressure drag(separation) ↑**
- **Interfacial velocity : friction drag ↓, pressure drag ↓**
- **Transient size reduction : increases drag**

- **Yuen : balance of reduction of friction drag with increase in pressure drag**

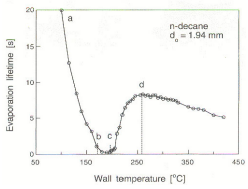
- **Drag curve for solid sphere can be used**
  - **Hill's vortex of internal circulation : not strong enough**



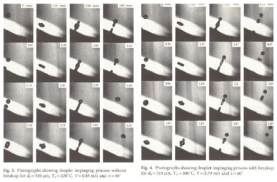
FD ↓ PD ↑ **FD ↓ PD ↓**

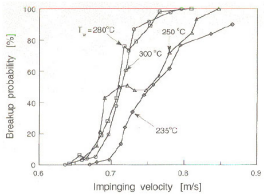
Droplet Impingement on Hot Plate

YS Ko, SH Chung. "An experiment on the breakup of impinging droplets on a hot surface," Exp. Fluids 21 (1996) 118-139.



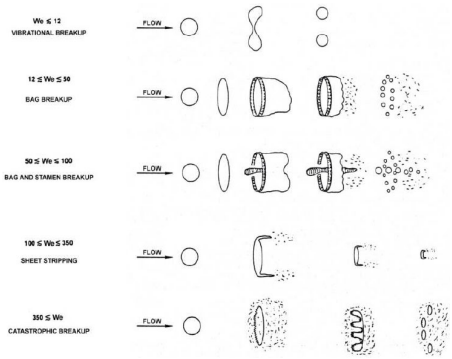
Leidenfrost phenomenon





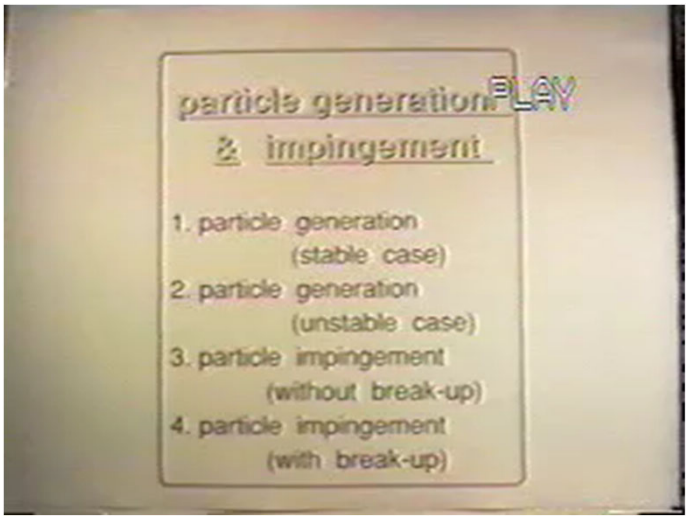
Webber number

$$\mathbf{We} = \frac{\rho v^2 d}{\sigma} = \frac{\textbf{Kinetic energy on impact}}{\textbf{surface energy}}$$

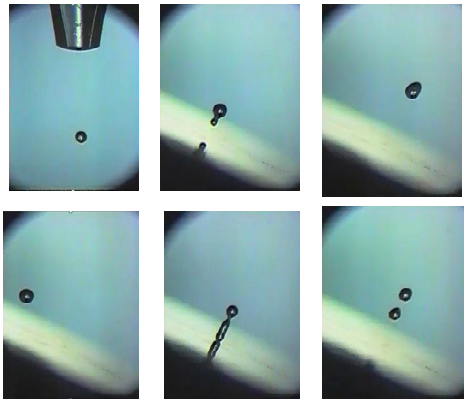


https://www.researchgate.net/figure/Secondary-breakup-zones-as-a-function-of-Weber-number-11_fig2_234154283

Droplet Generation and Impingement



Droplet Generation and Impingement



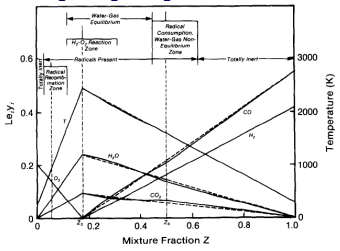
Generation-Impact-Bounce

Generation-Impact-Breakup

CO+H_2 Diffusion Flame

$CO + H_2O \rightarrow CO_2 + H_2$

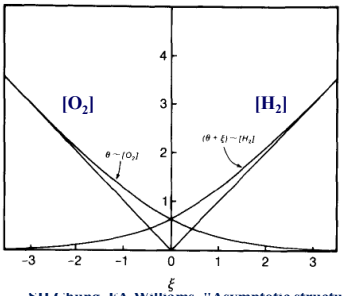
$2H_2 + O_2 = 2H_2O$

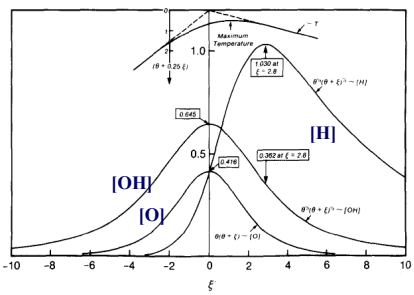


$$[O] = \frac{K_1 K_3 [O_2][H_2]}{[H_2O]},$$

$$[OH] = \left\{ \frac{K_1 K_3}{K_4} [O_2][H_2] \right\}^{1/2},$$

$$[H] = \left\{ \frac{K_1 K_3^3 [O_2][H_2]^3}{K_4 [H_2O]^2} \right\}^{1/2},$$

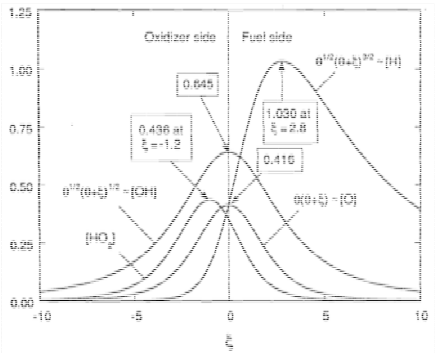




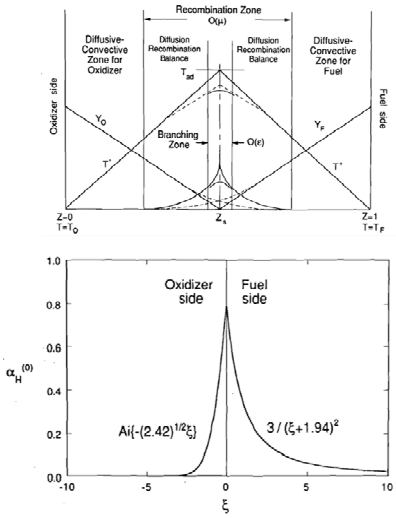
SH Chung, FA Williams, "Asymptotic structure and extinction of CO/H2 diffusion flames with reduced kinetic mechanisms," *Combust. Flame* 82 (1990) 389-410.

H_2 DF Structure

- **Small stain**
  - **I: $3H_2 + O_2 \rightarrow 2H_2O + 2H$**
  - **II: H+H+M → H2 + M**



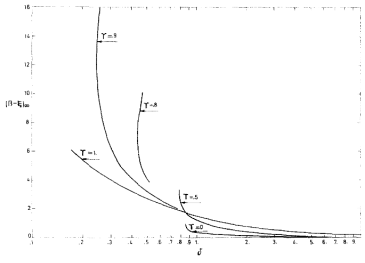
- **Moderate strain**

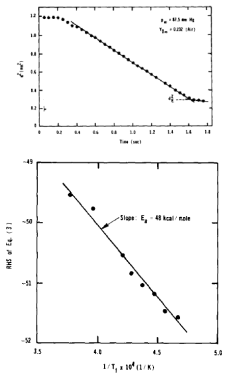


SR Lee, SH Chung, "On the structure of hydrogen diffusion flames with reduced kinetic mechanisms, *Combust. Sci. Technol.* 96 (1994) 247-277.

Diffusion Flame Extinction

- **Matched Asymptotic Expansion Technique**
  - **Liñán : Counterflow**
  - **Law : Droplet**



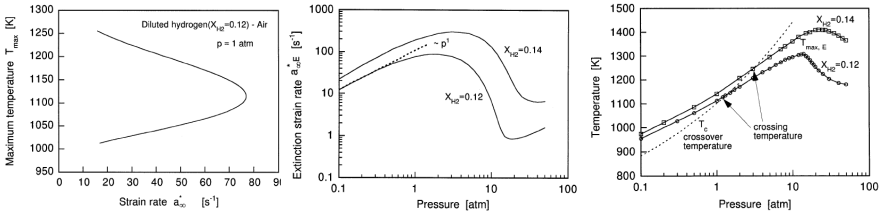


A Linan, Acta Astronautica, 1 (1974) 1007
CK Law CNF 24 (1975) 89

SH Chung, CK Law CNF 64 (1986) 237
Decane E_a = 48 kcal/mol

Diffusion Flame Extinction with P

- **Counterflow H_2 flame**



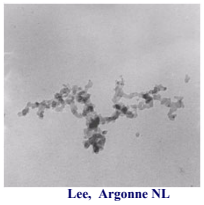
- **When considering Soret effect, a_E becomes 2-4 times larger by enhancing H and H_2 diffusion**
- **Relative intensities of chain branching (2-body) and recombination (3-body).**
- **At low P, two-body reactions are more influential: Higher pressure results in higher rates of two body reactions (a_E ↑ as P↑)**
- **Intermediate P, extinction controlled by 3-body reactions (a_E ↓ as P↑)**
- **For P > 20 atm, backward reactions become larger for OH + OH + M ↔ H_2O_2+M and H_2O_2 + H ↔ H_2 + HO_2 (a_E ↑ as P↑)**

CH Sohn, SH Chung, "Effect of pressure on the extinction, acoustic pressure response, and NO formation in diluted hydrogen-air diffusion flames," *Combust. Flame* 121 (2000) 288-300.

Soot Formation in DF

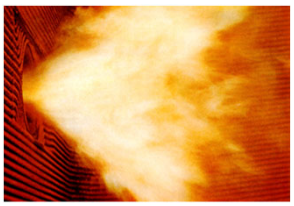
- **Visible Emission: Public awareness**
- **Health : Carcinogenic and Mutagenic**
- **Black Carbon : Global Warming**

- **Strictly Regulated Emission**



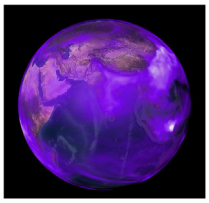
Lee, Argonne NL

- **Radiation Heat Transfer**
- **Incomplete Combustion : Efficiency**
- **Deposit : Burner Lifetime / Performance**



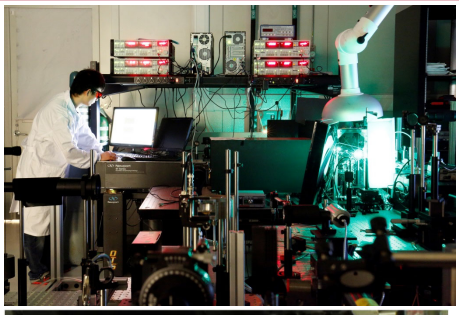
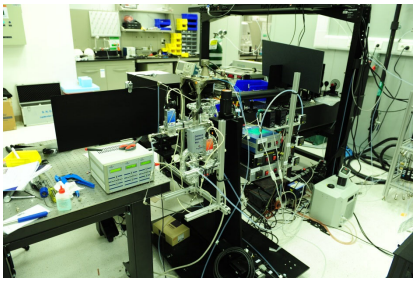
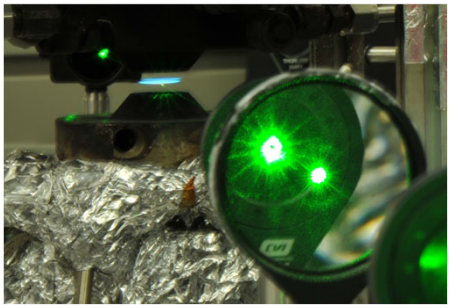
Fuel Oil Burner (VKW)

Gulf War (1991) Oil Well Fire, NG



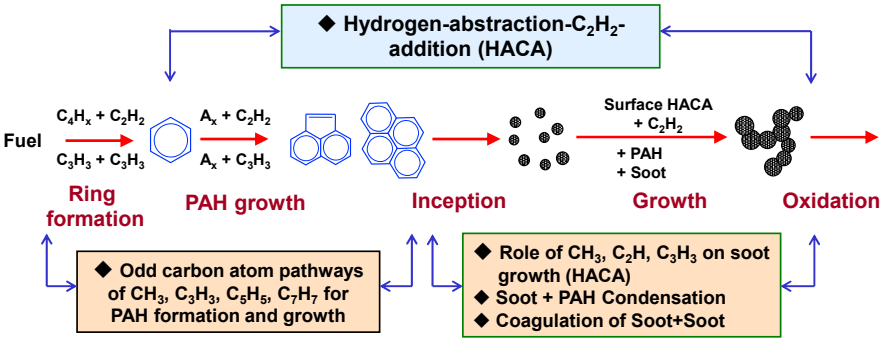
Wiki

KAUST Soot Lab


LE/LS, LII, PAH LIF, PIV, SMPS, TOF MS

Soot Formation Pathway



Issues

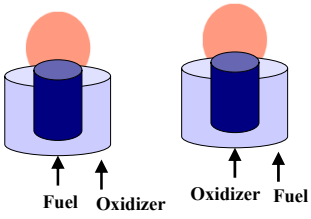
Incipient ring formation: C2+C4 vs C3+C3
PAH growth: HACA vs aromatic addition
Inception: A4 + A4 vs extension
Soot growth: Radical site
PAH condensation to soot
Oxidation of soot: O2 & OH

Wang, Chung, Soot formation in laminar counterflow flames, PECS 2019

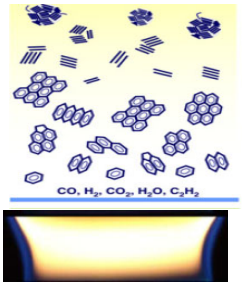
Configurations for Soot Studies

Coflow DF

NDF



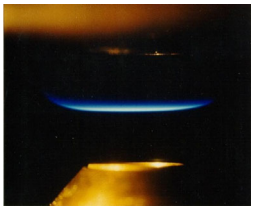
Premixed Flames

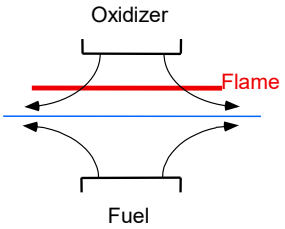


Hai Wang. PCI 2011

Hadef et al. I J Thermal Sci 2010

Counter flow DF

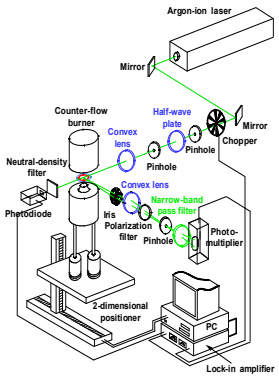


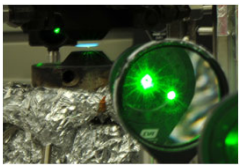


Soot models depend on flow configurations they are based on

Experiment

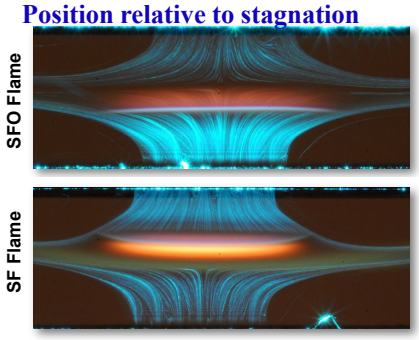
- **Counterflow flames**





- **Laser-based measurement**
  - LE/LS
  - LII
  - PAH fluorescence
  - LDV/PIV
  - CARS

- **Position relative to stagnation**

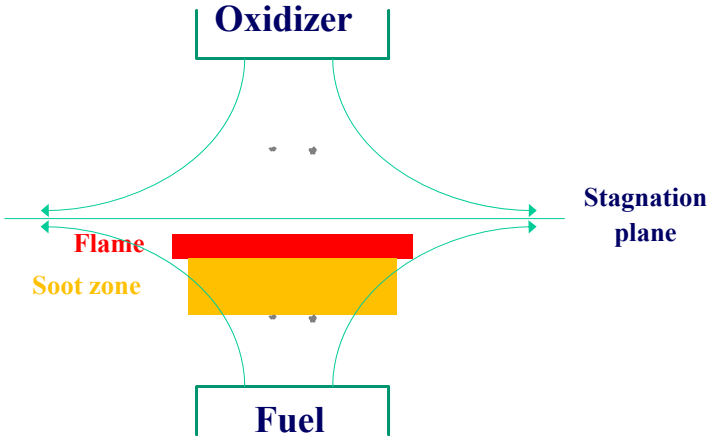


$X_{C2H4} = 0.106$ $X_{O2} = 0.833$

$X_{C2H4} = 0.745$ $X_{O2} = 0.257$

Counterflow Flames

KT Kang, JY Hwang, SH Chung, W Lee, "Soot zone structure and sooting limit in diffusion flames: Comparison of counterflow and coflow flames," *Combust. Flame* 109 (1997) 266-281.

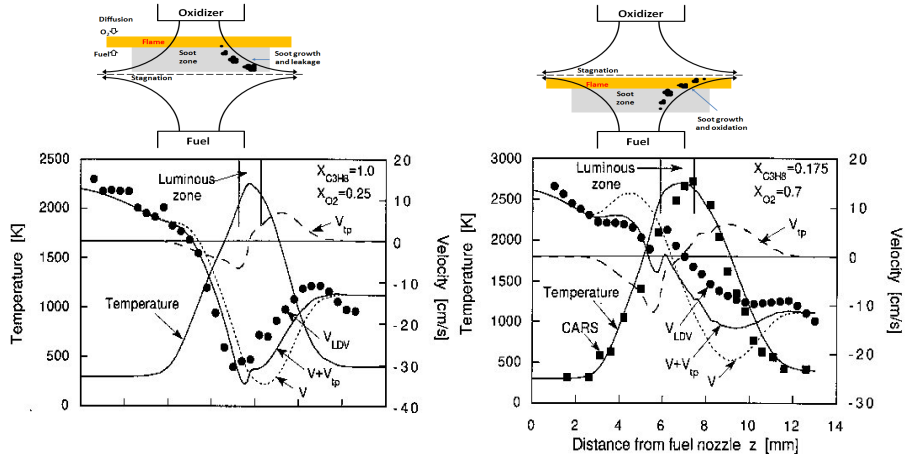


Soot formation/oxidation (SF/SO) flame

Abhijeet Raj
abhijeet.raj@kaust.edu.sa

Counterflow Flame Structure

- Soot Formation Flame
- Soot Formation/Oxidation Flame



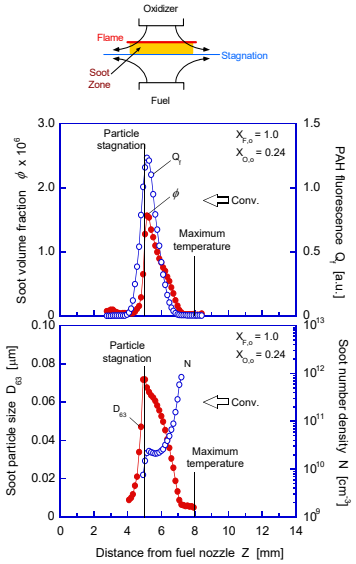
Thermophoretic Effect : Particle motion in temperature gradient by molecular collision

Thermophoretic velocity

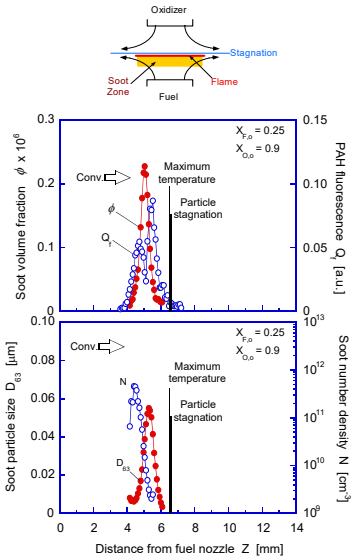
$$V_{tp} = -\kappa \frac{3\nu}{4(1+\pi a/8)} \frac{\nabla T}{T}$$

Soot Zone Structures

- **Soot formation flame**



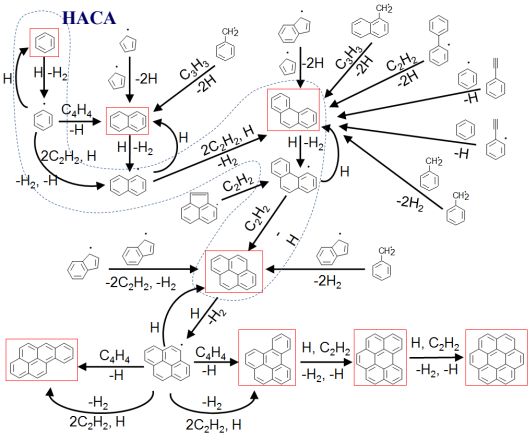
- **Soot formation/oxidation flame**



PAH Mechanism Development

PAHs

Benzene (A1)	Naphthalene (A2)	Phenanthrene (A3)	Pyrene (A4)
Benzyl[e]pyrene (A5)	Benzyl[ghi]perylene (A6)	Coronene (A7)	



Mechanism of Marshal et al. (2009)
154 species and 1404 reactions
up to pyrene

New mechanism up to coronene
231 species and 2126
(77 species and 722 reactions added)

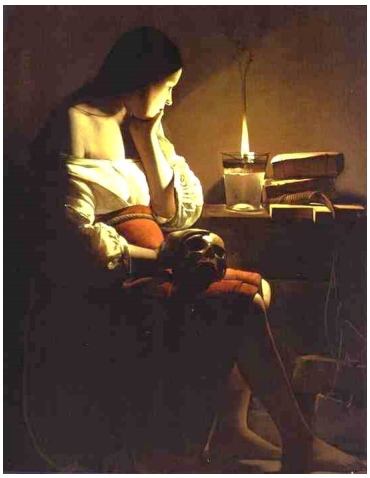
A Raj, IDC Prada, AA Amer, SH Chung, "A reaction mechanism for gasoline surrogate fuels for large polycyclic aromatic hydrocarbons," *Combust. Flame* 159 (2012) 500-515 **(KAUST PAH Mech 1)**

