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Introduction to combustion

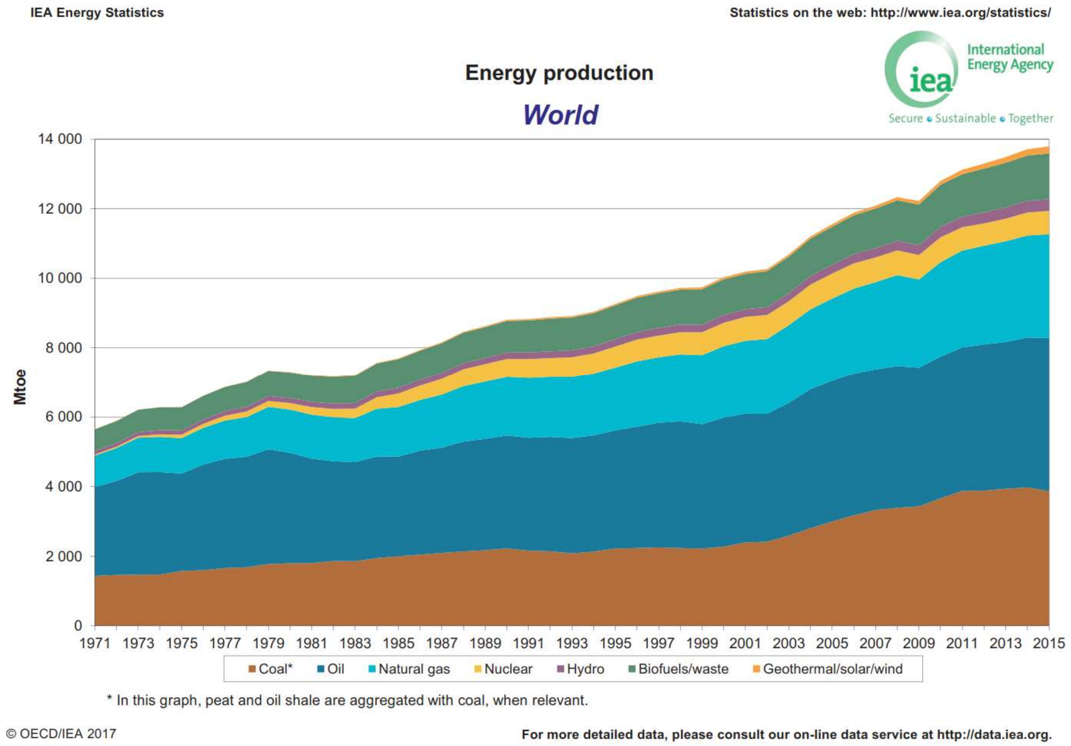
EEN-E2002 Combustion Technology
2019

D.Sc (Tech) Ossi Kaario

Motivation

- **Why learn about combustion ?**

- **Most of the energy in the world, 80% - 90%, is produced from different kinds of combustion processes**
- **Understanding of what is combustion**
  → how to make it more efficient or how to reduce emissions
- **This lecture is about fundamental flames and combustion chemistry**



* In this graph, peat and oil shale are aggregated with coal, when relevant.