Y Wang, A Raj, SH Chung, "A PAH Growth Mechanism and Synergistic Effect on PAH Formation in Counterflow Diffusion Flames," *Combustion and Flame* 160 (2013) 1667-1676 **(KAUST PAH Mech 2)**

Smoke Point Lamp

- ASTM D1322
- Maximum flame height obtainable without smoking

Watson et al.
Fuel 2013

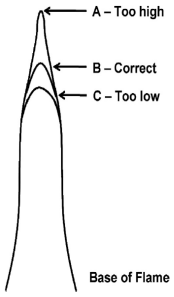


Magdalene with the Smoking Flame
Georges de La Tour 1640

Quantitative sooting metric based sooting limits

- **Existing sooting metrics**
  - **Threshold soot index (TSI)** *Calcote and Manos, CNF 1983*
  - **Normalized smoke point (NSP)** *Li and Sunderland, CST 2012*
  - **Yield soot index (YSI)** *McEnally and Pfefferle, CNF 2007*
  - **Oxygen extended sooting index (OESI)** *Barrientos et al, CNF 2013*

- **Based on smoke-point flame or co-flow flame**
  - **Competition between formation and oxidation**
  - **Low strain**
  - **Typically pure fuel / air**
    - **Dilution effect:** *Yelverton and Roberts, CST 2008*
  - **Subjectivity in determining smoke point position**
    - *Watson et al, Fuel, 2013*
  - **Coflow velocity** *Yelverton and Roberts, CST 2008*



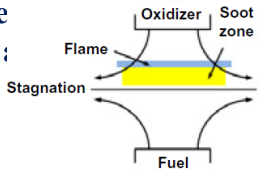
(a) Determination of the Smoke Point according to ASTM D1322

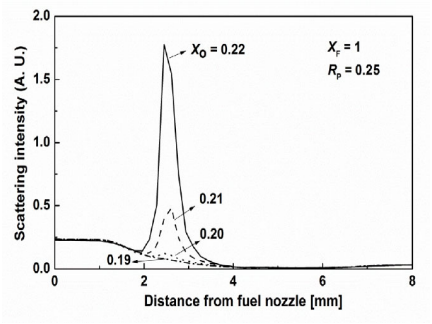
Watson et al. Fuel 2013

Sooting limit in counterflow: definition

- Critical sooting condition in counterflow diff usion flame represented by *sooting limit*

- Sooting limit is defined as critical fuel/oxyge n mole fraction ($X_{F,cr}$ / $X_{O,cr}$) when soot just bout to appear





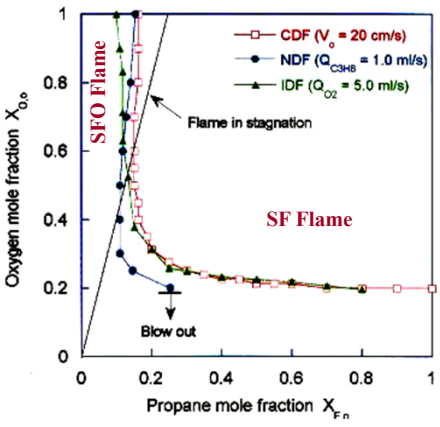
For fixed X_F

Increase X_O at 0.01 interval until local peak appears

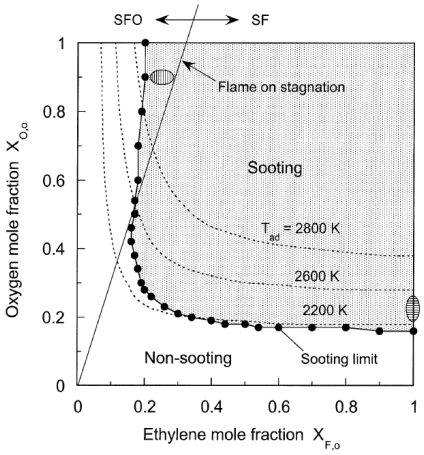
Following CK Law

Counterflow Sooting Limit Map

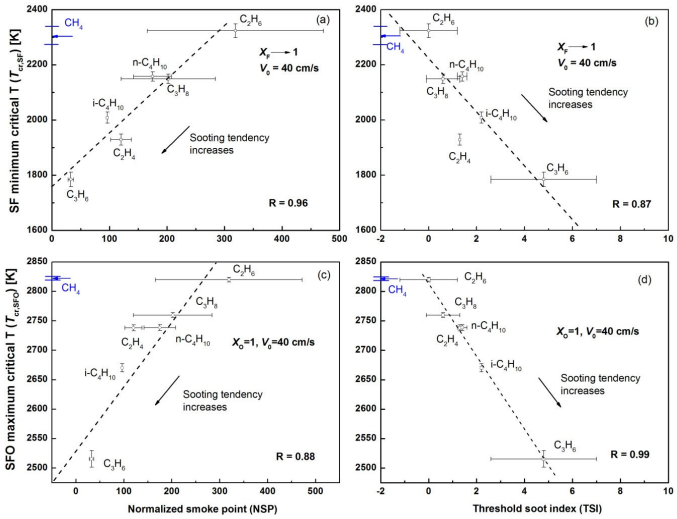
Kang et al., CNF 1998



Hwang & Chung, CNF 2001

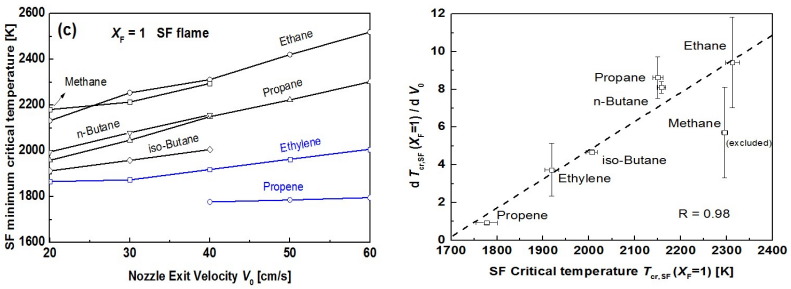


Sooting Temperature Index (STI)



Define the minimum/maximum temperature along sooting limit as STI
Correlation between STI and TSI/NSP is good
Uncertainty in STI may be much smaller

Strain Rate Effect on Sooting Limit



- **Critical temperature increases with V_0**
- **The sensitivity of STI to V_0 is fuel dependent**
- **Fuels having higher STI is more sensitive to V_0**
- **Define $dT_{cr,SF}/dV_0$ as sooting sensitivity index (SSI) to represent the effect of strain on sooting tendency**

Sooting Sensitivity Index (SSI) can be defined
SSI correlated wit STI

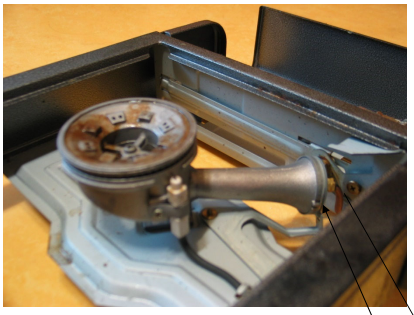
Premixed Flames

Introduction

- **Premixed Flame : Important Parameter S_L^o**
  - **Laminar Burning Velocity / Laminar Flame Speed**
  - **Propagation velocity of 1D, planar premixed flame in the absence of heat loss**
  - **Representing reactivity, exothermicity**
  - **Essential in the design of practical devices**

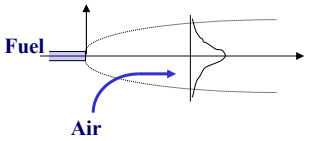
- **Relevant Phenomena**
  - **Flashback**
  - **Blowoff**

Gas Range

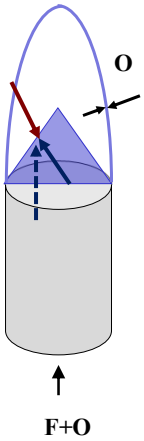


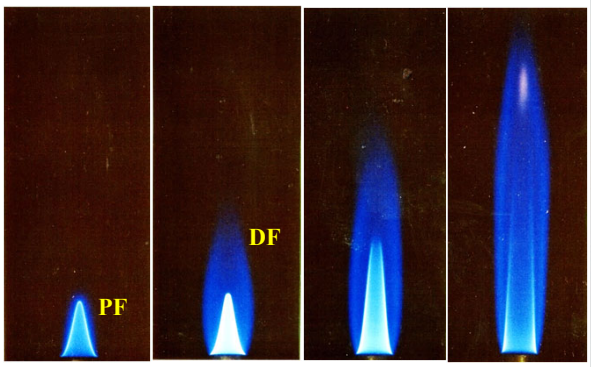
Fuel nozzle

Air entrainment



Premixed Flames w/ Decreasing Air

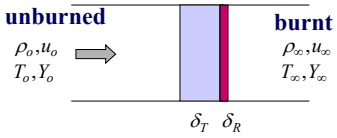




Decreasing air

Laminar Burning Velocity

- **Phenomenological Derivation**
  - **1D, Planar, Steady propagation**
  - **Flame stationary coordinate**
  - **Assume constant pressure:** $\Delta p/p=10^{-5}$
  - **Sufficiently off-stoichiometric**
  - **One-reactant reaction : [R] → [P]**



Preheat zone
Reaction zone

(1) Mass conservation $\rho_o u_o = \rho_\infty u_\infty = \rho_o S_L^o$

(2) Conv-Diff – Rea balance $\rho_o S_L^o Y_o = \rho D \frac{Y_0}{\delta_T} = Y_o \bar{\omega} \delta_R$

(3) Energy Balance $\lambda \frac{T_\infty - T_o}{\delta_T} = Y_o \bar{\omega} \delta_R Q$

(4) Energy conservation $Y_o Q = C_p \left(T_\infty - T_o \right)$

(5) Large activation energy $\frac{\delta_R}{\delta_T} = \varepsilon \equiv \frac{T_\infty}{E_a / R^o}$

Laminar Burning Velocity

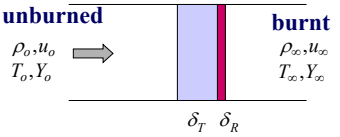
- **(3),(4) → (2)** $\frac{\lambda}{C_p} \frac{1}{\varepsilon \bar{\omega}} = \delta_T^2 \quad \therefore \delta_T = \sqrt{\frac{\lambda}{C_p} \frac{1}{\varepsilon \bar{\omega}}}$
- **Diffusion – Convection Balance**

$$\rho_o S_L^o Y_o = Y_o \bar{\omega} \delta_R = Y_o \bar{\omega} \varepsilon \delta_T$$

$$\therefore \; S_L^o = \frac{1}{\rho_o} \sqrt{\frac{\lambda}{C_p} \varepsilon \bar{\omega}}$$

- **Note:**

$$\rho_o \sim p$$
$$\bar{\omega} \sim p^n \exp(-E_a / R^o T_\infty)$$



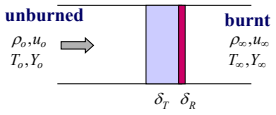
$$S_L^o \sim p^{n/2-1} \left(\frac{\lambda}{C_p}\right)^{1/2} \exp\left(-\frac{E_a}{2R^o T_\infty}\right)$$
$$T_\infty = T_o + Y_o Q / C_p$$

Kinetic factor : P, Arrhenius term
Transport factor : $(\lambda/C_p)^{1/2}$

For 2nd order reaction $n = 2$, S_L^o **independent of pressure**
HC fuels, S_l^o decreases with pressure

Laminar Burning Velocity

- From (2,5) $\delta_T = \frac{D}{S_L^o} = \frac{\lambda}{\rho_o C_p S_L^o}$ $S_L^o = \frac{1}{\rho_o}\varepsilon\bar{\omega}\delta_T$

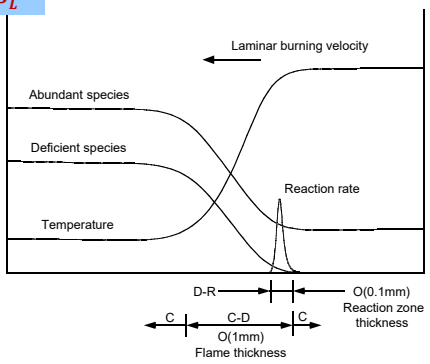


- From (3, 4) $\delta_T^2 = \frac{\lambda}{C_p}\frac{1}{\varepsilon\bar{\omega}}$ $\delta_T = \sqrt{\frac{\lambda}{C_p}\frac{1}{\varepsilon\bar{\omega}}}$

$$S_L^o = \frac{1}{\rho_o}\sqrt{\frac{\lambda}{C_p}\varepsilon\bar{\omega}}$$

- Flame thickness (Le=1) $\delta_T = \frac{\alpha}{S_L^o}$

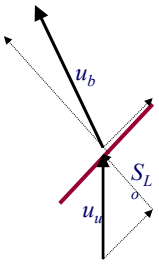
$\alpha = O(1\text{cm}^2/\text{s})$ at 1000K
$S_L^o = O(10 \sim 100\ \text{cm/s})$
$\delta_T = O(1\ \text{mm} \sim 0.1\ \text{mm})$
$\delta_R = O(0.1\ \text{mm} \sim 0.01\ \text{mm})$



Burning Velocity Measurement

- Difficulty :
  - 1D planar flame is difficult to stabilize (rarely exists)
  - Frequently flame is curved
  - Definition of flame front for curved one is difficult
  - Flame location depends on optical methods
    (direct photography, shadowgraphy, schlieren, interferometry)

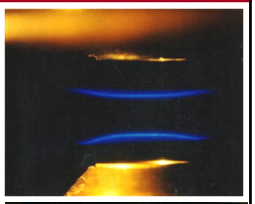
- Local burning velocity
  - For stationary surface
  - Normal: continuity of mass flux
  - Tangential: continuity of velocity

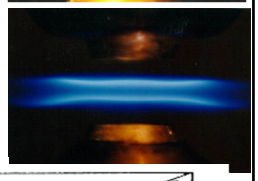


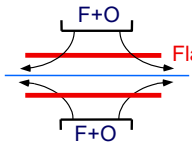
- Measurement
  - Outwardly Propagating Spherical Flame
  - Counterflow flames

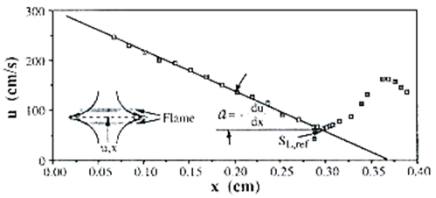
Aerodynamics

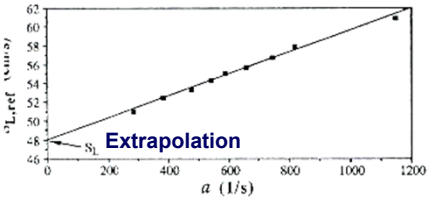
- Flame Stretch $\kappa \sim U_o/l$
- Laminar burning velocity is for planar flame w/ $\kappa = 0$
- Counterflow – planar flame stabilized
- Widely accepted as an accurate method





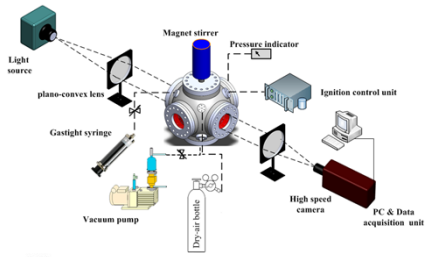


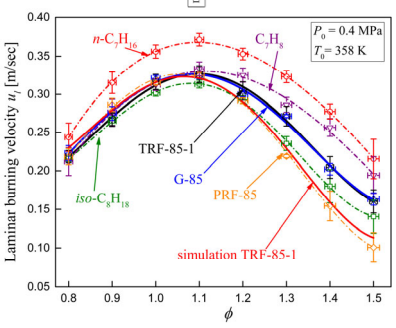


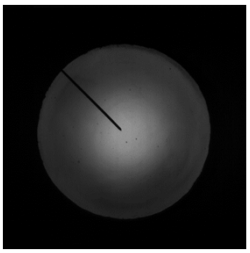


Law

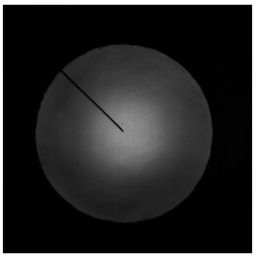
Spherical Flame Method







Gasoline50/Pentene50-1bar 358K-Stoich

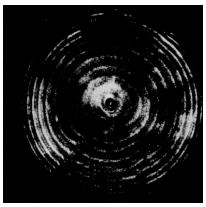


Gasoline50/Pentene50-5bar 358K-Stoich

Mannaa, Mansour, Roberts, Chung, "Laminar Burning Velocities at Elevated Pressures for Gasoline and Gasoline Surrogates Associated with RON", *Combust. Flame* 162 (2015) 2311–2321.

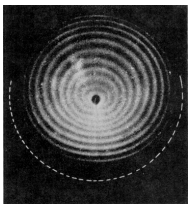
Spherical Flame Method

- **Factors need to be considered**
  - **Pressure rise**
  - **Ignition transient / Unsteady transition / Quasi-steady propagation / Chamber affect propagation**
  - **Extrapolation method**
    - o **Linear model**
    - o **Non-linear models**
- **Limitations**
  - **Cellular instability**
  - **Buoyancy effect for small S_L^o**



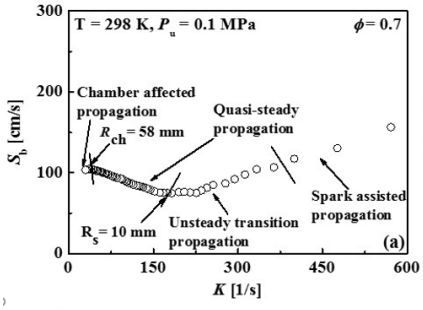
CO flame

Lewis and von Elbe



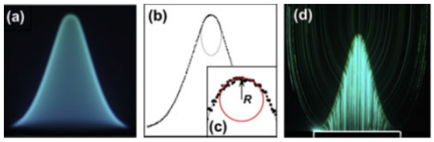
CO flame (very rich)

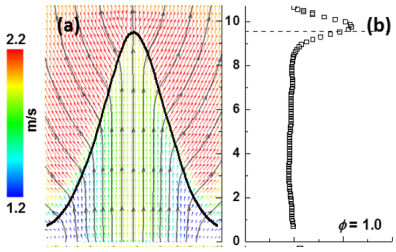
Slow burning case

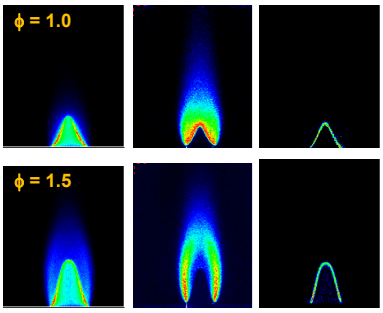


Kim, Van, Lee, Park, Chung, "Laminar flame speed, Markstein length, and cellular instability for spherically propagating methane/ethylene-air premixed flames," 214 (2020) 464

Bunsen Flame Structure





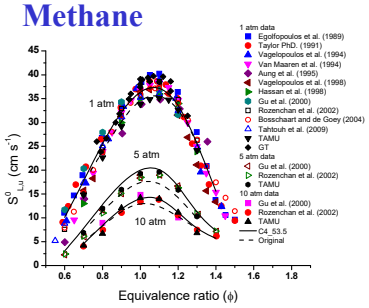


Direct | OH PLIF | CH Chemi-luminescence

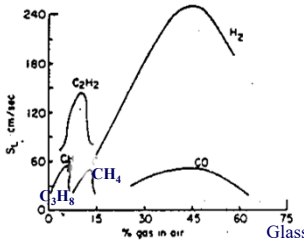
TM Vu, MS Cha, BJ Lee, SH Chung, "Tip opening of premixed bunsen flames: Extinction with negative stretch and local Karlovitz number," Combust. Flame 162 (2015) 1614–1621.

Laminar burning velocity

- **Methane**

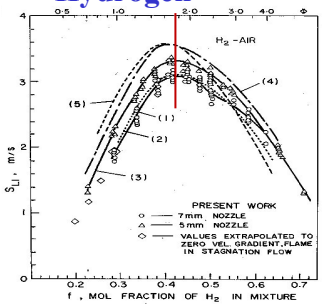


Maximum near near $\phi \approx 1.1$ Curran
for HC fuels



Glassman

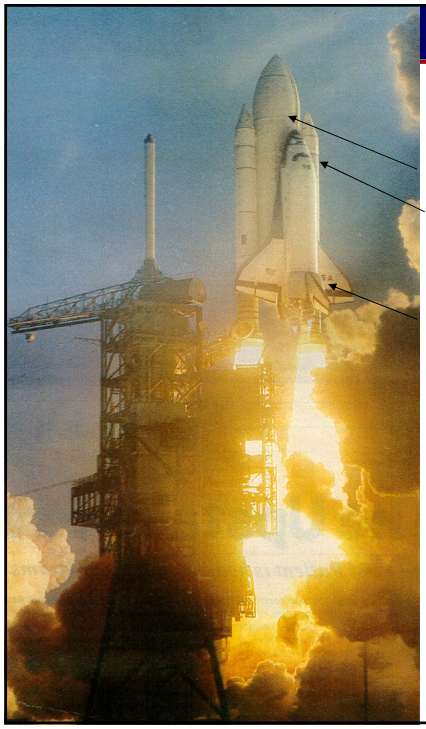
- **Hydrogen**



Maximum near $\phi \approx 1.8$ Law

- **Influenced by**
  - **Fuel type**
  - **Equivalence ratio**
  - **Transport properties**
  - **Initial temperature**
  - **Pressure**

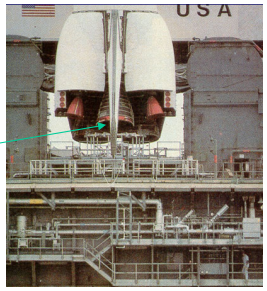
Space Shuttle



External fuel tank

Booster rocket

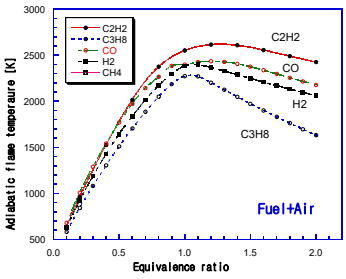
Shuttle



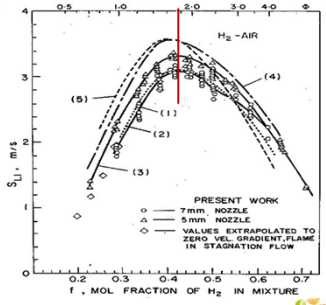
Main nozzle

Space Shuttle

- Total weight : 1215 Ton
- External fuel tank : h 47 m, d 8.6 m
  - Oxygen 585 ton + Hydrogen 100 ton
  - H/O mass ratio = 1: 5.8 (ϕ = 1.38)
  - Stoichiometry $H_2 + (1/2)\, O_2 \rightarrow H_2O$ (1:8)
  - Burning duration : 8 min, 1.4 ton/s
  - Why ϕ = 1.38?
- Booster Rocket
  - Oxygen 585 ton + Hydrogen 100 ton
  - Composite propellant : AP+ binder+ Al, Bo
  - Burning duration : 83 s

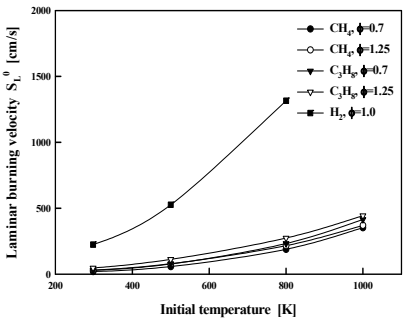


Adiabatic flame temperature

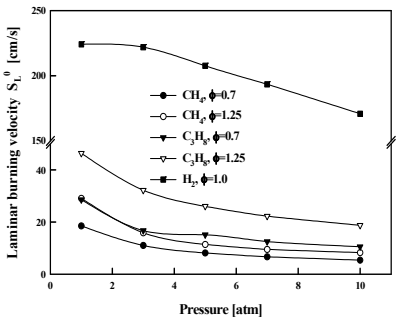


T_0 and P_0 Effect

- Effect of T_o
  - T_{ad} → Reaction rate through $T_\infty = T_o + Y_o Q/C_p$
  - Change in density $S_L \sim 1/\rho_o \sim T_o$



S_L^o for CH_4, C_3H_8, H_2 with T_0
Reasonably ~T_0^2



S_L^o for CH_4, C_3H_8, H_2 with P_0

ES Cho, TK Oh, SH Chung, "Local Karlovitz numbers at extinction for various fuels in counterflow premixed flames," *Combust. Sci. Technol.* 178 (2006) 1559-1584.

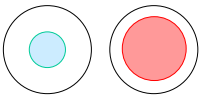
SI Engine

- SI Engine, Bore 10cm, 3000 rpm= 50 rps
- Combustion duration 36 CA = 2 ms available
- 5cm×500/s = 25m/s required: Maximum $S_l^o \approx 0.5$ m/s : 50 times faster
- During compression
  - $Tv^{r-1} = const$, $\gamma = 1.4$, CR = 10.5, $T_o = 770$K
  - $T_{max} = 2200$K for $\phi = 1$, $T_o = 300$K
  - For $T_{max} = 2670$K, $E_a = 20{,}000$K

$$\frac{S_L(E/G)}{S_L(STP)} = \frac{\exp(-E_a/2R^oT_{E/G})}{\exp(-E_a/2R^oT_{STP})} \approx 2.5$$

  - Considering S_L increase, the burning in SI E/G is still 20 times faster than S_L^o

- Burnt gas expansion effect 2670K vs 770K: 3 times
- Secondary compression
- Turbulence effect
  - Depends on speed
  - Turbulence generation and decay



Flammability Limit

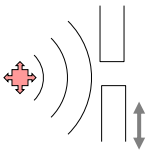
- Not all mixtures are flammable
- Standard: US Bureau of Mines
  - Glass tube ϕ=5.1 cm, 150cm (120-180) long
  - Once flame can not reach the top : Limit of flame propagation

Fuel	Flammability (ϕ)		d_q	E_{min}
	Lean	Rich	Abs min(mm)	Abs min(mJ))
Hydrogen H_2	0.14	2.54	0.61	0.018
Carbon monoxide CO	0.34	6.76	—	—
Methane CH_4	0.46	1.64	2.0	0.29
Propane C_3H_8	0.51	2.83	1.8	0.26
n-Octane C_8H_{18}	0.51	4.25	—	—
AcetyleneC_2H_2	0.19	∞	2.3 (ϕ=1)	0.03 (ϕ=1)
MethanolCH_3OH	0.48	4.08	1.5	0.14

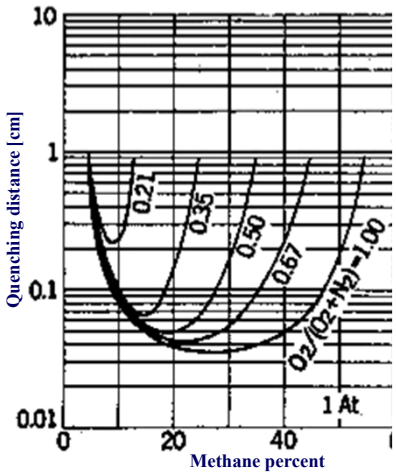
LvE F152
Cf: K p130

Quenching Distance (Diameter)

- Maximum distance that a flame can not penetrate
  - Application
    - Mine fire safety (grating or mesh)
    - Gas range nozzle hole
    - Flame arrester
  - Effect of wall
    - Heat loss
    - Radical destruction

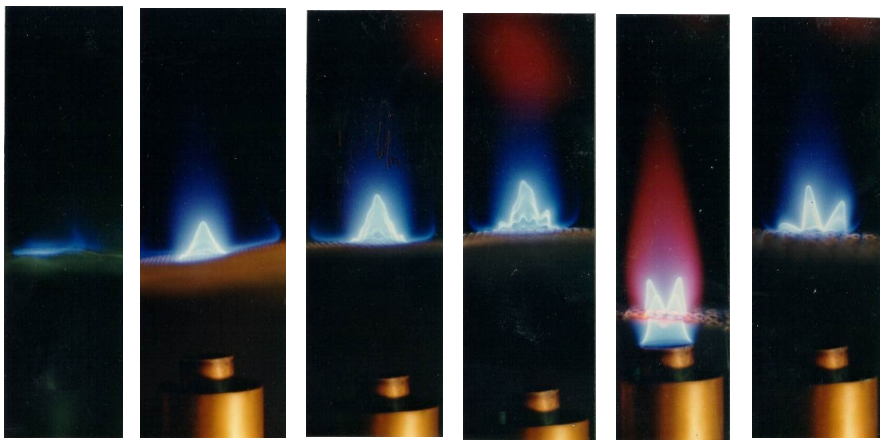


Stop gas flow &
Check whether
flashback

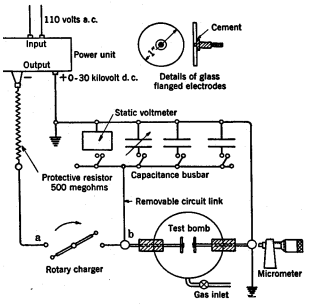


LvE F160

Flame Quenching

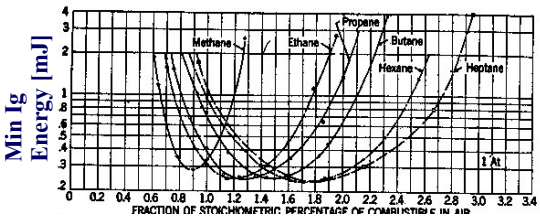


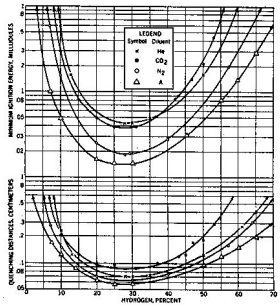
Minimum Ignition Energy



Combustion vessel D > 30cm
W/ glass flange

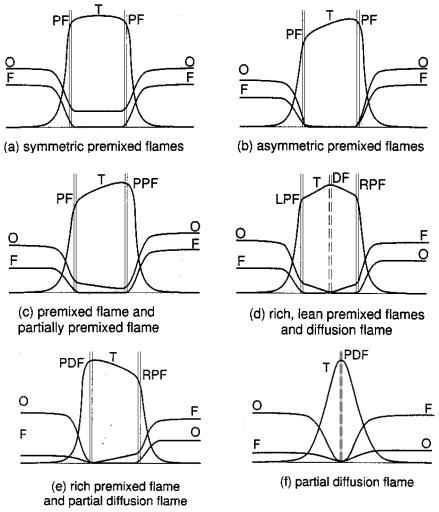
Scheme of apparatus for determining minimum ignition energies for electric-spark ignition (Blanc, Guest, von Elbe, and Lewis).





LvE F153

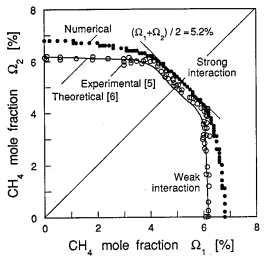
Flame Interaction: Flammability



(a) symmetric premixed flames
(b) asymmetric premixed flames
(c) premixed flame and partially premixed flame
(d) rich, lean premixed flames and diffusion flame
(e) rich premixed flame and partial diffusion flame
(f) partial diffusion flame

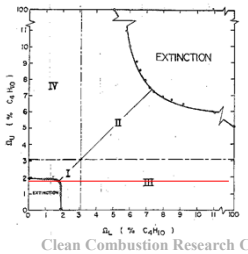
Possible modes of downstream interaction between two premixed flames (CK Law)

SH Chung, "Interaction of Flames," Chap 20, Handbook of Heat and Mass Transfer 4 (1990) 863-891, N.P. Cheremisinoff (Ed.), Gulf Publ. Co.

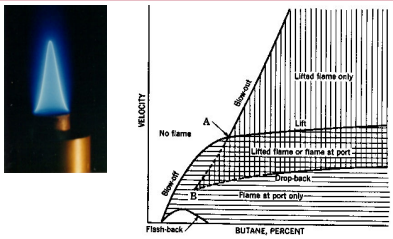


Extinction boundaries for lean methane/air mixture

Chung, Kim, Law, "Extinction of interacting premixed flames: Theory and experimental comparisons," *PCI* 21 (1986) 1845

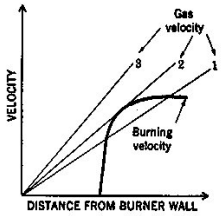


Flame Stability Map: Butane



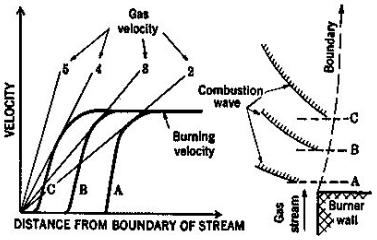
LvE

Flashback



Flame travels into tube
- **Penetration distance $d_p = d_q/2$**
- **Velocity near wall approximated as linear**

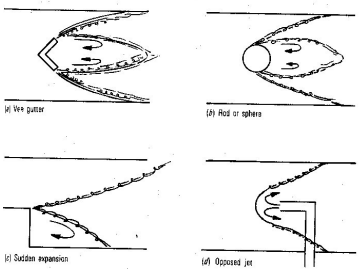
Blowoff

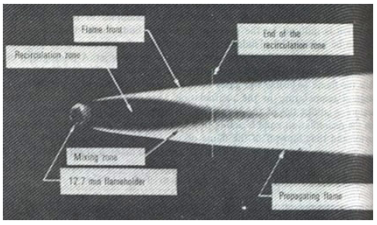


Velocity : Linear characteristics
Burning velocity: concentration

Flame Stabilization

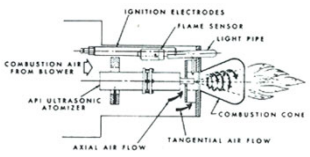
- **Flame holder : High velocity**
  - **Vee gutter, Bluff body**
  - **Sudden expansion, Opposed jet**



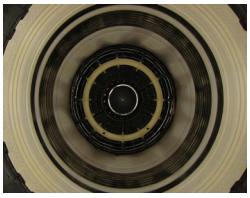


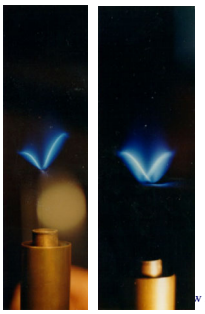
LvE

Swirl flow



Afterburner – T50



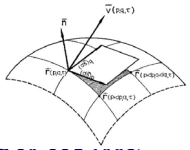


Factors Influencing Flame

- Aerodynamic Stretching
  - Convective non-uniformity & unsteadiness
  - Flame stretch
- Preferential Diffusion & Differential Diffusion
  - Unequal diffusion rates
  - Non-unity Lewis number effect
- Heat Loss : Non-adiabaticity
  - Conduction & Radiation
  - Mixing : Burnt gas
  - Flame interaction
- Intrinsic Instability
  - Diffusional - thermal instability
  - Hydrodynamic instability
  - Acoustic instability
  - Buoyancy-driven instability

Aerodynamics : Flame Stretch

- Representing Aerodynamic Effect on Flame: κ
- History
  - Karlovitz, 1953 du/dy
  - Williams, 1975 $\kappa = (1/A)(dA/dt)$ $[t^{-1}]$
  - Buckmaster (Acta Astro 6:741 1979), Matalon (CST 29:225 1983)
  - Chung & Law (CNF 55:123, 1984)



$$\kappa = \nabla_t \cdot V_t + (V \cdot n)(\nabla_t \cdot n)$$

Tangential flow non-uniformity
Curvature of propagating flame

  - $V_t = v_t$: flow velocity along tangential to flame
  - V : Flame surface velocity
  - Curvature : $(\nabla_t \cdot n)$
- The effect arises from the difference between streamline (convection) and flame normal (diffusion) directions
  - Flame temperature, burning velocity, extinction etc.
  - Flame stretch represents the inverse of characteristic flow time
  - Related to Damköhler number

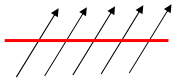
Chung, Law, "An invariant derivation of flame stretch," *Combust. Flame* 55 (1984) 123-125.

Flame Stretch

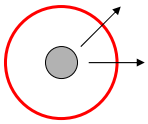
$$\kappa = \nabla_t \cdot \mathbf{v}_t + (\mathbf{V}\cdot\mathbf{n})(\nabla_t \cdot \mathbf{n})$$

Tangential non-uniformity
+ Curvature of propagating flame

- No Stretch Effect



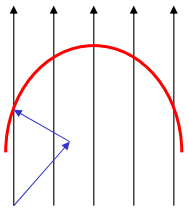
Uniform tangential velocity field



Steady spherical flame

- Stretch Effect

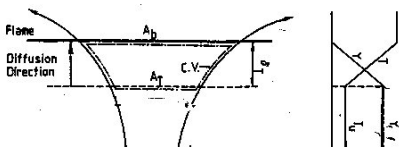
Non-uniform tangential velocity field



Curved flame in uniform field

Stretch Effect (Le=1)

- Planar Flame in Diverging Flow



Continuity $\rho_b \upsilon_b A_b = \rho_u \upsilon_u A_T$

Energy Conservation

$$C_p\left(\rho_b \upsilon_b A_b T_b - \rho_T \upsilon_T A_T T_u\right) + \left(A_b - A_T\right)\lambda\frac{T_b - T_u}{\delta} = \left\{\rho_T \upsilon_T A_T Y_u + \left(A_b - A_T\right)\rho D\frac{Y_u}{\delta_T}\right\}Q$$

Convection out | Convection in | Diffusion out | Convection | Diffusion | Generation

$$C_p\left(T_b - T_u\right)\left[1 + \frac{A_b - A_T}{A_b}\frac{\lambda}{C_p}\frac{1}{\delta}\frac{1}{\rho_b \upsilon_b}\right] = Y_u Q\left[1 + \frac{A_b - A_T}{A_b}\rho D\frac{1}{\delta}\frac{1}{\rho_b \upsilon_b}\right] \qquad \therefore C_p\left(T_b - T_u\right) = Y_u Q$$

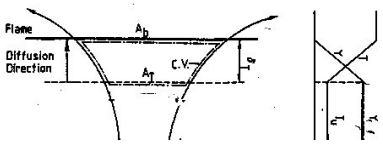
Diffusion-Reaction Balance

$$\lambda\frac{T_b - T_u}{\delta}A_b = Y_u \bar{\omega}\delta Q A_b \qquad \therefore \delta = \sqrt{\frac{\lambda}{C_p}\frac{1}{\bar{\omega}}}$$

Chung, Law, An integral analysis of the structure and propagation of stretched premixed flames, *CNF* 72 (1988) 325

Stretch Effect (Le=1)

- **Planar Flame in Diverging Flow**



Convection-Diffusion Balance

$$\rho D\frac{Y_u}{\delta}A_b = Y_u\rho_u\upsilon_u A_T + \rho D\frac{Y_u}{\delta}\left(A_b - A_T\right)$$

$$\upsilon_u = \frac{1}{\rho_u}\frac{\lambda}{C_p}\frac{1}{\delta} = S_f^o$$

Burning rate $\rho_b\upsilon_b \equiv \rho_u S_f$

Velocity at upstream $\rho_b\upsilon_b = \frac{A_T}{A_b}\rho_u\upsilon_u = \rho_u S_f = \frac{A_T}{A_b}\rho_u S_f^o$

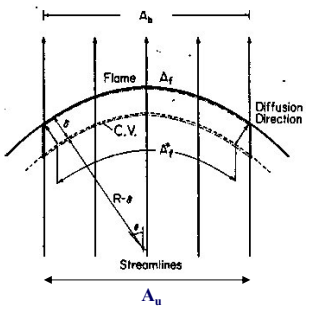
$$\therefore \frac{S_f}{S_f^o} = \frac{A_T}{A_b} = 1 - \frac{A_b - A_T}{A_b}$$

Flame stretch $\kappa = \frac{A_b - A_T}{A_b}\frac{S_f^o}{\delta}$

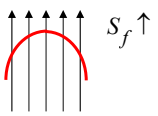
$$\boxed{\frac{S_f}{S_f^o} = 1 - \frac{\lambda}{\rho_u C_p}\frac{\kappa}{S_f^{o2}}}$$

Positive stretch decreases burning rate

Curved Flame in Uniform Flow Field



Negative curvature



Continuity $\rho_u\upsilon_u A_u = \rho_b\upsilon_b A_b \quad A_u = A_b$

$$\therefore \rho_u\upsilon_u = \rho_b\upsilon_b = \rho_u S_f$$

D-R Balance $\lambda\frac{T_b - T_u}{\delta} = \rho D\frac{Y_u}{\delta}Q = Y_u\bar{\omega}\delta Q$

Energy Conservation $Y_u Q = C_p(T_b - T_u) \;\therefore \delta = \sqrt{\frac{\lambda}{C_p\bar{\omega}}}$

Convection-Diffusion Balance

$$\rho D\frac{Y_u}{\delta}A_f = Y_u\rho_u\upsilon_u A_u - \rho D\frac{Y_u}{\delta}\left(A_f - A_f^*\right)$$

$$\therefore S_f = \frac{1}{\rho_u}\bar{\omega}\delta\frac{2A_f - A_f^*}{A_u} \qquad A_f = R_1R_2\left(4\theta_1\theta_2\right)$$

Geometric Relation $A_f^* = \left(R_1 - \delta\right)\left(R_2 - \delta\right)\left(4\theta_1\theta_2\right)$

$$A_u = R_1R_2\left(4\sin\theta_1\sin\theta_2\right)$$

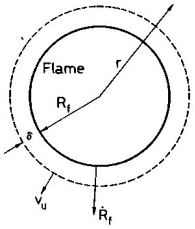
Since $S_f^o = \frac{1}{\rho_u}\sqrt{\frac{\lambda}{C_p}\bar{\omega}}$

$$\therefore \frac{S_f}{S_f^o} = 1 + \left(\frac{\delta}{R_1} + \frac{\delta}{R_2}\right) \qquad \text{as } \theta \to 0$$

Stretch $\kappa = -S_f^o\left(\frac{1}{R_1} + \frac{1}{R_2}\right) \quad \frac{S_f}{S_f^o} = 1 - \frac{\delta}{S_f^o}\kappa$

Spherically Propagating Flame

$\nabla_t \cdot \mathbf{v}_t = 0 \quad (\mathbf{V}\cdot\mathbf{n}) = \dot{R}_f \qquad \nabla_t \cdot \mathbf{n} = \frac{2}{R} \qquad \kappa = 2\dot{R}_f / R_f$



Density change $\rho_b \rightarrow \rho_b$

Rate of change of mass in burnt region = Mass dispersion rate

$$(\rho_u - \rho_b)\frac{d}{dt}(\frac{4}{3}\pi R_f^3) = \rho_u 4\pi r^2 \dot{r} \quad \text{for } r > R_f + \delta \qquad (1-\frac{\rho_b}{\rho_u})R_f^2 \dot{R}_f = r^2 \dot{r}$$

At $r = R_f + \delta$: $\dot{r} = v_u$

$$v_u \simeq (1 - \frac{\rho_b}{\rho_u})\dot{R}_f(1 - \frac{2\delta}{R_f})$$

Flame fixed coordinate $v_{rel} \equiv \dot{R}_f - v_u = \frac{\rho_b}{\rho_u}\dot{R}_f + \frac{2\delta}{R_f}\dot{R}_f(1-\frac{\rho_b}{\rho_u})$

Thermal diffusion-Mass diffusion -Reaction Balance $\lambda\frac{T_b - T_u}{\delta} = \rho D\frac{Y_u}{\delta}Q = Y_u\bar{\omega}\delta Q$

Energy Conservation $Y_u Q = C_p(T_b - T_u) \qquad \therefore \delta = \sqrt{\frac{\lambda}{C_p\bar{\omega}}}$

Mass Diffusion – Reactant supply Balance $\rho D\frac{Y_u}{\delta}R_f^2 = Y_u\rho_u v_{rel}(R_f + \delta)^2$

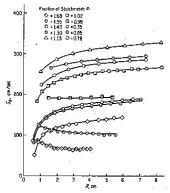
Relative velocity in burnt side which is stagnant $\rho_b \dot{R}_f = \rho_u S_f$

Flame speed relation

$$\frac{S_f}{S_f^o} = 1 - \frac{2\delta}{R_f}\{(\frac{\rho_b}{\rho_u} - 1) + 1\}$$