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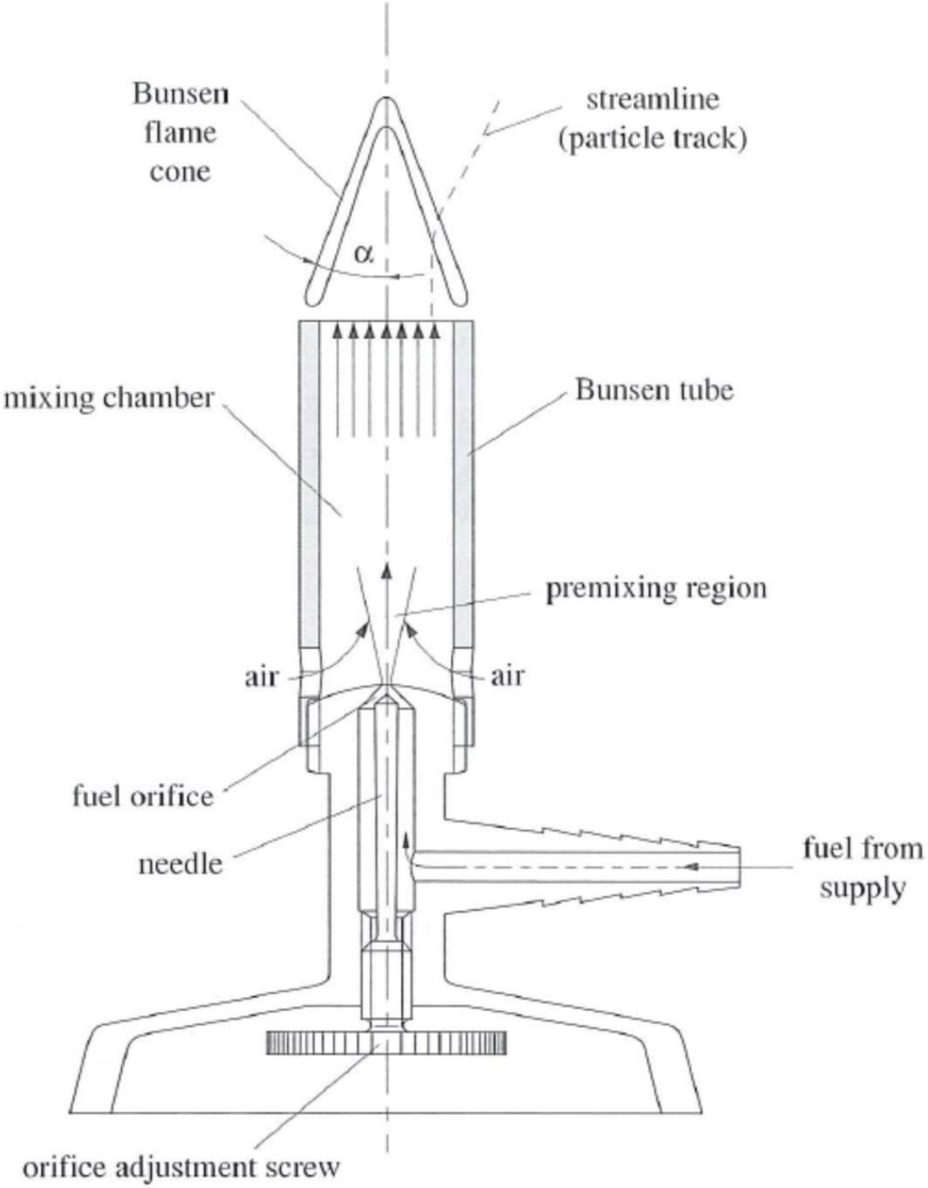
For more detailed data, please consult our on-line data service at http://data.iea.org.

> 80% from combustion

Contents

- Bunsen flame
- Fundamental flame types
- Reaction mechanism and Lambda
- Combustion kinetics
- Ignition
- Adiabatic flame temperature