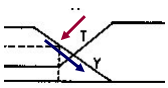
↓ area change

↓ gas motion



Preferential Diffusion

- **Thermal diffusion acts as heat loss from flame**
- **Mass diffusion acts as heat gain by reactant supply**

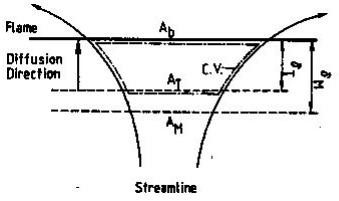


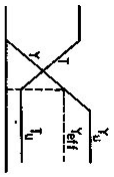
- **Relative intensity can be characterized by Lewis number Le**

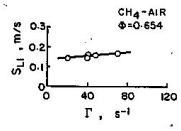
$$Le = \frac{\lambda/\rho C_p}{D} = \frac{\text{Thermal diffusivity}}{\text{Mass diffusivity}}$$

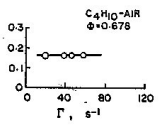
- **Lewis number may affect flame characteristics**
  - **Flame temperature**
  - **Flame speed**
  - **Flame stability : Diffusional – Thermal Instability**
  - **Extinction characteristics**

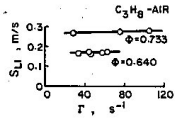
Flame Stretch & Preferential Diffusion

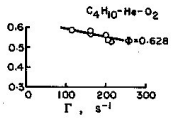












$$T_b = \left(T_u + \frac{Y_u Q}{C_p}\right) + \frac{Y_u Q}{C_p}\left(\frac{1}{Le} - 1\right)\left(\frac{\lambda}{\rho_u C_p}\right)\frac{\kappa}{S_f^{o2}}$$

$$\frac{S_f}{S_{f\,Le}^o} = 1 + \bar{K}\left[\frac{T_a Y_u Q}{2C_p T_{ad}^2}\left(\frac{1}{Le} - 1\right) + \left(\frac{1}{Le} - 1\right) - 1\right]$$

Temp Thickness

$$\bar{K} = \frac{\lambda}{\rho C_p}\frac{\kappa}{S_f^{o2}}$$

Stretch at Le=1

Law

If Le < 1, fast mass diffusion supplies chemical energy to flame
Increases flame speed for positive stretch

Ma & Ka

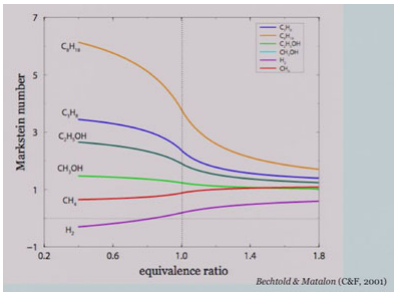
- **Karlovitz number: Non-D stretch effect**
- **Markstein number: Influence of stretch on flame speed**

$$S_f = S_L - \mathcal{L}K$$ stretch

$$\mathcal{L} = \left\{\frac{\sigma}{\sigma-1}\int_1^\sigma \frac{\lambda(x)}{x}dx + \frac{\beta(Le_{ff}-1)}{2(\sigma-1)}\int_1^\sigma \frac{\lambda(x)}{x}\ln\left(\frac{\sigma-1}{x-1}\right)dx\right\} l_f$$ = Markstein length

$$\frac{S_L}{S_L^o} = 1 - \mathrm{KaMa}$$

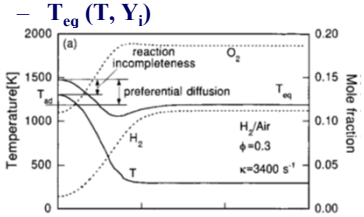
$$\mathrm{Ka} = \frac{\kappa}{S_L^o/\delta_o}$$

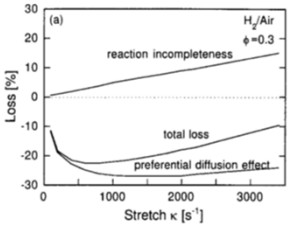


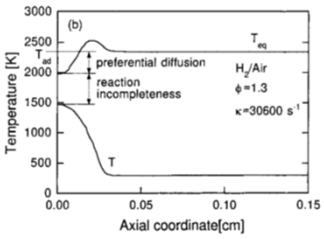
Local Equilibrium Temperature

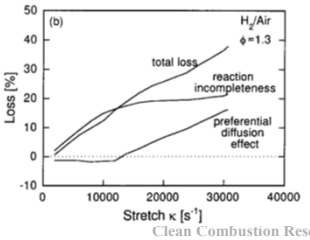
- How to quantify from numerical simulation
  - Insufficient time leading to incomplete reaction
  - Preferential effect
- Local Equilibrium Temperature
  - T_{eg} (T, Y_i)

Lee et al, "Local equilibrium temperature as a measure of stretch and preferential diffusion effects in counterflow H2/air premixed flames," *PCI* 27 (1998) 579



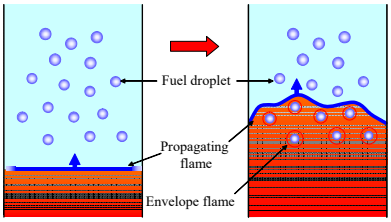




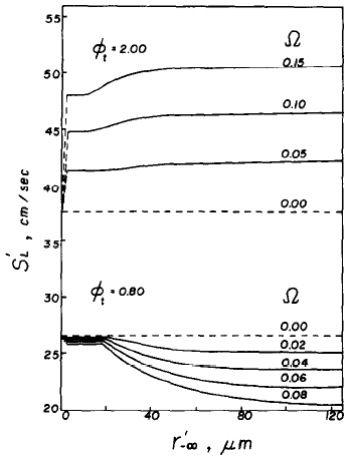


Premixed flame passing through sprays

Kobayashi



(a) n-decane spray. (b) n-octane spray.
Photograph of propagating flame front in microgravity.
(Nunome, Y., et al., Proc.Combust.Inst.29, 2002)



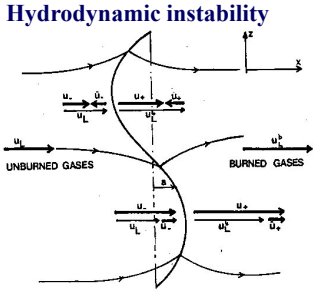
T.H. Lin, C.K. Law, S.H. Chung, "Theory of laminar flame propagation in off-stoichiometric dilute sprays," *Int. J. Heat Mass Trans*. 31(1988) 1023-1034

Combustion Instability

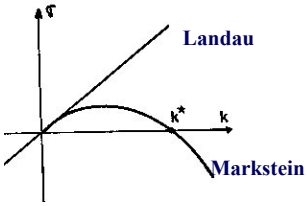
- **Intrinsic Instability**
  - Chemical kinetic instability
  - Hydrodynamic instability
  - Diffusional - thermal instability
- **Chamber Instability**
  - Acoustic instability
  - Shock instability
  - Fluid dynamic in chamber
- **System Instability**
  - Feed system interaction
  - Exhaust system interaction

Instability

Hydrodynamic instability

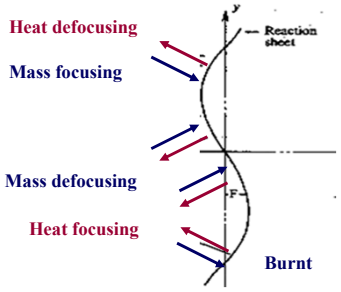


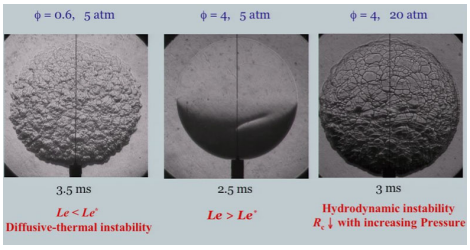
Amplitude growth rate vs wave number k (inverse of amplitude)



Small k (large wave length) : unstable
Large k (small wave length) : stable

Diffusional-Thermal instability

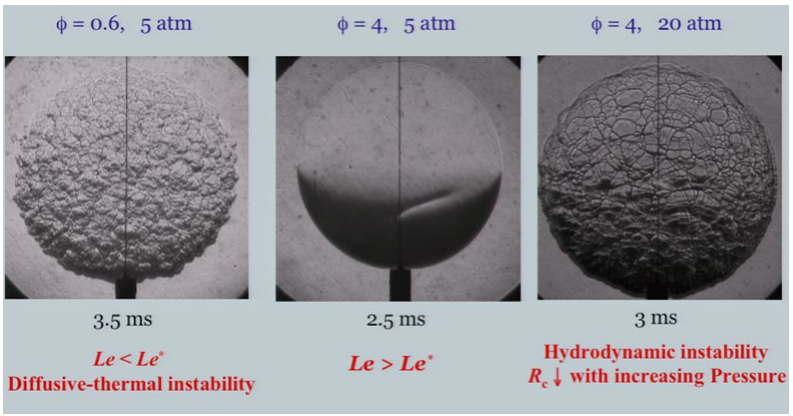




Hydrogen-Air Spherical Flame (CK Law)

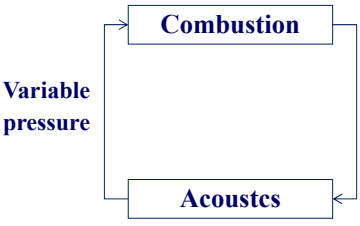
Diffusive-Thermal Instability

- **Hydrogen-Air Spherical Flame**
  - **CK Law**



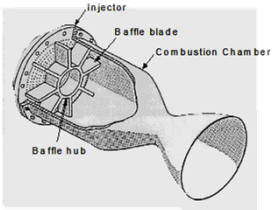
Acoustic Instability

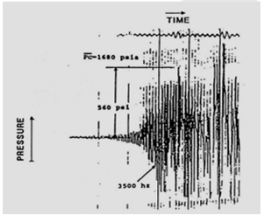
- **Thermo-acoustic instability**
- **Feedback mechanism (ref. Candel, 1992)**

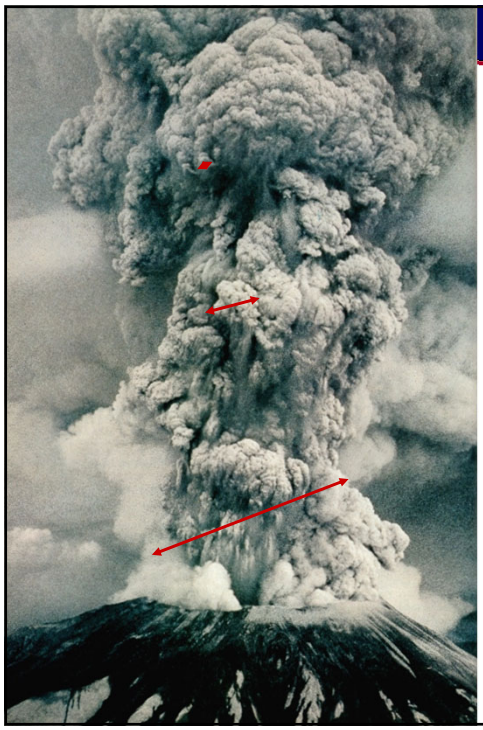


Rayleigh criterion

$$R = \int_T p'q'\,dt$$







Turbulent Jet

- Mt. St. Hellens eruption (80.5)
- Multiple scales
  - Integral scale (l_0)
  - Taylor microscale (λ)
  - Kolmogorov scale (η_K)
- Energy cascade
  - From large to small scales
  - Dissipation at smallest scale
- Flame thickness (δ)

NG

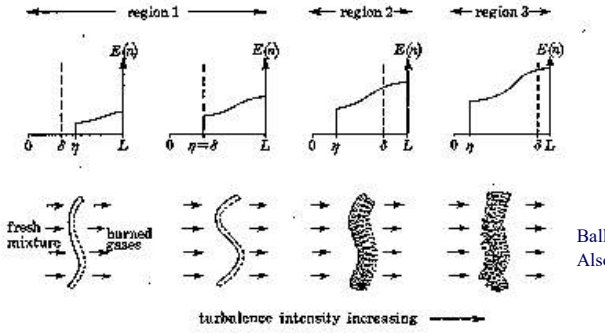
Scales

- Turbulent Flow
  - System characteristics
  - Length scales : integral scale, Kolmogorov scale
  - $k = 3u'^2/2 \quad \varepsilon = u'^3/l$
- Chemical scale
  - Flame speed S_L
  - Flame thickness δ

	Length	Time	Velocity
Integral scale	$l = (u'^3/\varepsilon)$	$\tau_l = l/u'$	$u' = (2k)^{1/2}$
Kolmogorov scale	$\eta_k = (\nu^3/\varepsilon)^{1/4}$	$\tau_k = (\nu/\varepsilon)^{1/2}$	$\upsilon_k = (\nu\varepsilon)^{1/4}$
Chemical scale	δ	$\tau_c = \nu/S_L^{o2} = \delta/S_L^o$	$u_c = S_L^o$

Turbulent Combustion Mode

- Relative Scales
  - Flow l, η_k versus chemical δ



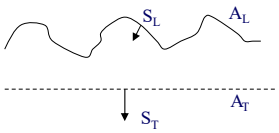
Ballal and Lefebvre
Also I Toong

Laminar Flamelet

Distributed Reaction Zone Model

Limiting Behavior

- **Large scale, low intensity regime ($\delta < \eta_k$)**
  - **Wrinkled laminar flamelet**
  - **$\rho_o S_T A_T = \rho_o S_L A_L$:**
  - **Damköhler (1940)** $\boxed{S_T/S_L^o = A_L/A_T}$
  - **Many models**
  - **e.g.: $A_L/A_T = 1+u'/S_L^o$: $S_T = S_L + u'$**



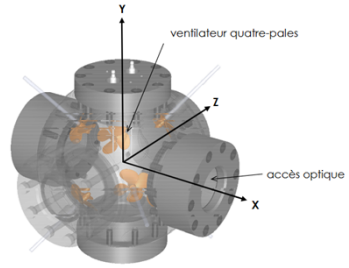
- **Small scale, high intensity regime ($\delta > l$)**

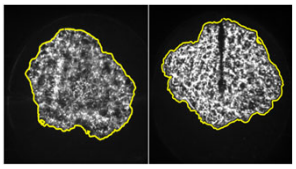
$$S_T = \frac{1}{\rho_o}\sqrt{(\lambda/C_p)_T \omega_T} \qquad S_L^o = \frac{1}{\rho_o}\sqrt{(\lambda/C_p)_T \omega_L}$$

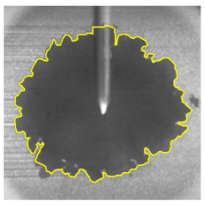
  - $\omega_L = \omega_T$ $\quad \frac{S_T}{S_L^o} = \sqrt{\frac{(\lambda/C_p)_T}{(\lambda/C_p)_L}}$
  - Turbulent diffusivity proportional to $u'l$ $\quad \boxed{\frac{S_T}{S_L^o} \sim R_l^{1/2}}$

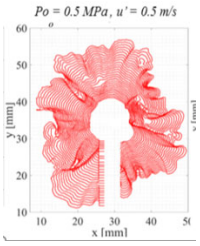
Turbulent Flame Speed Measurement

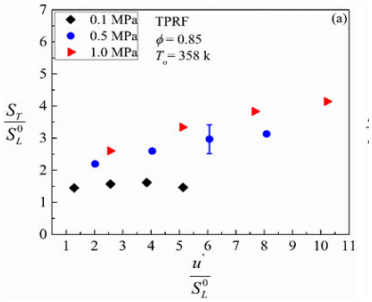
- **Spherical Chamber 4.2 L**
  - 6 identical four-blade fans







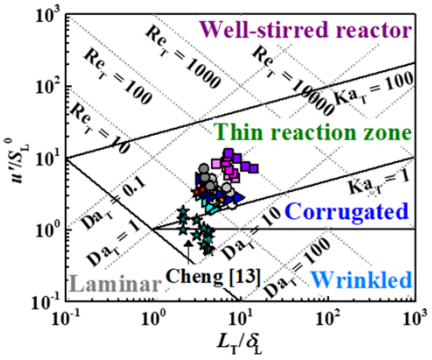


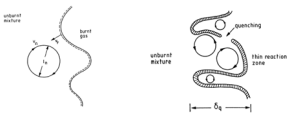


O. Mannaa, P. Brequigny, C. Mounaim-Rousselle, F. Foucher, S.H. Chung, W.L. Roberts, "Turbulent burning characteristics of FACE gasoline and TPRF blend associated with the same RON at elevated pressures," Experimental Thermal and Fluid Science 95 (2018) 104–114.

Turbulent Premixed Flames

- **Damköhlor number** $\mathrm{Da}_l = \dfrac{\text{integral time}}{\text{chemical time}} = \dfrac{\tau_l}{\tau_c} = \dfrac{l/u'}{\delta/S_L} = \dfrac{l/u'}{\delta^2/\nu} = (\dfrac{l}{\delta})^2 R_l^{-1}$
- **Karlovitz number** : $\mathrm{Ka} = \dfrac{\text{Chemical time}}{\text{Kolmogorov time}} = \dfrac{\tau_c}{\tau_k} = \dfrac{\delta/S_L}{\tau_k} = (\dfrac{\delta}{\eta_k})^2 = \mathrm{D}_l^{-1}\mathrm{R}_l^{1/2}$
- **Turbulent Reynolds number** : $\mathrm{R}_l = \dfrac{u'l}{\nu} = \dfrac{u'}{S_L}\dfrac{l}{\delta} = \mathrm{D}_l^2\mathrm{Ka}^2$
- Ka = 1 : Klimov-Williams limit
- **Borghi-Peters Diagram**





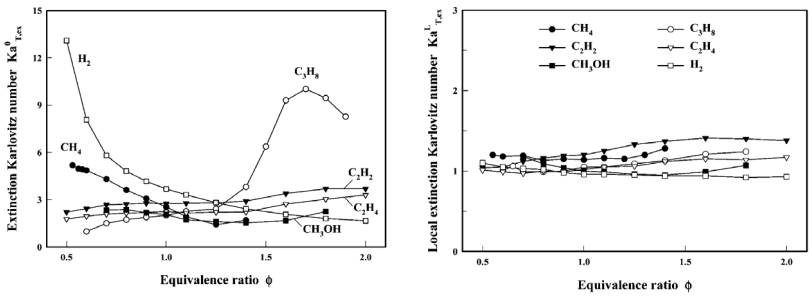
N Peters

Turbulent flame Speed

- $S_T/S_L^0 = 1 + a(u'/S_L^0)^b$
- $S_T/S_L^0 = a\mathrm{Re}_T^{1/2}$
- $S_T/S_L^0 = (\mathrm{Re}_T\mathrm{Le}^{-1})^{1/2}$ Nguyen et al.
- $S_T/S_L^0 = 1 + a\mathrm{Le}^{-1}\mathrm{Re}_T^{1/2}$ Bradley
- $S_T/S_L^0 \approx [1 + \mathrm{Sc}\mathrm{Re}_\lambda^{1/2}](\delta_L^0/\lambda)$ Gülder

Local Karlovitz Number Concept

- **Turbulence Karlovitz number defined in terms of turbulence time scales can be used as a criterion for flamelet quenching**
- **Corresponding Kalovitz number in laminar flames** $Ka^0 = (\delta_0/S_L^0)\kappa$
  - **Ratio of two time scales: chemical reaction time of unstretched flame and physical flow time of stretched flame**
- **Local Karlovitz number : Ratio of the two for stretched flame**
  - **Independent of pressure and initial temperature** (Ka^L_{ext} =1) $Ka^L = (\delta/S_L)\kappa$



E-S Cho, SH Chung "Local Karlovitz numbers at extinction for various fuels in counterflow premixed flames," *CST* 178 (2006) 1559

Critical Phenomena

Critical Phenomena

- Ignition/extinction
  - Transient in time
  - Highly abrupt process by large activation energy
  - Criticality Test : Steady-state analysis
    - Test whether state state solution exists?
    - Ignitable or extinguishable?
  - Penalties
    - Time lag
    - Existence of multiple solution
      - ✓ uniqueness & physical existence should be tested from transient analysis
      - ✓ Some process may not have steady state : transient analysis

Relevant Studies

- **Transient Analysis**
  - Thermal explosion
- **Steady-state Analysis**
  - Ignition of premixture between two flat plates
  - Ignition by a hot particle
  - Premixed flame extinction: stretch or heat loss
  - Counterflow ignition/extinction
  - Droplet ignition/extinction
  - Stagnation-point flow ignition/extinction

Phenomenological Ignition Analysis

- Frank-Kamenetskii / Kapila & Kassoy
- Combustion system w/ characteristic temp T_c

Heat generated $q\exp(-T_a/T_c)$

Inflexion point at $T_c = T_a/2$

Heat loss by conduction & convection

Assume linear $k(T_c - T_o)$

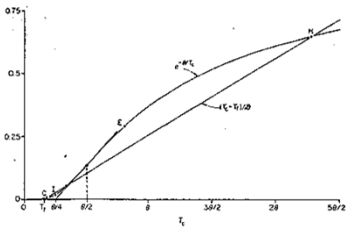
Equilibrium

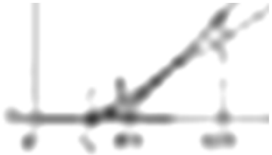
$$\exp(-T_a/T_c) = \frac{k}{q}(T_c - T_o) = \frac{T_c - T_o}{D}$$

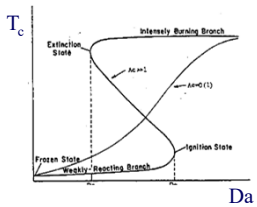
Damköhler number $D \equiv \frac{q}{k}$

For $T_o < T_a/4$: 1 or 3 solution(s)