Bunsen burner



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Butane global chemistry

$$C_4H_{10} + 6.5(O_2 + 3.77N_2) \rightarrow 4CO_2 + 5H_2O + 24.5N_2$$

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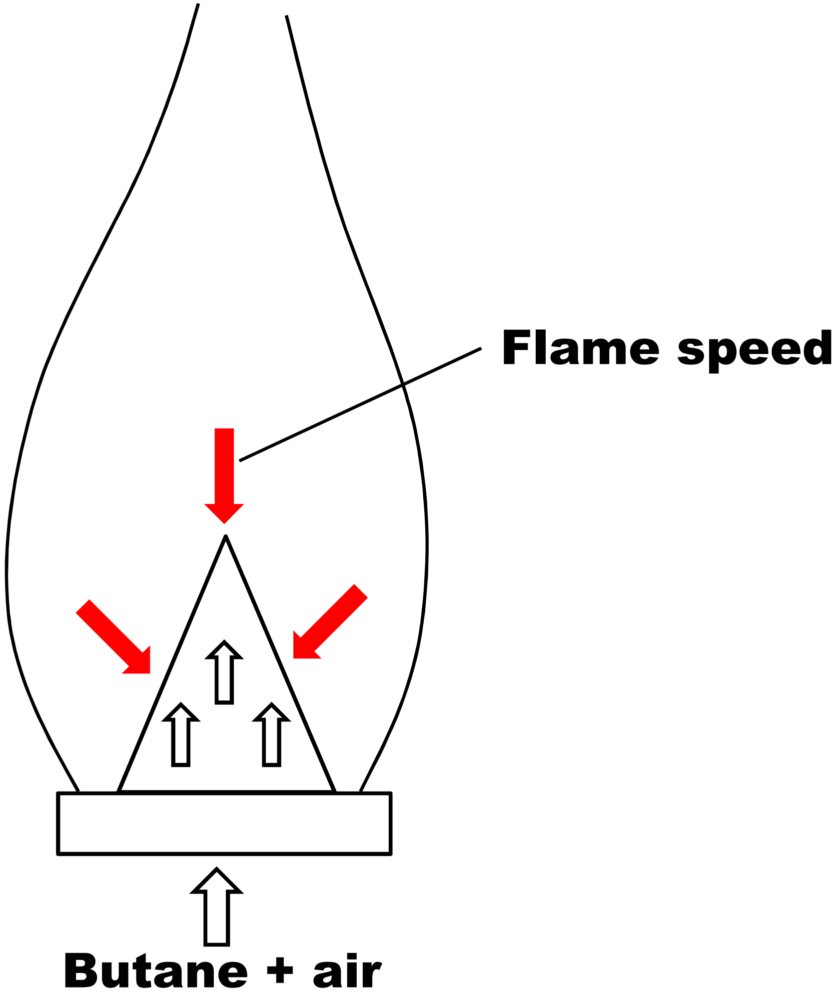
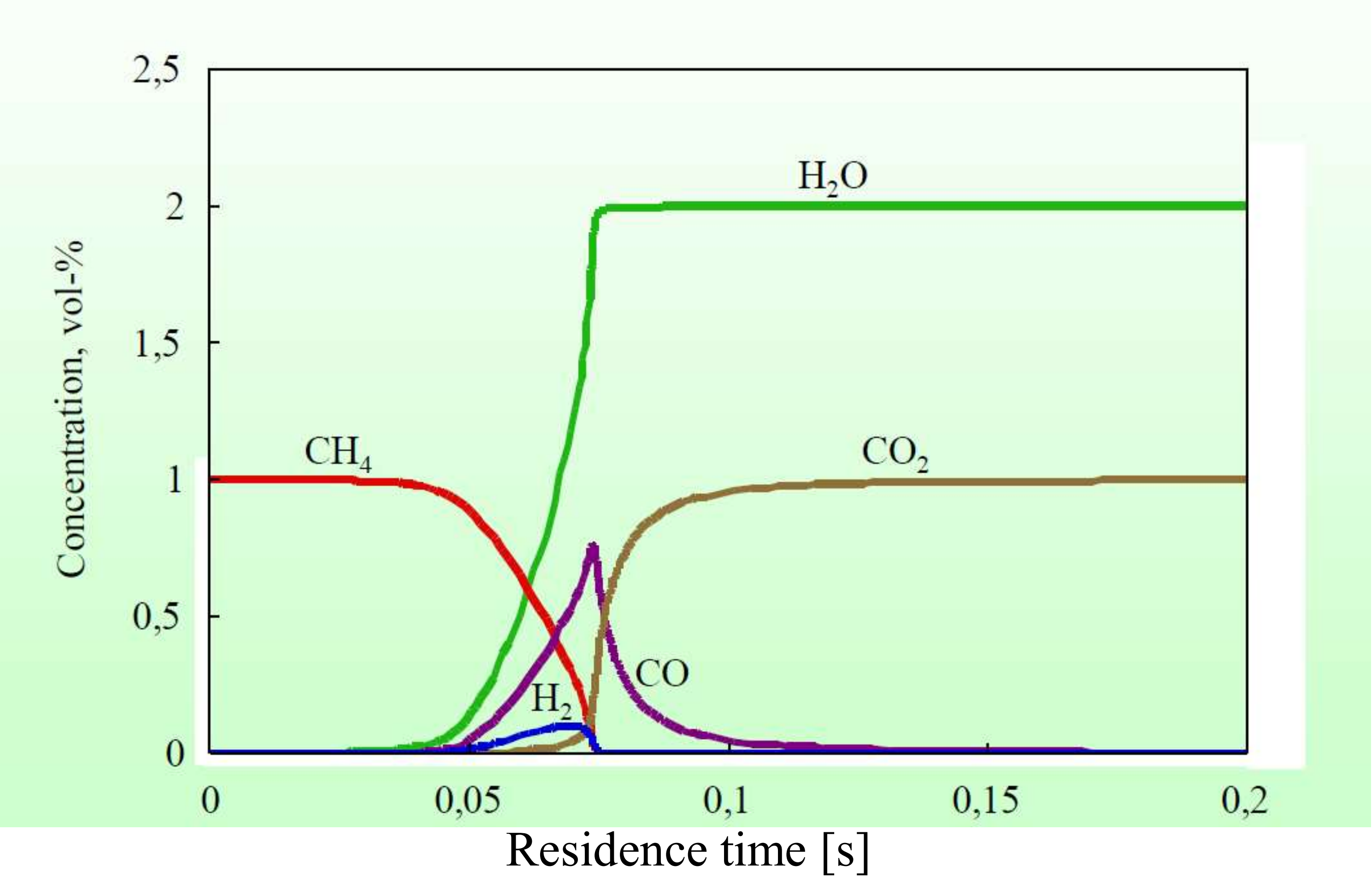
Premixed Bunsen flame