For $T_o > T_a/4$: 1 solution







Homogeneous Explosion

- **Thermal Explosion**
  - **Spatially homogeneous system**
  - **No heat loss**
  - **Steady-state cannot be attained for any D**

$$\frac{dT}{dt} = D e^{-T_a/T}, \quad T = T_o \quad t = 0$$

$$e^{T_a/T} dT = D dt$$

$$Dt = \int_{T_o}^{T} e^{T_a/T} dT = T_a \int_{T_o}^{T} (-\frac{e^X}{x^2}) dx = T_a \left[\frac{1}{x} e^x - \int \frac{e^x}{x} dx \right]_{T_o}^{T}$$

$$\frac{T_a}{T} = x, \quad -\frac{T_a}{T^2} dT = dx, \quad dT = -\frac{T_a}{x^2} dX$$

$$\therefore Dt = T_a [f(T) - f(T_o)]$$

$$f(T) = \frac{T}{T_a} e^{T_a/T} - E_i(\frac{T_a}{T})$$

$$E_i(x) = \int_{-\infty}^{x} \frac{e^x}{x} dx$$

Cauchy integral using principle value

Exact solution

Thermal Explosion

- **Asymptotic series expansion**

$$Dt = T_a \int_{T_a/T_o}^{T_a/T} (-\frac{1}{x^2} e^x) dx = T_a [-\frac{1}{x^2} e^x - \int \frac{1}{2x^3} e^x dx]$$

$$\simeq -T_a [\frac{T^2}{T_a^2} e^{T_a/T}]_{T_o}^{T} + \cdots \quad \text{as } T_a \to \infty$$

$$Dt = \frac{T_o^2}{T_a} e^{T_a/T_o} - \frac{T^2}{T_a} e^{T_a/T} + \cdots$$

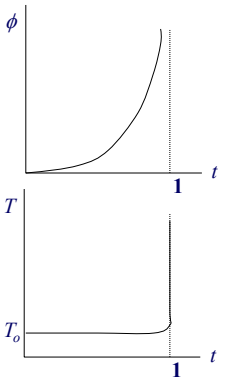
$$D \frac{T_a}{T_o^2} e^{-T_a/T_o} t = 1 - (\frac{T}{T_o})^2 e^{T_a/T - T_a/T_o} + \cdots$$

where $\delta = D \frac{T_a}{T_o^2} e^{-T_a/T_o}, \quad \tilde{t} = \delta t$

$$\therefore \tilde{t} = \tilde{t}_e - (\frac{T}{T_o})^2 e^{T_a/T - T_a/T_o} + \cdots$$

Let $T = T_o + \frac{T_o^2}{T_a} \phi + \cdots \qquad \phi = -\ln(\tilde{t}_e - \tilde{t})$

$$\tilde{t}_e = 1 \qquad D \frac{T_a}{T_o^2} e^{-T_a/T_o} t_{ig} = 1 \qquad t_{ig} \propto e^{T_a/T_o}$$



Time to explosion : Thermal Runaway

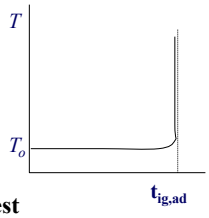
Time takes for T to deviate from T_o by more than O($1/T_a$)

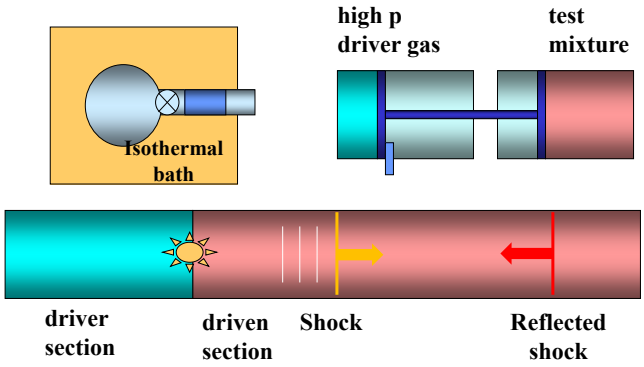
Induction period

Fuel depletion

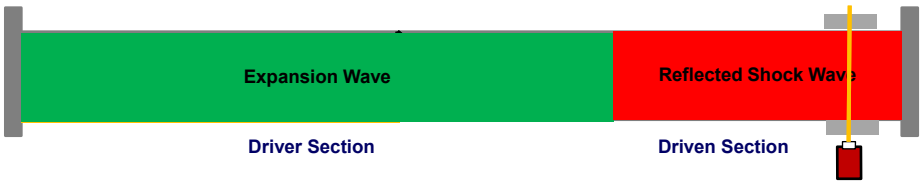
Autoignition : Experiment

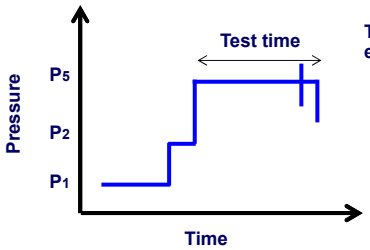
- **Experiment : Delay time to explosion**
  - 0-D characteristics of reactivity
  - Preheated vessel : t_d ~1 s to 1 hr
  - Adiabatic compression : RCM ~10^{-1} to 10^{-2} s
  - Shock compression : Shock tube ~10^{-3} s



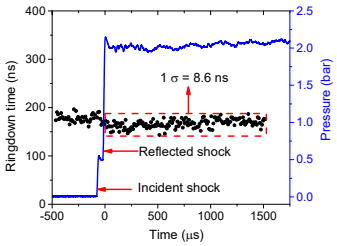


Shock tube experiment





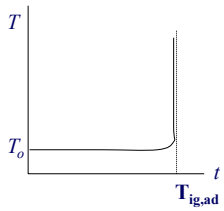
Test times are O (ms) – fast time response sensors required to measure species time histories

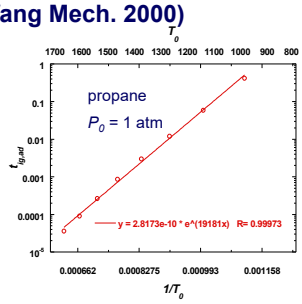


A Farooq: KAUST

Adiabatic Ignition Delay Time

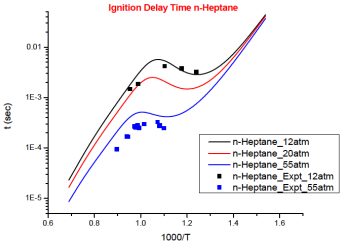
- Adiabatic ignition delay time ($t_{ig,ad}$) calculation
  - CONP code (Sandia National Lab. 1985)
  - Propane diluted with nitrogen (Wang Mech. 2000)
  - $t_{ig,ad}$ ~ exp (20,000 / T_0)





- Ignition delay time sensitivity
- 1000 K : e^{20} ~ 1 ms
- 300 K : e^{66} ~ 1ms × e^{46}

  = 1 ms × (10^{20}) = 10^{17} s = 3 × 10^9 yrs



Sample Calculations: Molecules

- O_2 molecules at 1 atm
  - Maxwell-Boltzmann : Avg. velocity
  - Avogadro number N_A= 6.022 ×10^{23} /mole
  - d = 3.1 ×10^{-10} m, σ = 3.02 ×10^{-19} m^2
  - m = 5.32 ×10^{-23} g = 5.32 ×10^{-26} kg

Temp [K]	300	1000	2000
n [particles/m^3]	2.69×10^{25} 2.7×10^{19}/cm^3	0.806×10^{25}	0.403×10^{25} 0.4×10^{19}/cm^3
Avg. v [m/s]	445	812	1150
z [coll/s]	3.62 ×10^9 3.6/ns	1.98 ×10^9 1.98/ns	1.40 ×10^9 1.4/ns
λ [m]	0.084 ×10^{-6} 0.084 μm 84 nm	0.26 ×10^{-6} 0.26 μm 260 nm	0.58×10^{-6} 0.58 μm 580 nm

$$\bar{v} = \left(\frac{8kT}{\pi m}\right)^{1/2}$$

$$z = n\sigma\bar{v}$$

$$\lambda = \frac{1}{\sqrt{2}\sigma n} = \frac{\bar{v}}{z}$$

$$\bar{v} = \left(\frac{8kT}{\pi m}\right)^{1/2} \propto T^{1/2}$$

$$z = n\sigma\bar{v} \propto PT^{-1/2}$$

$$\lambda = \frac{\bar{v}}{z} \propto \frac{T}{P}$$

- Thermal explosion
  - Z = 2×10^9 /s
  - T_a/T = 20
  - exp(–20000/1000)=10^{-9}
  - 1 s required. Reality 1 ms
  - WHY???

$$\varphi = -\ln(\tilde{t}_e - \tilde{t})$$

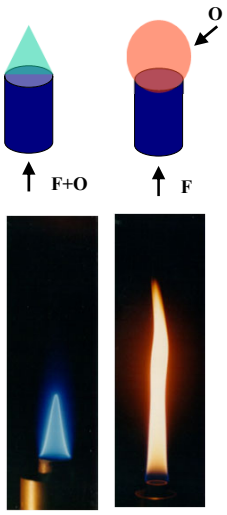
$$T = T_o\left(1 + \frac{T_o}{T_a}\varphi + \cdots\right)$$

Flame Stabilization

Tribrachial flame and mild combustion

Classification of Flames : Mixing

	Premixed Flame	Diffusion Flame Nonpremixed flame
Fuel / Oxidizer	Mixed in molecular level initially	Initially separated Molecular mixing at flame through diffusion and convection
Controlling Mechanism	Reaction Diffusion	Diffusion
Flame Position	Wave propagation	Self-adjust to maximize flame intensity (Stoichiometry)
F/O Consumption at Flame	Complete consumption of lean component	Complete consumption of fuel/oxidizer
Analysis	Finite rate kinetics	Infinite rate kinetics

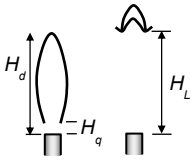


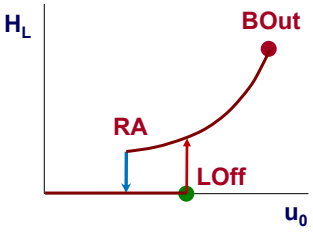
Partially-premixed flames?

Jet Flame Stabilization

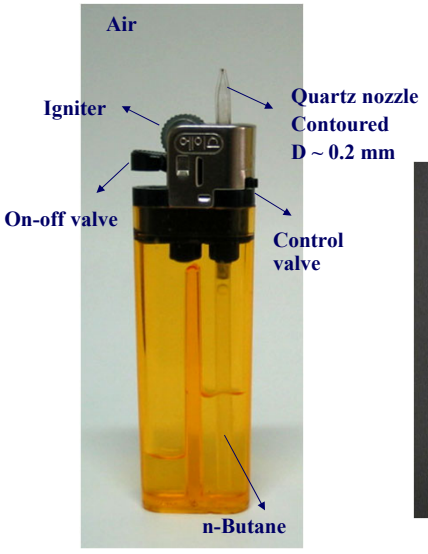
- Nozzle-Attached Flame
- Liftoff (LO) / Blowoff (BO)
- Lifted Flame
- Blowout (BOut)
- Reattachment (RA)

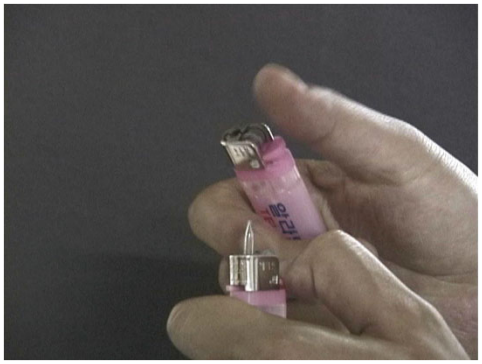
- Importance
  - Safety of burner systems
  - Limiting factor for burner capacity
  - Entrainment of air into fuel core
  - Flame structure and sooting





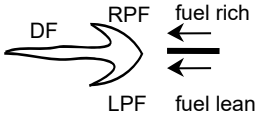
Classroom Experimental Setup



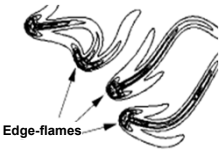


Mixing Layer Flames

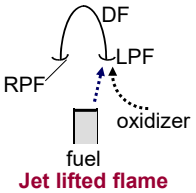
Stratified through lean-rich conditions



2D stagnant layer
(Phillips, 1965)

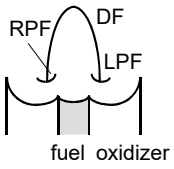


Autoignition front
(Vervisch & Poinsot, 1998)

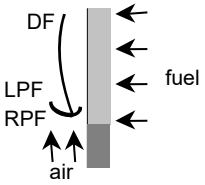


Jet lifted flame
(Chung & Lee, 1991; Savas & Gollahali)

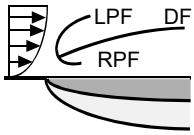
Heat loss free



Composite propellant
(Price 1995)
Corner flame model (Candel)



Boundary layer
(Ko & Chung 1992)



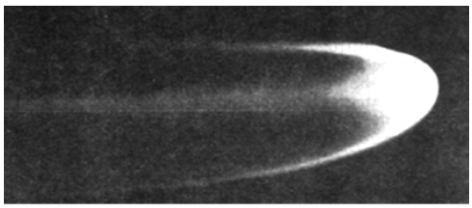
Flame spread
(Wichman, 1992)

Nozzle Attached Flame

Heat loss

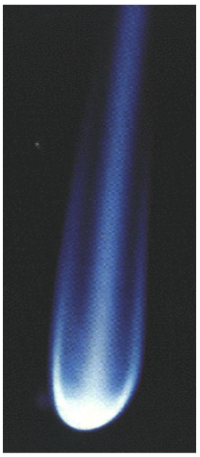
Chung, PCI 2007

Observed Tribrachial Flames

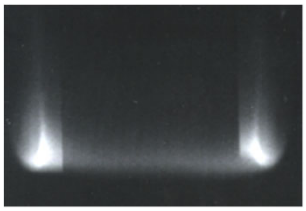


2D Stagnant Layer (Phillips, 1965)

Fuel Jet
(Chung & Lee, 1991)



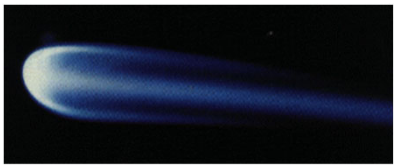
2D Mixing Layer
(Peters, 1995)

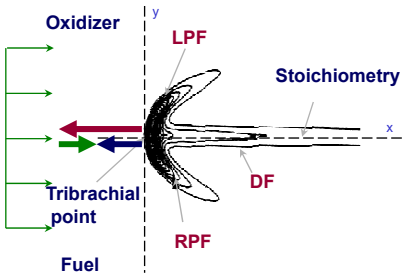


Cylindrical Boundary Layer
(Ko (Chung), 1992)

Flame Spread
(Miller & Easton, 2002)

Characteristics of Tribrachial Flame





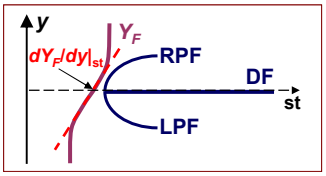
- Coexistence of DF, RPF, LPF
  - Tribrachial point along Stoichiometry
- Front wings of premixed flames (RPF & LPF)
  - Propagation Speed S_e

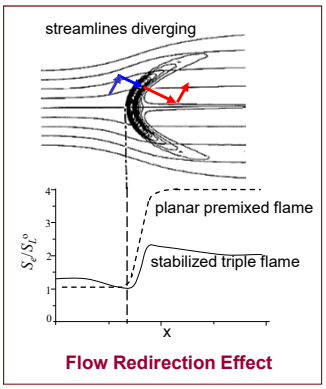
Balance Mechanism

$$S_e = S_d + u_L$$

Propagation Speed

- Fuel Concentration Gradient ($dY_F/dy|_{st}$)
  - Determine curvature of premixed wings (Ko & Chung 1999)
  - Affect local S_L^0 along premixed wings
  - Dold, Se↓ as Gradient↑ (1989, 1991)
- Flow Redirection Effect
  - Reutch et al. (1995)
  - Landau's Hydrodynamic Instability Mechanism
  - Streamline divergence by gas expansion
  - S_e can be larger than $S_L^0|_{st}$
  - Limiting Cases
    - Upper bound for $(dY_F/dy|_{st}) \rightarrow 0$
    - $S_{e,max} \propto S_L^0(\rho_u/\rho_{b,st})^{1/2}$
    - $(dY_F/dy|_{st}) \rightarrow \infty : S_e < S_L^0$

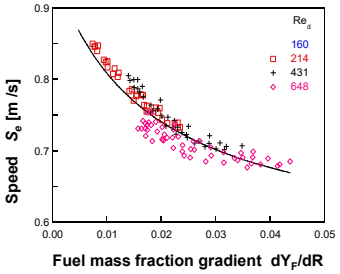




Flow Redirection Effect

Propagation Speed Measurement

- **Methane**

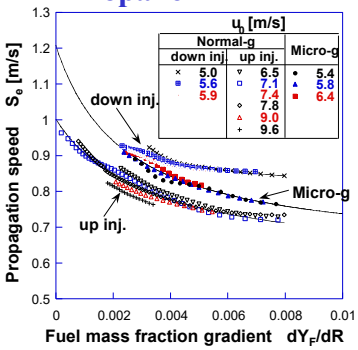


$$\frac{S_e}{S_L^0|_{st}} = 0.01663\left[\frac{dY_F}{dR}\bigg|_{st} + 0.01664\right]^{-1} + 1.398$$

- Inverse proportionality
- Extrapolated : 0.96 m/s
- $S_L^0(\rho_u/\rho_{b,st})^{1/2}$ = 1.09 m/s
- $S_e > S_L^0$

YS Ko, SH Chung, "Propagation of unsteady tribrachial flames in laminar nonpremixed jets," *Combust. Flame* 118 (1999) 151-163.

- **Propane**



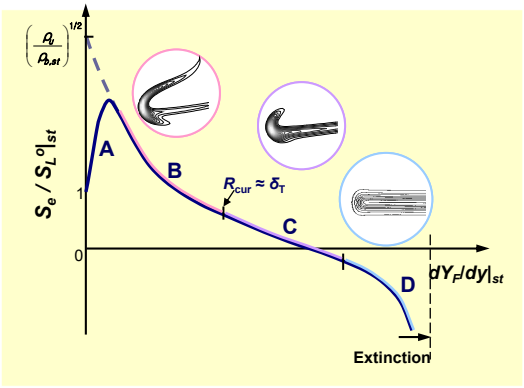
$$\frac{S_e}{S_L^0|_{st}} = 0.00313\left[\frac{dY_F}{dR} + 0.00237\right]^{-1} + 1.42$$

- Inverse proportionality
- Extrapolated : 1.21 m/s
- $S_L^0(\rho_u/\rho_{b,st})^{1/2}$ = 1.10 m/s
- $Se > S_L^0$

JS Lee, SH Won, SH Jin, SH Chung, O Fujita, K Ito, "Propagation speed of tribrachial (triple) flame of propane in laminar jets under normal and microgravity conditions," *Combust. Flame* 134 (2003) 411-420.

Transition Regime

- As $dY_F/dy|_{st} \rightarrow 0$ in Tribrachial Regime: $S_{e,max} \rightarrow S_L^0(\rho_u/\rho_{b,st})^{1/2}$
- When $dY_F/dy|_{st} = 0$ for Homogeneous Case: $S = S_L^0$
- Transition Regime should exist



YS Ko, TM Chung, SH Chung, "Characteristics of propagating tribrachial flames in counterflow," *KSME Int. J.* 16 (2002) 1710-1718

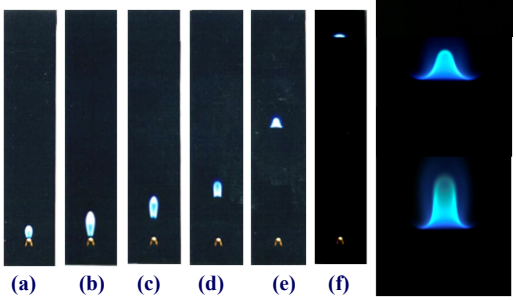
NI Kim, JI Seo, KC Oh, HD Shin, "Lift-off characteristics of triple flame with concentration gradient," Proc. Combust. Inst. 30 (2005) 367-374.

Die Hard II

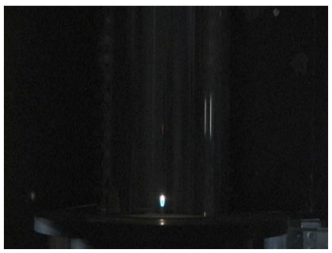
- Takeoff velocity 280 km/hr (70 m/s)

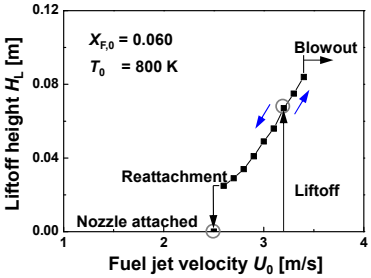
Laminar Jet Flame Stabilization

- Nozzle-attached flame
- Liftoff
- Lifted flame
- Blowout



(a) (b) (c) (d) (e) (f)



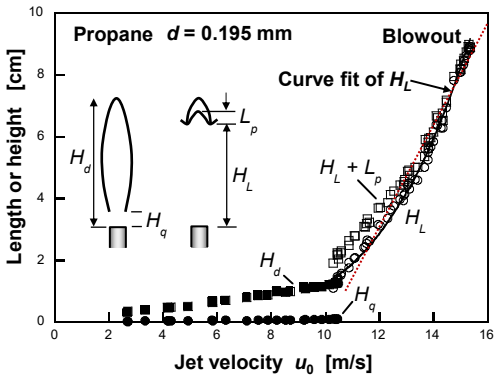


Free Jet, d = 0.195 mm; Propane

(a) Q=0.195 (b)17.3 (c)18.3 (d)20.3
(e)22.3 (f)26.4 ml/min

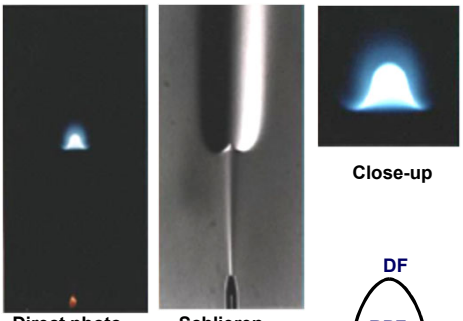
SH Chung, BJ Lee, "On the characteristics of laminar lifted flames in a nonpremixed Jet," *Combust. Flame* 86 (1991) 62-72.