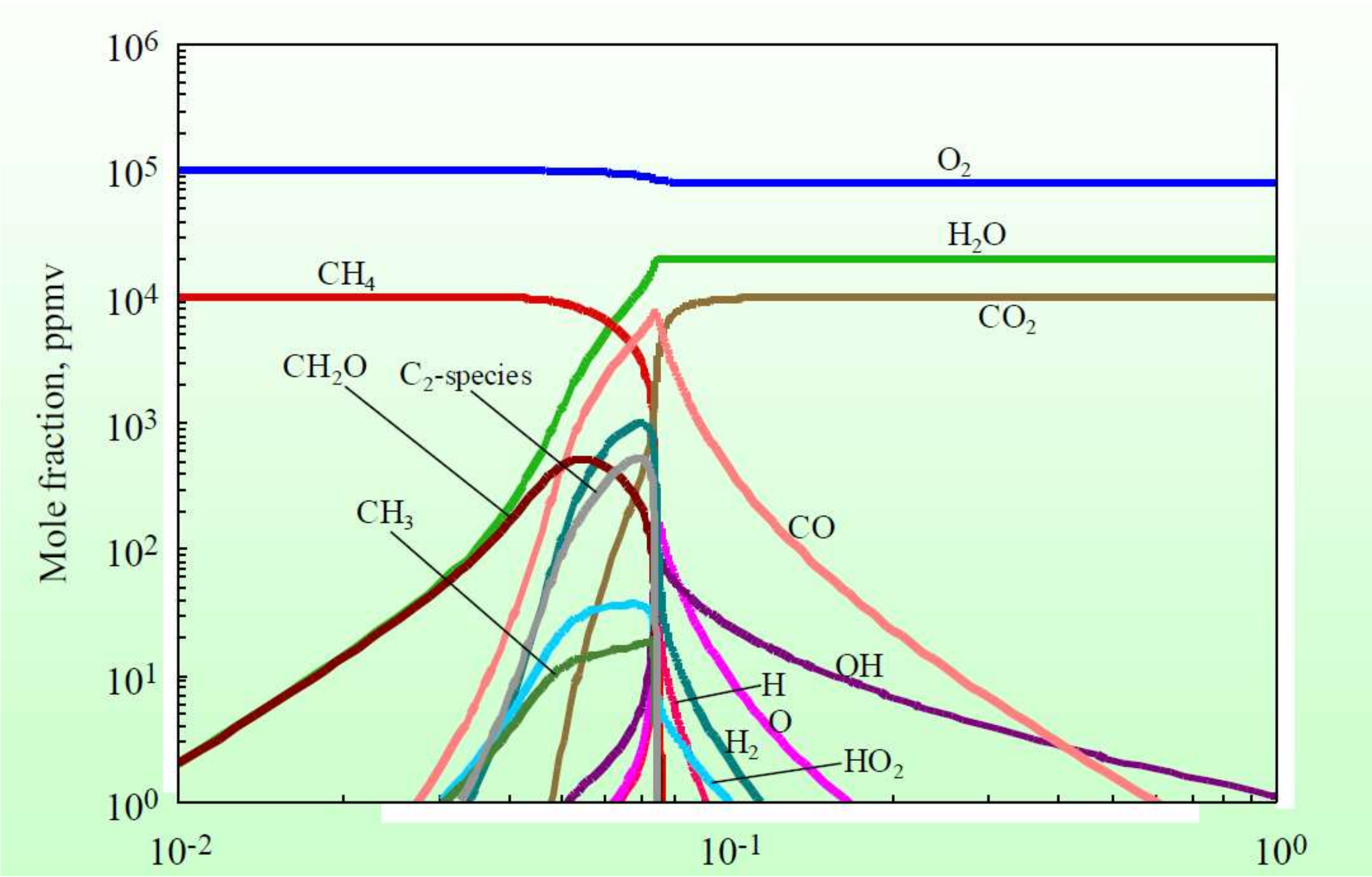


Premixed methane – air mixture combustion



Kilpinen, 1997

Premixed methane – air mixture combustion