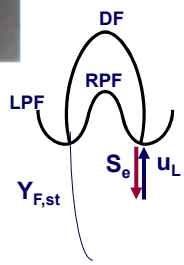
Liftoff Height H_L with Jet Velocity



- Turbulent case : Linear $H_L \propto u_0^1$
- Highly nonlinear with u_0 : $H_L \propto u_0^{4.7}$ (Propane) , $u_0^{3.6}$ (n-Butane)

Liftoff Height Prediction





- Tribrachial Structure
  - Stoichiometry
  - Propagation S_e
- Stabilization
  - Balance Mechanism

$S_e = u_L$ (Stationary)

- Schlieren
  - Cold jet upstream of flame
  - Similarity solutions

Similarity Solutions

- **Similarity Solutions (Schlichting for velocity)**

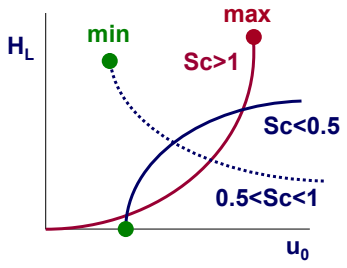
$$u=\frac{3}{8\pi\nu x}\frac{J}{\rho}\frac{1}{\left(1+\eta^2/8\right)^2} \qquad v=\frac{1}{2}\sqrt{\frac{3}{8\pi}\frac{J}{\rho}}\frac{\eta}{x}\frac{\left(1-\eta^2/8\right)^2}{\left(1+\eta^2/8\right)^2} \qquad Y_F=\frac{(2Sc+1)}{8\pi\nu x}\frac{I}{\rho}\frac{1}{\left(1+\eta^2/8\right)^{2Sc}}$$

where $\eta=\sqrt{\frac{3}{32}}\frac{u_0 d}{\nu}\frac{r}{x}$ $\qquad J=\frac{\pi\rho u_0^2 d^2}{4}$ $\qquad I=\frac{\pi\rho u_0 d^2 Y_{F,0}}{4}$

- **Sc = ν/D_F: Schmidt number**
- **Tribrachial point (x^*, η^*) : $H_L = x^*$, $u^* = S_e$, $Y_F = Y_{F,st}$**

$$\frac{H_L}{d^2}\frac{\nu}{S_e}=\left(\frac{3}{32}\frac{3}{2Sc+1}\frac{Y_{F,st}}{Y_{F,0}}\right)^{\frac{1}{Sc-1}}\left(\frac{u_0}{S_e}\right)^{\frac{2Sc-1}{Sc-1}}$$

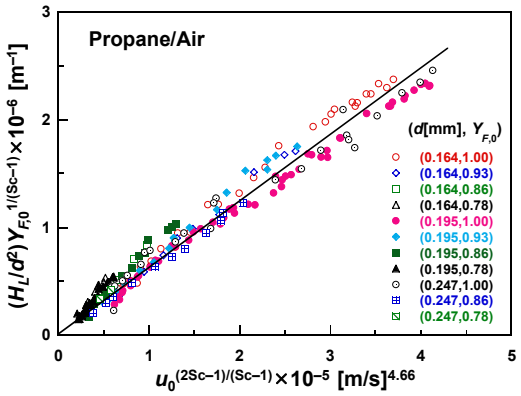
$$\eta^{*2}/8=\left(\frac{3}{2Sc+1}\frac{Y_{F,st}}{Y_{F,0}}\frac{u_0}{S_e}\right)^{\frac{1}{2(Sc-1)}}-1$$



Liftoff Height Correlation

- **Partially premixed propane (Air partial premixing to fuel)**
  - **Stoichiometry maintained**
  - **$S_L^o|_{st}$ thus S_e maintained**

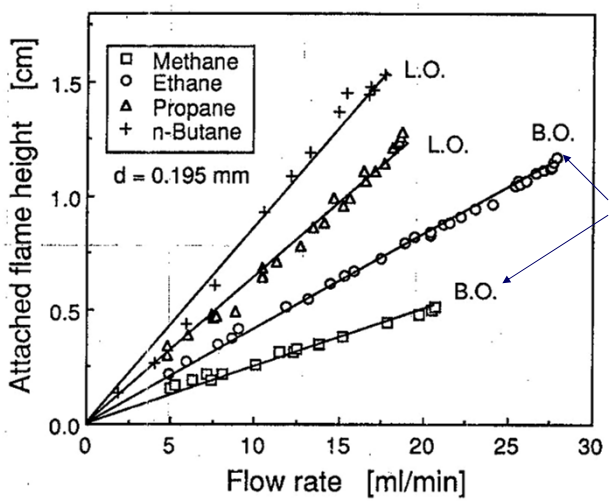
$$\left(\frac{H_L}{d^2}\right)Y_{F,0}^{\,1/(Sc_F-1)}=\text{const}\times u_0^{(2Sc_F-1)/(Sc_F-1)}$$



Sc = 1.376
(2Sc-1)/(Sc-1) = 4.66

B.J. Lee, M.S. Cha, S.H. Chung*, "Characteristics of laminar lifted flames in a partially premixed jet," *Combust. Sci. Technol.* 127 (1997) 55-70

Fuel Dependence



Direct blowoff
No lifted flame
CH_4, C_2H_6

Laminar lifted flames do not exist for ethane and methane in free jets

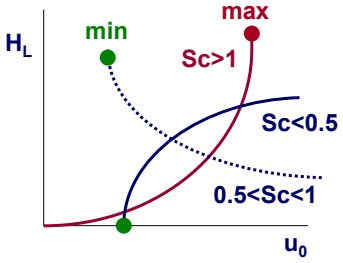
Schmidt Number Dependence

- Prediction

$$H_L \sim d^2 u_0^{(2Sc-1)/(Sc-1)}$$

- Experimental curve fitting

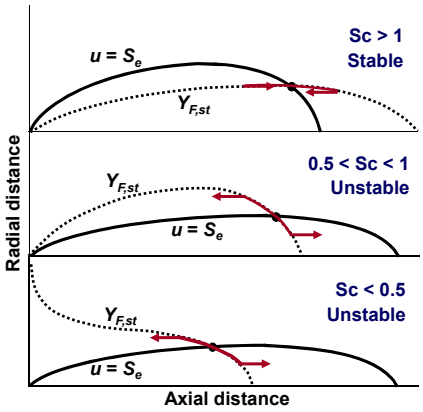
Fuel	Sc Table	Sc Exp
CH_4	0.704	Blowoff
C_2H_6	1.064	Blowoff
C_3H_8	1.376	1.36 – 1.43
C_4H_{10}	1.573	1.61 – 1.74
H_2	0.204	No liftoff



Physically unrealistic

Stability of Lifted Flames

- Iso-Velocity Contour : S_e
- Iso-Concentration Contour : $Y_{F,st}$



- Sc = ν/D_F: Schmidt number

Lifted edges in free jet
Stable for Sc > 1
Unstable for Sc < 1

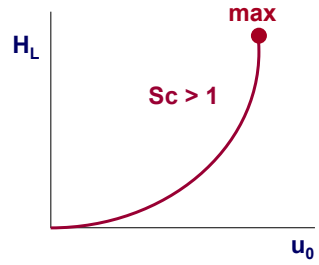
Can explain fuel dependence

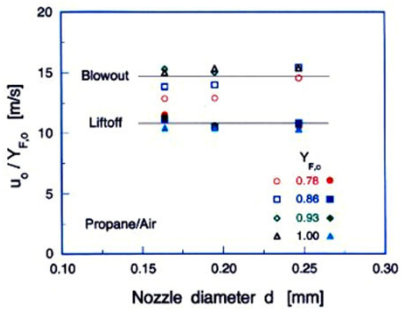
BJ Lee, SH Chung, "Stabilization of lifted tribrachial flames in a laminar nonpremixed jet," *Combust. Flame* 109 (1997) 163-172

Critical Conditions : Blowout

$$\eta^{*2}/8 = \left(\frac{3}{2\mathrm{Sc}+1} \frac{Y_{F,st}}{Y_{F,0}} \frac{u_0}{S_{tri}} \right)^{-\frac{1}{2(\mathrm{Sc}-1)}} - 1$$

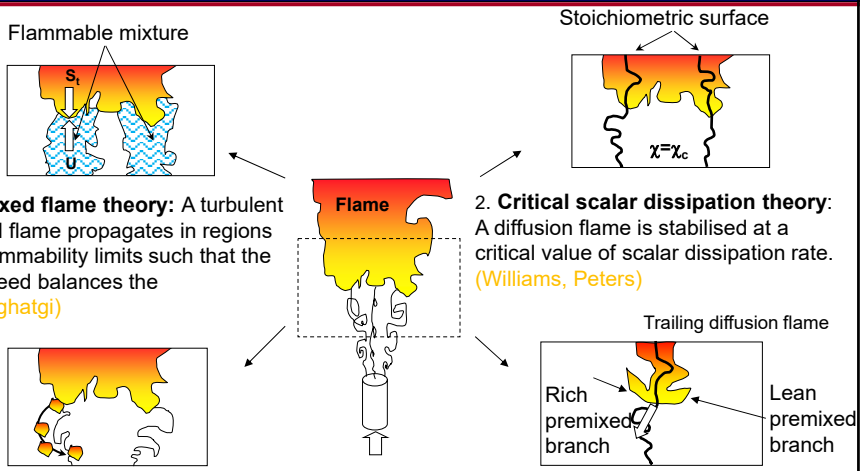
- Sc > 1: $\dfrac{u_0}{S_e} < \dfrac{2Sc+1}{3Y_{F,st}}$
  - Corresponds to blowout condition
  - u_{BO} independent of d





BJ Lee, SH Chung, "Stabilization of lifted tribrachial flames in a laminar nonpremixed jet," *Combust. Flame* 109 (1997) 163-172

Turbulent Flame Stabilization



1. **Premixed flame theory:** A turbulent premixed flame propagates in regions within flammability limits such that the flame speed balances the flow.(Kalghatgi)

2. **Critical scalar dissipation theory**: A diffusion flame is stabilised at a critical value of scalar dissipation rate. (Williams, Peters)

3. **Large eddy theory**: pockets of hot burned products are transported upstream and ignite fuel/air mixture. (Broadwell)

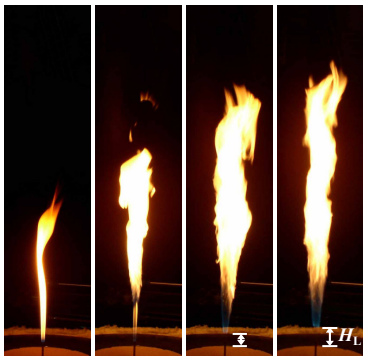
4. **Edge flame theory:** a partially premixed edge-flame stabilizes by self-propagation relative to the flow. (Branches may be collapsed.) (Chung, Peters)

Curtesy of Evatt Hawkes UNSW

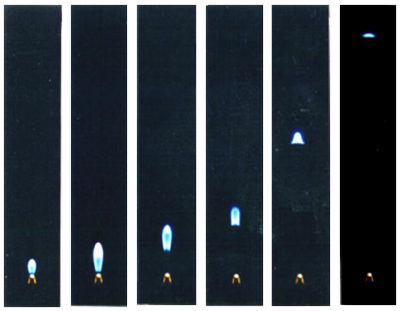
UNSW

Turbulent Lifted Flames

- **Premixed Flame Model**
  - **Vanquickenborne & van Tigglen (1966); Kalghatgi (1981)**
- **Large-scale Mixing Model**
  - **Broadwell et al. (1984); Miake-Lye & Hammer (1988)**



Laminar : Tribrachial Structure

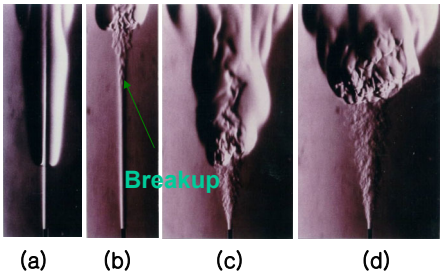


Chung & Lee, CNF 1991

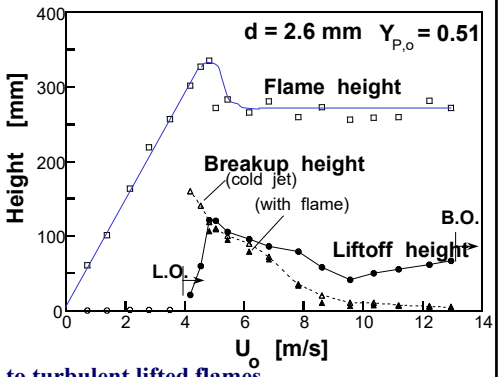
KN Kim, SH Won, SH Chung, "Characteristics of turbulent lifted flames in coflow jets with initial temperature variation," *Proc. Combust. Inst.* 31 (2007) 1591-1598

Laminar to Turbulent Transition

Premixed Flame Model (Kalghatgi, 1984)
Large Scale Mixing Model (Broadwell, Dahm, Mungal, 1984)
Extinction Model (Williams & Peters)



u_0 = 4.50, 4.80, 9.56, 12.23 m/s

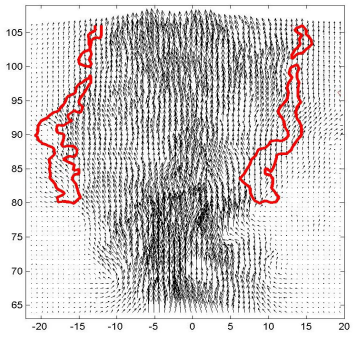


Continuous transition from laminar to turbulent lifted flames
Imply the importance of tribrachial flame on turbulent lifted flames

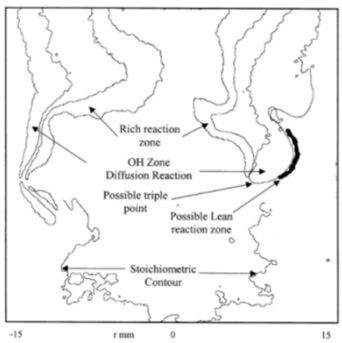
BJ Lee, JS Kim, SH Chung, "Effect of dilution on the liftoff of nonpremixed jet flames," *Proc. Combust. Inst.* 25 (1994) 1175-1181

Local Structure of Turbulent Lifted Flame Edges

- **Various Laser-Based Measurement (PIV, LIF, …)**
  - **Muniz & Mungal 1997, Schefer & Goix 1998, Watson, Lyon et al. 1999, Maurey et al. 2000, Mansour 2003, Cessou et al. 2004, …**
  - **Local Vel. at Lifted Edge ~ Laminar Burning Vel.**
  - **Turbulent Lifted Flame Edge: Ensemble of Edge Flames**



PIV and CH LIF data
(Muniz & Mungal, CF 1997)

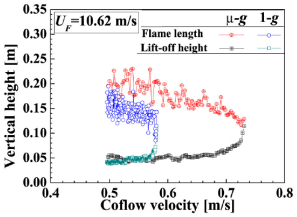


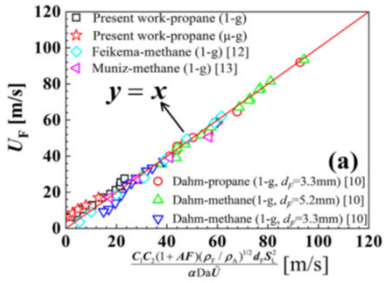
OH and C_2H_x LIF data with Rayleigh image
(Mansour et al., CF 2003)

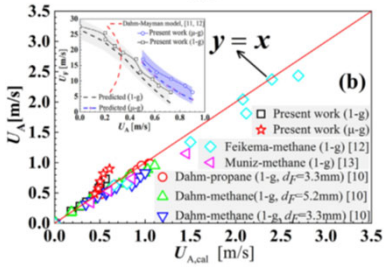
Turbulent Blow-out

- Free jet, coflow jet, and gravity effects considered

(a) (U_F [m/s], U_A [m/s]) = (6.37, 0.5)
(b) (10.6, 0.5)



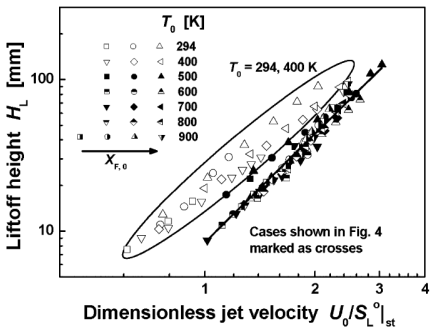




Q Wang, L Hu, S Wang, S Wang, SH Chung, O Fujita, "Blowout of non-premixed turbulent jet flames with coflow under microgravity condition," Combust. Flame 210 (2019) 315-323

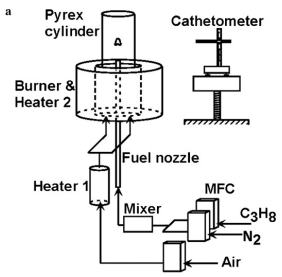
Temperature effect (Laminar Jet)

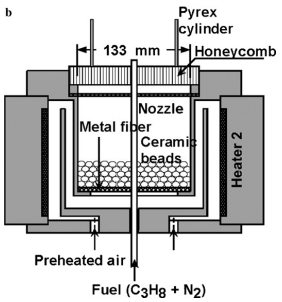
- Correlated with $U_0/S_L^o|_{st}$
- Buoyancy effect for 294 & 400 K



- Richardson no decreases with T_0

$$Ri = (\Delta\rho g d)/(\rho_u U_0^2)$$



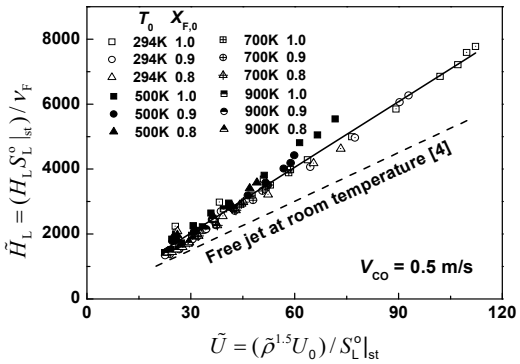


KN Kim, SH Won, SH Chung, "Characteristics of laminar lifted flames in coflow jets with initial temperature variation," *Proc. Combust. Inst.* 31 (2007) 947-954

Scaling Laws for Turbulent jet

- Initial Temperature variation up to 900 K
- Premixed Flame Model can be still valid (Kalghatgi, 1984)
- Large Scale Model does not provide satisfactory correlation

$$\tilde{U}_0 = \frac{U_0}{S_L^0|_{st}}\tilde{\rho}^{1.5}, \quad \tilde{H}_L = \frac{H_L S_L^0|_{st}}{\upsilon_F}$$



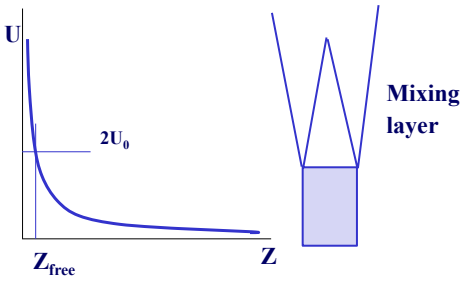
Mixing of fuel and air in the upstream region is important rather than large-scale mixing by burnt gas in scaling liftoff height and blowout velocity

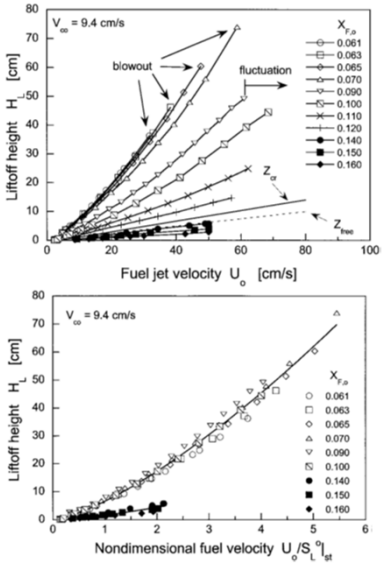
Partially Premixed Model
Premixed Flame Model
Both based on the Balance between Propagation and Local Velocity

KN Kim, SH Won, SH Chung, "Characteristics of turbulent lifted flames in coflow jets with initial temperature variation," *Proc. Combust. Inst.* 31 (2007) 1591-1598

Jet Development

- Length of jet developing region
- $Z_{free}/d = 0.0165 \times Re_d$



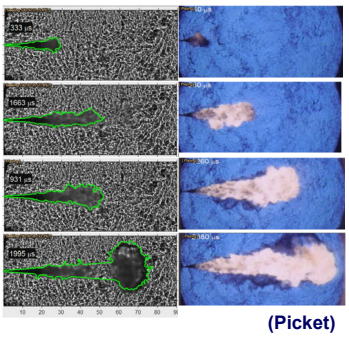


S.H. Won, M.S. Cha, S.H. Chung, B.J. Lee, "Lifted flame stabilization in developing and developed regions of coflow jets for highly diluted propane," *Proc. Combust. Inst.* 28 (2000) 2093-2099

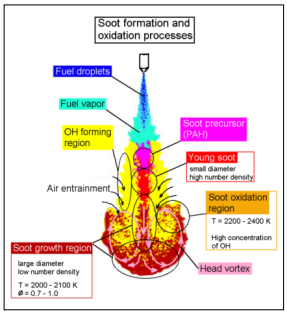
Jet Flame Stabilization: Autoignition

Diesel Spray Flames

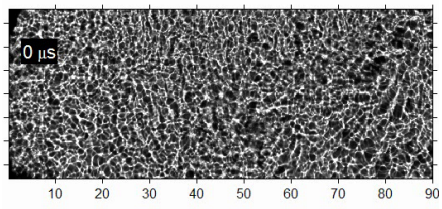
- **Diesel Engine Combustion**
  - **High temperature after compression**
  - **Autoignition initiates combustion**
  - **Lifted flame after ignition**
  - **Liftoff height controls air entrainment**
  - **Air entrainment affects soot formation**



(Picket)

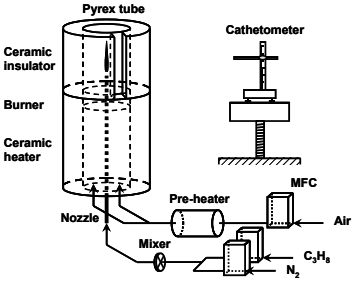


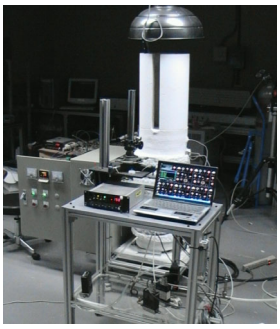
H.Kosaka et al. (Journal of Engine Research)



Experiment 1

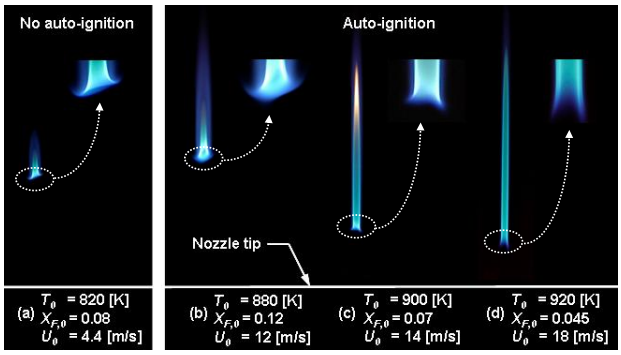
- Coflow burner
  - Fuel nozzle : i.d. 3.76 mm, L 750 mm
  - C_3H_8 diluted with N_2
  - Coflow air : i.d. 150 mm
- Heating system
  - Pre-heater 2.5 kW
  - Ceramic heater 7.5 kW (PID logic)
  - Representation of T_0 : fuel nozzle tip
- Mass flow controllers
- Cathetometer
- Camcorder and high speed camera





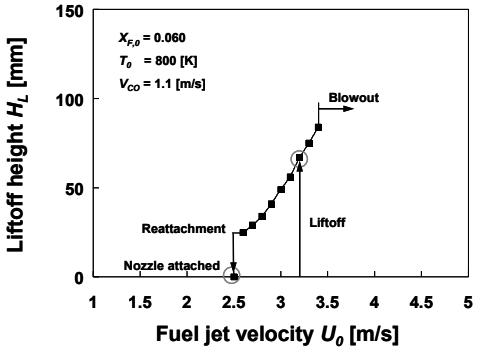
Flame Behavior

- T_0 below 860 K
  - Flame was generated by external ignition source.
  - Conventional lifted flame having tribrachial structure
- T_0 above 860 K
  - Flame was auto-ignited without any external ignition source.
  - Edge structure exhibited tribrachial (or bibrachial) flame

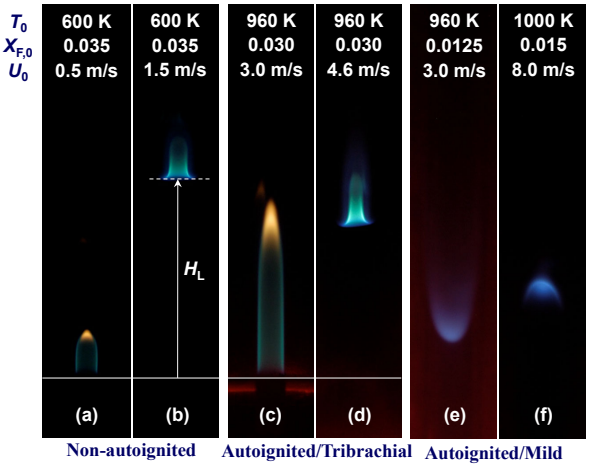


Non-autoignited Lifted Flames

- As jet velocity increases
  - Attached flame lifted from nozzle.
  - Liftoff height increases nonlinearly.
- At excessively large jet velocity
  - Blowout occurred.
- When the jet velocity decrease from a lifted flame,
  - Reattachment occurred.