Residence time [s]

Kilpinen, 1997

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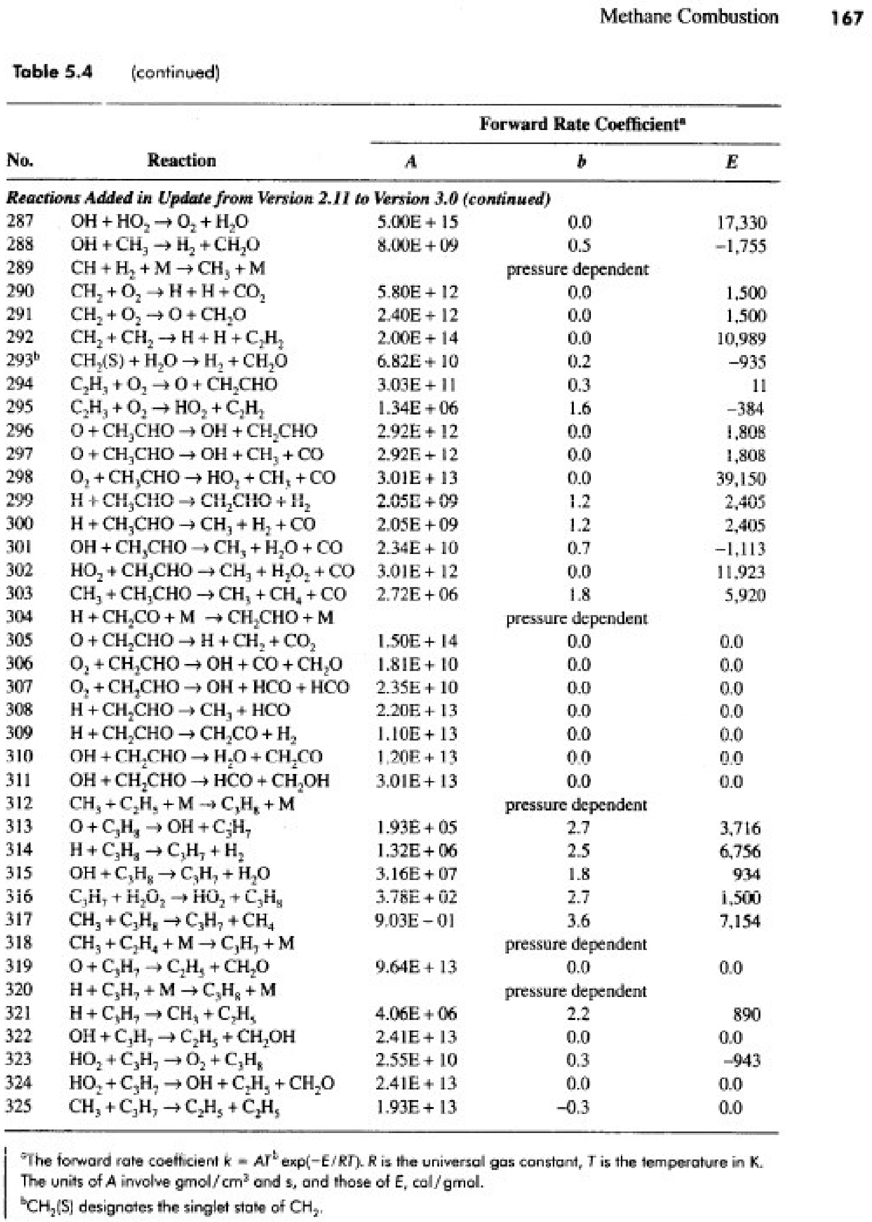
Elementary reactions