Non-autoignited & Autoignited Flames



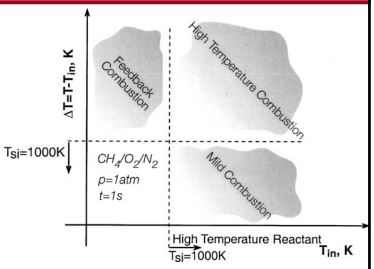
Nozzle-attached flames and lifted flames of *n*-heptane with various fuel jet velocities in the non-autoignited and autoignited regimes.

Mild Combustion

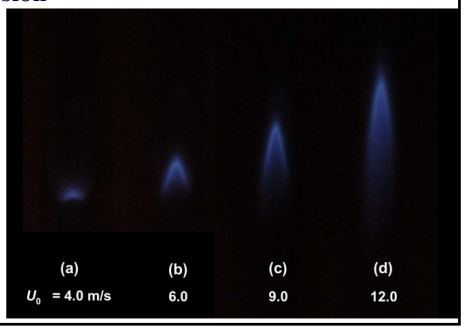
- Highly heated air: $T_0 > T_{ig}$
- Small heat release: $(T_{max} - T_0) < T_{ig}$

- Can be realized
  - High dilution or Low BTU fuel, e.g., s yngas
  - High EGR
  - Results in low NOx and soot emission

- Flameless combustion
- HiCOT (High temperature air combustion technology)



A. Cavaliere, M. de Joannon, PECS 30 (2004) 329–366

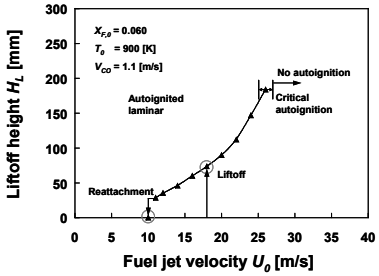


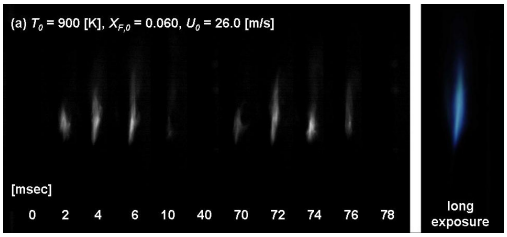
$X_{F,0} = 0.014$
$T_0 = 900$ K.

Autoignited Lifted Flame w/ Tribrachial Edge

- With jet velocity
  - Liftoff and reattachment.
  - Liftoff height increases nonlinearly.

- Critical liftoff height
  - Lifted flame exhibited a repetitive behavior of autoignition and extinction.
  - Autoignition height ≈ Liftoff height



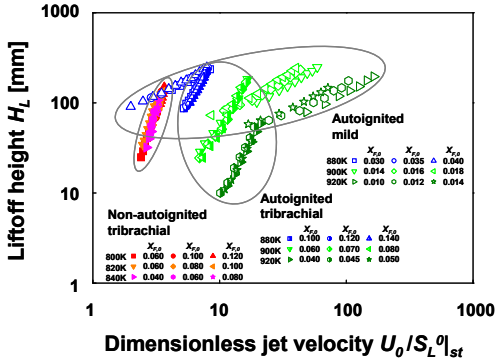


Stabilization: Non-autoignited Lifted Flame

- Balance mechanism between propagation speed of tribrachial edge and local flow velocity, regardless of the initial temperature
  - Kim, Won, & Chung, 2007
  - H_L correlated well with $S_L^0|_{st}$

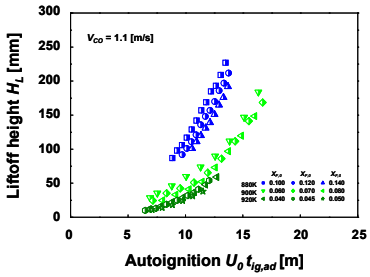
$$H_L[mm] = 0.69 \times \left(U_0 / S_L^0|_{st}\right)^{4.16}, \; R = 0.98$$

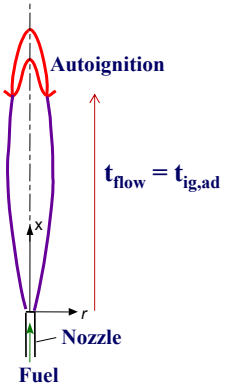
- Autoignited lifted flames did not correlated with $S_L^0|_{st}$
  - May be related to adiabatic ignition delay time



Correlation of $t_{ig,ad}$ and Liftoff Height

- First look
  - Flow time : $t_{flow} = H_L/U_0$
  - Ignition delay time $t_{ig,ad}$
  - $H_L \approx U_0 t_{ig,ad}$
- Not working

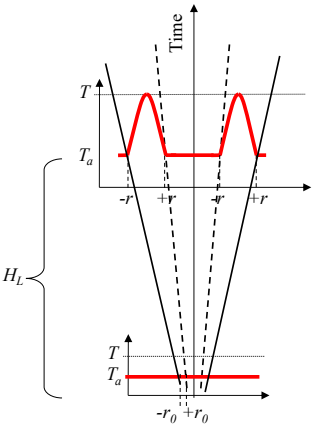




- As chemical reaction proceeds, heat loss is inevitable.

Thermal Explosion Theory

- Thermal balance between heat generated by reaction and conduction heat loss



r : stoichiometric mixing layer half thickness

- Energy equation by Frank-Kamenetskii

Heat loss $-\lambda \frac{d^2T}{dr^2} = \rho QCA \times \exp\left(\frac{-E_a}{RT}\right)$

- Ignition delay time - T. Boddington, 1984

$$\frac{t_{ig}}{t_{ig,ad}} = \frac{M(B_i)}{(\delta/\delta_{cr} - 1)^{1/2}}$$

where $\delta_{cr} < \delta < 2\delta_{cr}$

- Non-adiabatic Ignition delay time

$$\left(\frac{t_{ig,ad}}{t_{ig}}\right)^2 \propto \delta \approx Da \approx \frac{t_{flow}}{t_{ig}}$$

$t_{flow} \propto H_L / U_0$

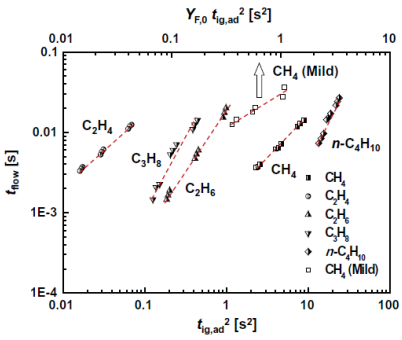
$$t_{ig} \propto \frac{t_{ig,ad}^{\ 2}}{t_{flow}}$$

Second Look

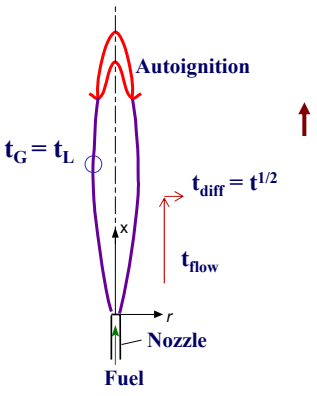
- As chemical reaction proceeds, heat loss is inevitable
- Thermal balance between heat generation and heat loss time scales
- Heat generation: $t_G = t_{ig}$
- Heat loss (diffusion): $t_L = t_{diff} = (t_{flow})^{1/2} = (H_L/U_0)^{1/2}$

$t_{flow} \propto t_{ig}^{\ 2}$

$H_L/U_0 \sim t_{ig}^{\ 2}$

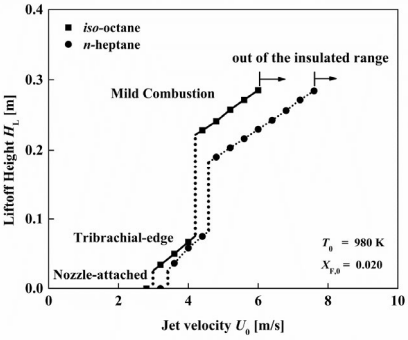


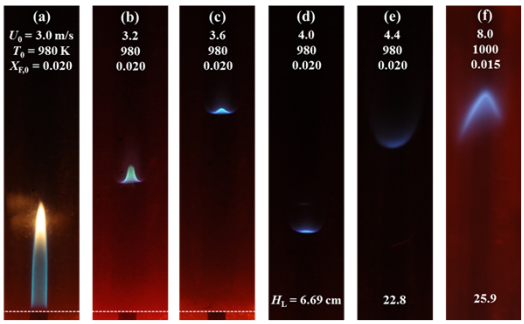
Combustion and Flame 2009, 2010



Iso-Octane: Two Transitions

- Self ignition & flame stabilization
- Tribrachial lifted flame
- MILD combustion
  - Concave & convex shapes



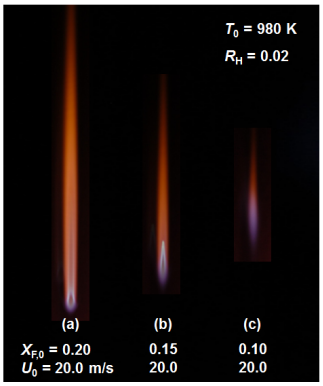


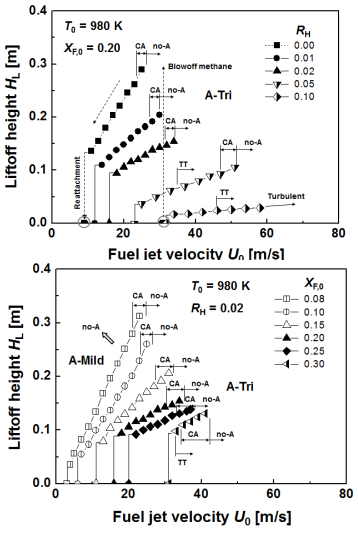
- Two transitions of flame stabilization
  Attached – Tribrachial – MILD
- H_L for *iso*-octane is higher
  Ignition delay time is longer

SM Al-Noman, SK Choi, SH Chung, "Autoignition Characteristics of Laminar Lifted Jet Flames of Pre-vaporized*Iso*-Octane in Heated Coflow Air," *Fuel* 162 (2015) 171–178

Hydrogen-Methane Autoignition Regime

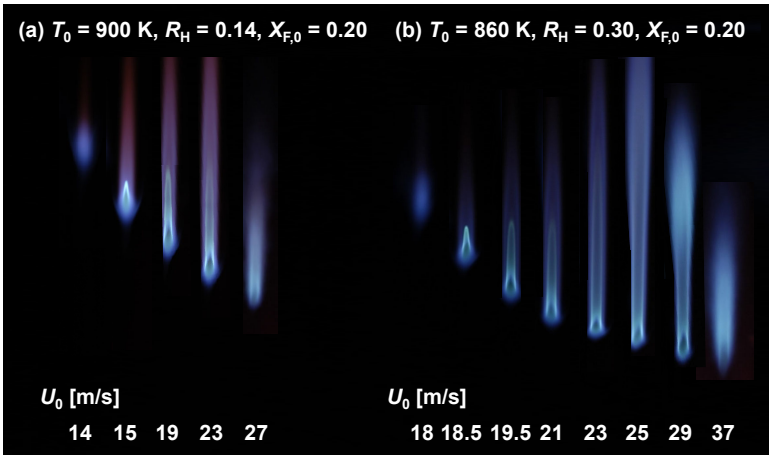
- Variables : T_0, $X_{F,0}$, R_H and U_0
- High-temperature regime : H_L↑ as U_0↑; H_L↓ as R_H↑





Decreasing Liftoff Height Regime

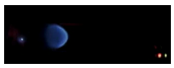
- Low temperature regime: 900 & 860 K



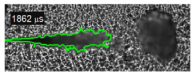
Engine Fuels

Canonical Flames in Combustion Research

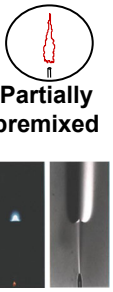
Flame propagation



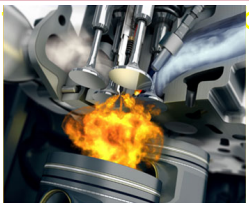
Autoignition
(HCCI, Diesel)

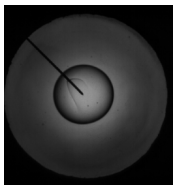


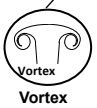
Pickett



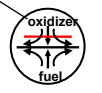
Partially premixed



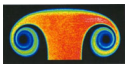


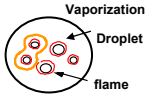


Vortex dynamics



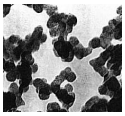
Aerodynamic Effect



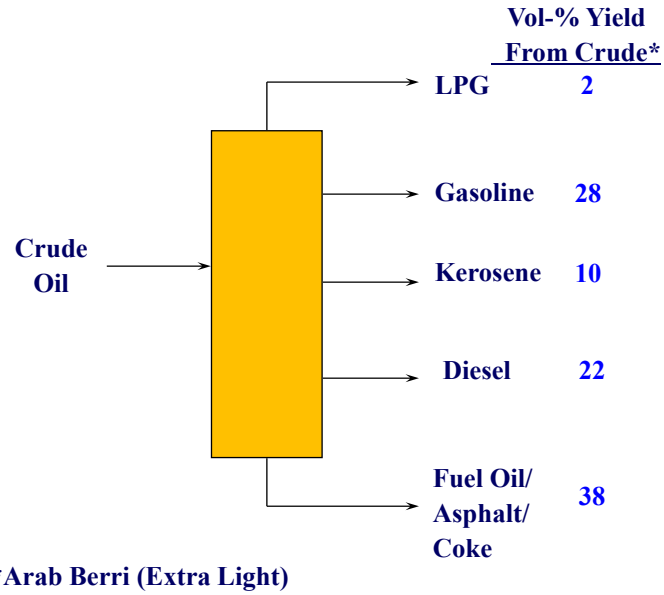


Spray/Droplet Combustion

Emission
(Soot, NOx)



Refining: Product Yield from Crude



*Arab Berri (Extra Light)

Chris Gosling, Honeywell (Future of transport fuel Workshop, KAUST 2014)

Engineering Indices of Fuel

- Research Octane number (RON)
- Motor octane number (MON)

} Gasoline

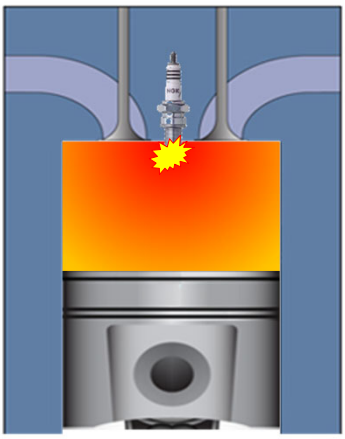
- Threshold soot index (TSI)
- Derived cetane number (DCN)

} Jet fuel Diesel

SI Engine

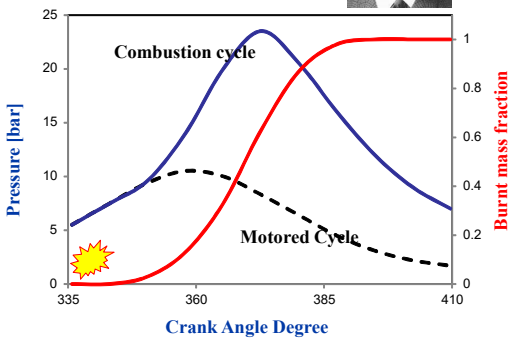
Spark starts the propagation of a turbulent flame front

Controlled Temperature and Pressure increase



Nikolaus August Otto (1832–1891)

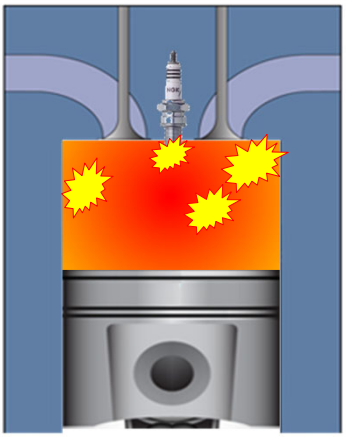
Otto Engine (1876)

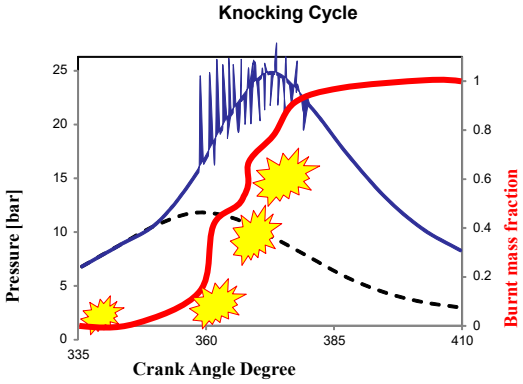


Credit to Marco Mehl, LLNL, 2014

Knocking

- When the compression ratio increases or ON is too low, anomalous combustion behavior lead to engine failure



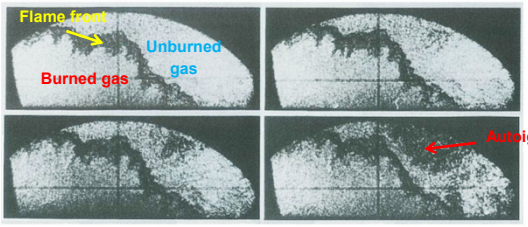


Credit to Marco Mehl, LLNL, 2014

- Click to edit Master text styles
  - Second level
    - Third level
      - Fourth level
        - » Fifth level

Knock

- Click to edit Master text styles
  - Second level
    - Third level
      - Fourth level
        - » Fifth level



Schlieren images of end gas autoignition (Spicher, 1991)

CFR engine

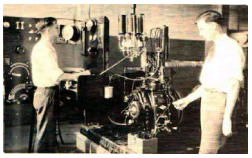
Octane Rating : Knock Propensity

Cooperative Fuel Research (CFR) engine (1928)

- Cabureted variable CR engine
- Determine critical CR when knock reaches a prefixed intensity
- Compare reference fuel mixtures of n-heptane (PRF0) and iso-octane (PRF100)

RON: - ASTM 2699
- 600 rpm / 325K /Spark Advance 13

Representative of idling / low load conditions



CFR Engine (1929)

MON: - ASTM 2700
- 900 rpm / 422K / Spark Advance 19-26°

Representative of road / high load conditions

Today's octane ratings are still based on the same tests

Cetane Number

- **Cooperative Fuel Research (CFR) engine**
  - ASTM D613
  - Increase CR till **fuel injection to ignition to be 2.407 ms**
  - Compare mixtures of cetane (hexadecane) and iso-cetane (2,2,4,4,6,8,8-heptamethylnoname)

- **Ignition Quality Tester (IQT)**
  - ASTM D6890, Advanced Engine Technology Ltd.
  - More reliable than CFR test
  - Fixed volume of duel spray injected into constant volume combustion chamber
  - Measure ignition delay time and calculate **Derived Cetane Number** (DCN) in the range 40-60

DCN

- **ASME D6890**
- **P_0 = 21.37 ± 0.07 bar, P_{inj} = 225 bar**
- **Calibration: n-heptane IDT to be 3.78± 0.01 ms (average of 3 runs) by adjusting temperature (818 ± 30 K) : present 835–845 K**
- **Each run involves 15 pre-injections to create a stable operating environment for the succeeding 32 main injections to average**
- **For IDT 3.1 – 6.5 ms (DCN 33–64)**

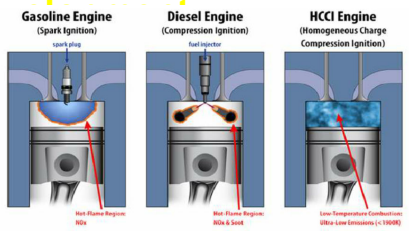
$$DCN = 4.46 + \frac{186.6}{\tau_{id}[ms]}$$

- **Outside the range c. 3.1 – 6.5 ms**

$$DCN = 83.99[(\tau_{id}[ms] - 1.512)^{-0.658}] + 3.547$$

- **DCN is more reliable than CN**

- Click to edit Master text styl
  - Second level
    - Third level
      - Fourth level
        - » Fifth level



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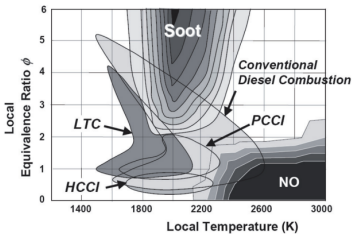
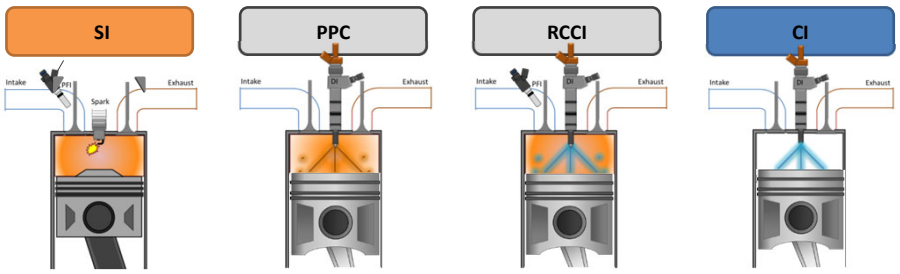


Neely et al. (2005) SAE Technical Paper No. 2005-01- 1091

Combustion Modes in IC Engines

Knocking (Autoignition) Efficiency limiting factor

Autoignition Operation limiting factor



Fuel Reactivity

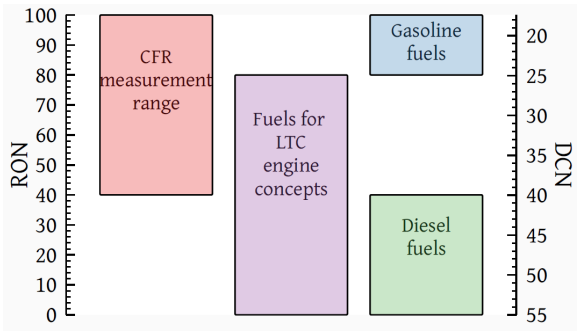
Low (e.g., gasoline)
Prevents Auto-Ignition

High (e.g., diesel)
Promotes Auto-Ignition

Advance engines may require fuel characteristics in-between gasoline and diesel

Robert Wagner, ORNL
Saudi Aramco/KAUST Workshop
"Future of Transport Fuels" March 24-26, 2014

RON and DCN Ranges

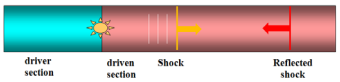


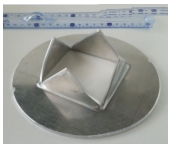
Measurement ranges of ONs and CNs and those for typical gasoline and diesel fuels.

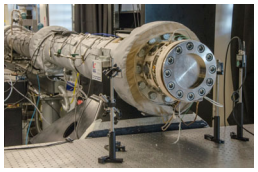
Can be extend DCN towards gasoline?

Autoignition Studies

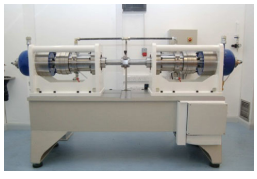
- **Shock tube**
  - Homogeneous, O(1-10 ms)





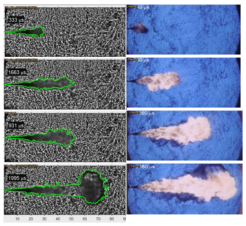


- **RCM**
  - Homogeneous, O(100 ms)



- **IQT**
  - Const. volume combustion chamber
  - Transient
  - Inhomogeneous

Picket (Sandia)



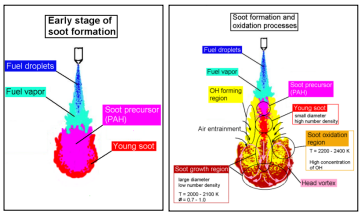
- **Diesel autoignition**
  - Variable volume
  - Lifted flame: Partially Premixed
  - Soot

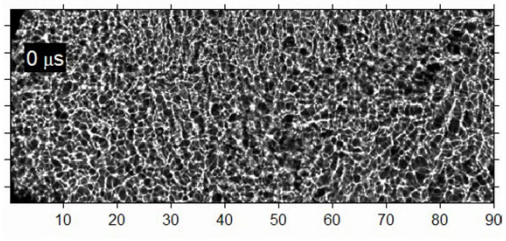
- **Link between shock tube ignition delay time and spray jet ignition**

Diesel Spray Flames

- **Diesel Engine Combustion**
  - **High temperature after compression**
  - **Autoignition initiates combustion**
  - **Lifted flame after ignition**
  - **Liftoff height controls air entrainment**
  - **Air entrainment affects soot formation**

(L Picket)





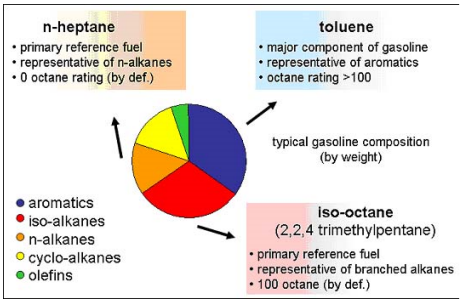
Conceptual model of diesel spray flame based on optical diagnostics
H.Kosaka et al. (Journal of Engine Research)

Courtesy of Tets Aizawa, TIT

Ignition delay= Physical + Chemical
Physical: Evaporation + Mixing

Surrogate Fuels : Gasoline

- **Kinetic modeling for gasoline fuel**
  - **PRF : Primary reference fuel (iso-octane + n-heptane)**
  - **TRF : Toluene Reference Fuels (Toluene + n-heptane)**
  - **TPRF : Toluene Primary Reference Fuels (Toluene + PRF)**
  - **ERF : Ethanol Reference Fuel (Ethanol+n-heptane)**
  - **EPRF**
  - **ETPRF**



Gauthier *et al. [52] found that* experimentally measured ignition delay times for 60% isooctane, 20% toluene, and 17% n-heptane mixture gave good agreement with shock tube ignition delay times

Table 2. Molar composition and octane numbers of the proposed surrogate fuel mixtures for gasoline.

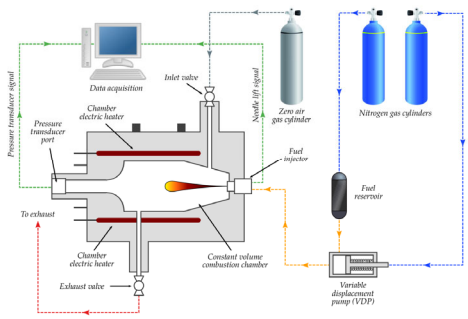
% Molar Composition	Mixture 1	Mixture 2	Mixture 3
iso-Octane	60	40	40
n-Heptane	8	10	20
Toluene	20	10	10
Methyl cyclohexane	8	40	30
1-Pentene	4	0	0
RON (linear)	92.9	82.2	74.5
MON (linear)	90.6	80.0	72.7
RON (blend)	96.3	92.9	82.5
MON (blend)	92.9	84.9	76.3

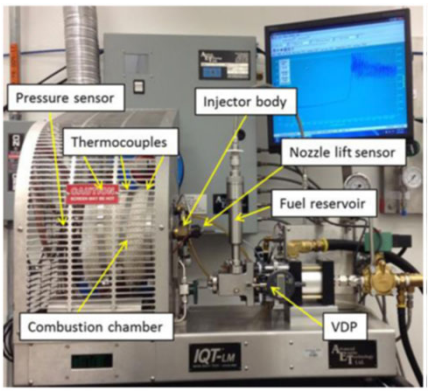
Ref. W. Pitz, C. Westbrook, O. Herbinet, E.J. Silke Prog. In Chemical Kinetic Modeling for Surrogate Fuels
08 COMODIA, Sapporo, Keynote Paper

IDT Measurement in IQT

KAUST Research-Ignition Quality Tester (KR-IQT)

- Conventional IQT : Injection of constant volume of fuel
  - Equivalence ration changes with fuel and chamber temperature
- KR-IQT could control fuel mass (volume) to test at a fixed equivalence ratio
  - Variable displacement pump (VDP)

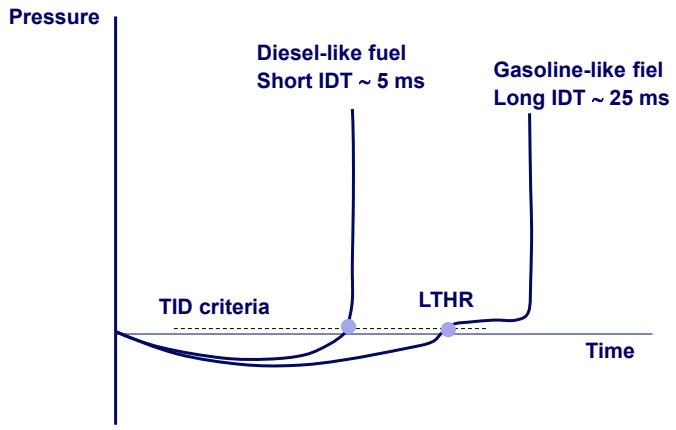




Determination of Ignition Delay

- Start of injection of fuel spray into CVCC (Soln) from max needle lift data
  - Evaporative cooling reduces pressure
  - Pressure recovery to initial pressure by heat transfer from chamber + exothermic reaction
- Ignition delay time (τ_{id}) from start of injection to significant heat release
  - IQT standard: P_0+138 kPa (20 psi)
  - Considering fuels with low temperature heat release (LTHR), Bogin proposed P_0+276 kPa (40 psi)
- For fuels with long ignition delay with significant LTHR, these definitions may lead to erroneous results for fuels such as iso-octane and gasoline-like fuels

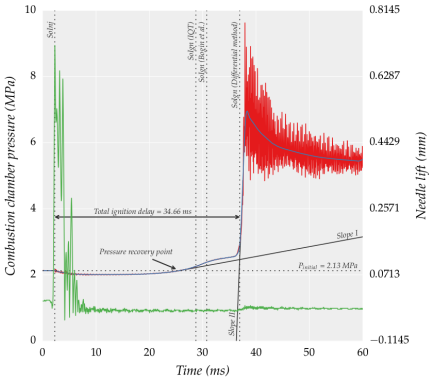
Determining Ignition Delay Time

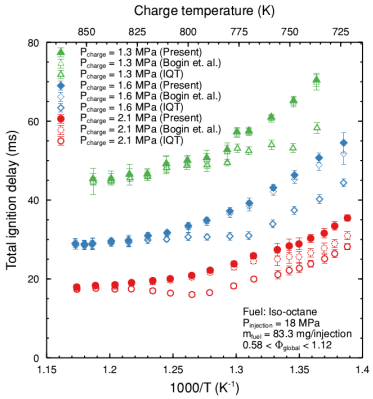


Error in IDT measurement for long IDT fuel by LTHR !
Total ignition delay (TID) = physical + chemical
Physical ID : Evaporation and mixing

Gradient Method and Temperature-Sweep Method

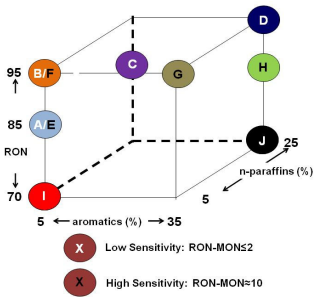
- **Gradient method**
  - Crossing of gradients at pressure recovery point and maximum gradient
- **Temperature sweep method**
  - Turn off the electrical heater then the chamber temperature decreases at a rate of about 5.5 K/min

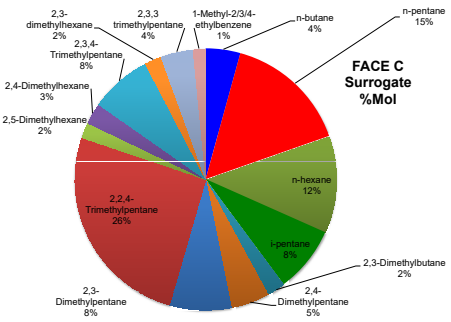




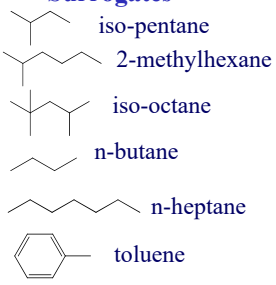
SY Yang, N Naser, J Cha, SH Chung, "Effect of temperature, pressure and equivalence ratio on ignition delay in ignition quality tester (IQT): diesel, *n*-heptane, and *iso*-octane fuels under low temperature conditions." *SAE Intl. J. Fuel Lubr.* 8 (2015) 537-548.

Fuels for Advanced Combustion Engines (FACE) Gasolines





Surrogates



- **Detailed Hydrocarbon Analysis (DHA)**
- **~ 100 species identified**
- **Linear alkanes at lighter end (butane, pentane).**
- **Branched alkanes are primarily mono-methylated C5 to C7 isomers**
- **Large number of trimethylpentanes (iso-octane)**

Courtesy by M Sarathy

RON and DCN Relation

- **Methodology in predicting octane index (RON /MON)**
  - **Basic principle is that fuels with the same octane index(OI) operating under the same pressure/time history have the same autoignition phasing**
  - **Two different fuels have the same octane index at the same temperature and pressure when they have the same total ignition delay times**

N. Naser, S.Y. Yang, G. Kalghatgi, S.H. Chung, "Relating fuel octane numbers to ignition delays measured in an ignition quality tester (IQT)," Fuel 187 (2017) 117-127

Fuel Matrix

- **Primary reference fuels (PRF)**
  Binary mixture of iso-octane and n-heptane
- **Toluene reference fuels (TRF)**
  Binary mixture of Tolune and n-heptane
- **Toluene primary reference fuels (TPRF)**
  Ternary mixture of toluene, iso-octane and n-heptane
- **Real fuels**
  FACE & Certificate gasolines

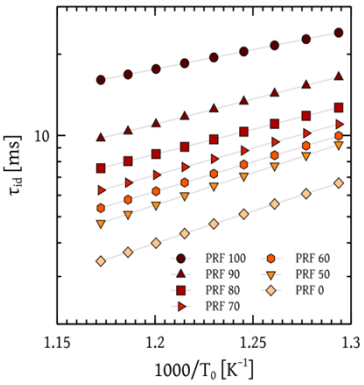
Table 2. Fuel matrix of FACE and certification gasolines

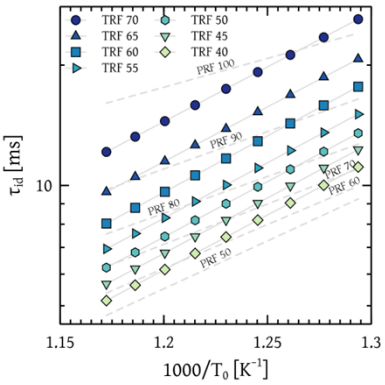
Fuel	RON	MON	Ref.
FACE A	83.5	83.6	COA**
FACE F	94.4	85.8	COA
FACE I	70.3	69.6	COA
FACE J	71.8	68.8	COA
Coryton gasoline	97.5	86.6	COA
Haltermann gasoline	91.0	83.4	COA

* Blending rule in Kalghatgi et al. (SAE 2015-01-0757)
**Certificate of analysis

Ignition delay times of PRFs & TRFs

- IDT for PRFs at P_0 = 21.3 bar (DCN condition) and ϕ = 0.7 and temperature in the range 753 – 853 K.
- The equivalence ratio can take any values as long as the same values for the primary and non-primary reference fuels are used.
- Crossing of TRF data (high sensitivity) with PRF data

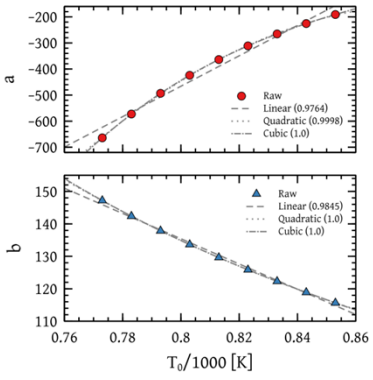




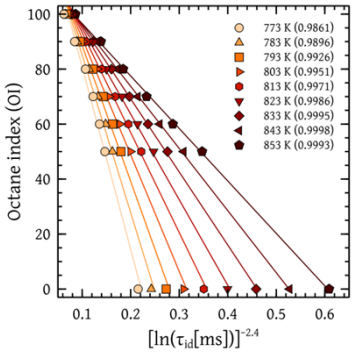
$\tau \sim \exp(E_a/RT)$
$\log \tau \sim E_a/RT$

Determining correlation between OI of PRF and τ_{id}

- A linear relation between OI and ignition delay is obtained when n = –2.4 with a and b as fn(T)
- An examination of the curve fit parameters a and b indicate that they are strongly dependent on the temperature.
- Fit parameters have a quadratic variation with charge temperature



Curve fit parameters versus charge temperature



Linear curve of octane index of primary reference fuels values in parentheses indicate R^2

$$OI = a[\ln\tau_{id}]^n + b$$

$$a = -26088\,(T_0/1000)^2 + 46839\,(T_0/1000) - 21162$$

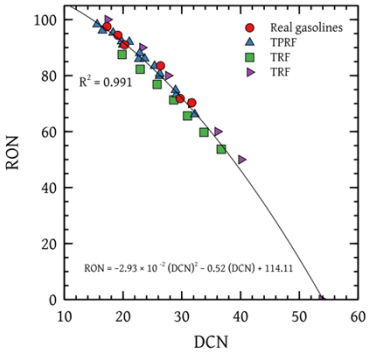
$$b = 1422\,(T_0/1000)^2 - 2799\,(T_0/1000) + 1481$$

DCN - RON correlation

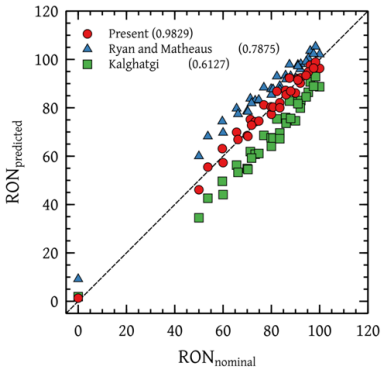
- **Excellent correlation between DCN and RON**

  $RON = -293(DCN/100)^2 - 52(DCN/100) + 114.1$

- **Note that the correlation between DCN and MON is poor as expected because of fuel sensitivity, such that a single DCN cannot simultaneously correlate with both RON and MON.**



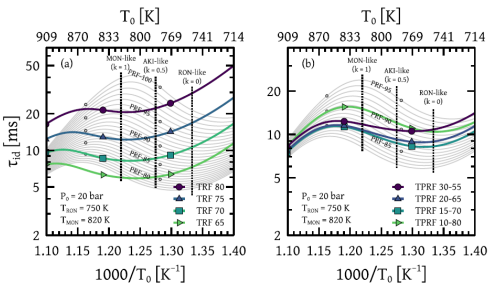
Correlation between DCN and RON

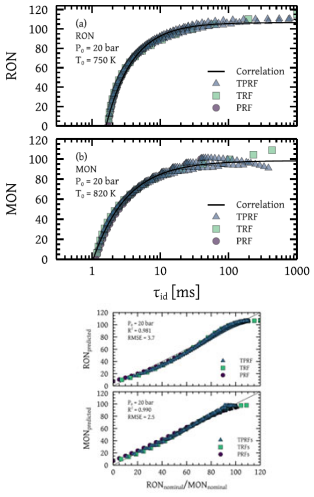


Comparison of predicted RON from DCN and from correlations available in the literature (values in parentheses indicate R^2).

RON / MON Estimation from IDT Calculation

Simulated IDT of PRFs (gray) and TRFs and TPRFs at = 20 bar.
RON/MON-like conditions determined from best correlations





N Naser, MS Sarathy, SH Chung, "Estimating fuel octane numbers from homogeneous gas-phase ignition delay times," Combust. Flame 188 (2018) 307-323.

Combustion Research Trends

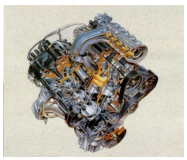
- Combustion : Multi-physics, multi-scale phenomena
- Click to edit Master text styles
  - Fluid, heat & mass transfer, chemical kinetics
  - Second level
    - Reaction zone thickness O(0.1 mm)
      - Third level
        - Fourth level
          - Fifth level

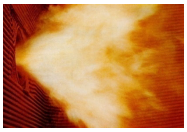
	1980’	1990’	2000’	2010’
Experiment	Flame and soot visualization	Laser diagnostics	Time-resolved	Validation data
Kinetics	H2, CH4	C4	C16	High C fuels Low-Temp
Computation	Detailed chemistry 1D	2D Transient	Turbulent High C fuels	Realistic Turbulent

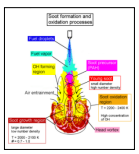
Engineering-based — Science-based

Combustion Applications

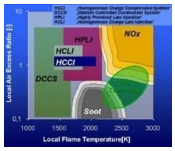
Issues	Topics
Efficiency Emission Fuel issues	Direct injection Low temp. combustion HCCI/PCCI Hybrid Fuel characterization Alternative Fuels
Low NOx Lean Premixed C Fuel CC, Cogeneration	Thermo-acoustics Flame-vortex interaction Ignition / Autoignition Lean blowout Flashback
Low emission Aftertreatment CCS Fuel	Oxy-fuel combustion CO_2 capture IGCC
Safety Security	Fire Explosion Low sooting flare



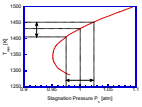


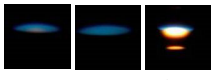


Kosaka



Kamimoto / Maier





iso-Octane n-Heptane Toluene