- **Methane chemistry**
- Detailed methane (CH_4) chemistry involves 53 species and 325 reactions (GRI 3.0 mechanism)



Methane Combustion 167

Table 5.4 (continued)

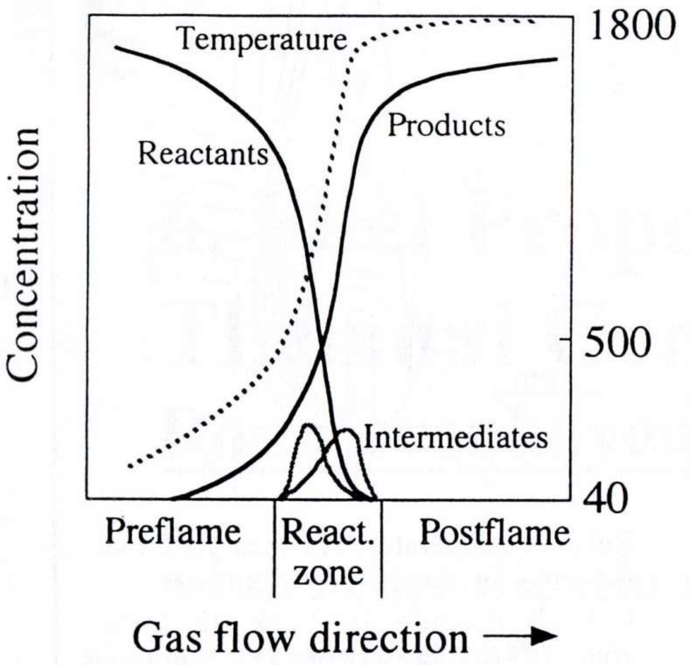
No.	Reaction	Forward Rate Coefficient[a] A	b	E
Reactions Added in Update from Version 2.11 to Version 3.0 (continued)				
287	$OH + HO_2 \rightarrow O_2 + H_2O$	5.00E + 15	0.0	17,330
288	$OH + CH_3 \rightarrow H_2 + CH_2O$	8.00E + 09	0.5	−1,755
289	$CH + H_2 + M \rightarrow CH_3 + M$		pressure dependent	
290	$CH_2 + O_2 \rightarrow H + H + CO_2$	5.80E + 12	0.0	1,500
291	$CH_2 + O_2 \rightarrow O + CH_2O$	2.40E + 12	0.0	1,500
292	$CH_2 + CH_2 \rightarrow H + H + C_2H_2$	2.00E + 14	0.0	10,989
293[b]	$CH_2(S) + H_2O \rightarrow H_2 + CH_2O$	6.82E + 10	0.2	−935
294	$C_2H_3 + O_2 \rightarrow O + CH_2CHO$	3.03E + 11	0.3	11
295	$C_2H_3 + O_2 \rightarrow HO_2 + C_2H_2$	1.34E + 06	1.6	−384
296	$O + CH_3CHO \rightarrow OH + CH_2CHO$	2.92E + 12	0.0	1,808
297	$O + CH_3CHO \rightarrow OH + CH_3 + CO$	2.92E + 12	0.0	1,808
298	$O_2 + CH_3CHO \rightarrow HO_2 + CH_3 + CO$	3.01E + 13	0.0	39,150
299	$H + CH_3CHO \rightarrow CH_2CHO + H_2$	2.05E + 09	1.2	2,405
300	$H + CH_3CHO \rightarrow CH_3 + H_2 + CO$	2.05E + 09	1.2	2,405
301	$OH + CH_3CHO \rightarrow CH_3 + H_2O + CO$	2.34E + 10	0.7	−1,113
302	$HO_2 + CH_3CHO \rightarrow CH_3 + H_2O_2 + CO$	3.01E + 12	0.0	11,923
303	$CH_3 + CH_3CHO \rightarrow CH_3 + CH_4 + CO$	2.72E + 06	1.8	5,920
304	$H + CH_2CO + M \rightarrow CH_2CHO + M$		pressure dependent	
305	$O + CH_2CHO \rightarrow H + CH_2 + CO_2$	1.50E + 14	0.0	0.0
306	$O_2 + CH_2CHO \rightarrow OH + CO + CH_2O$	1.81E + 10	0.0	0.0
307	$O_2 + CH_2CHO \rightarrow OH + HCO + HCO$	2.35E + 10	0.0	0.0
308	$H + CH_2CHO \rightarrow CH_3 + HCO$	2.20E + 13	0.0	0.0
309	$H + CH_2CHO \rightarrow CH_2CO + H_2$	1.10E + 13	0.0	0.0
310	$OH + CH_2CHO \rightarrow H_2O + CH_2CO$	1.20E + 13	0.0	0.0
311	$OH + CH_2CHO \rightarrow HCO + CH_2OH$	3.01E + 13	0.0	0.0
312	$CH_3 + C_2H_5 + M \rightarrow C_3H_8 + M$		pressure dependent	
313	$O + C_3H_8 \rightarrow OH + C_3H_7$	1.93E + 05	2.7	3,716
314	$H + C_3H_8 \rightarrow C_3H_7 + H_2$	1.32E + 06	2.5	6,756
315	$OH + C_3H_8 \rightarrow C_3H_7 + H_2O$	3.16E + 07	1.8	934
316	$C_3H_7 + H_2O_2 \rightarrow HO_2 + C_3H_8$	3.78E + 02	2.7	1,500
317	$CH_3 + C_3H_8 \rightarrow C_3H_7 + CH_4$	9.03E − 01	3.6	7,154
318	$CH_3 + C_2H_4 + M \rightarrow C_3H_7 + M$		pressure dependent	
319	$O + C_3H_7 \rightarrow C_2H_5 + CH_2O$	9.64E + 13	0.0	0.0
320	$H + C_3H_7 + M \rightarrow C_3H_8 + M$		pressure dependent	
321	$H + C_3H_7 \rightarrow CH_3 + C_2H_5$	4.06E + 06	2.2	890
322	$OH + C_3H_7 \rightarrow C_2H_5 + CH_2OH$	2.41E + 13	0.0	0.0
323	$HO_2 + C_3H_7 \rightarrow O_2 + C_3H_8$	2.55E + 10	0.3	−943
324	$HO_2 + C_3H_7 \rightarrow OH + C_2H_5 + CH_2O$	2.41E + 13	0.0	0.0
325	$CH_3 + C_3H_7 \rightarrow C_2H_5 + C_2H_5$	1.93E + 13	−0.3	0.0

[a] The forward rate coefficient $k = AT^b \exp(-E/RT)$. R is the universal gas constant, T is the temperature in K. The units of A involve gmol/cm³ and s, and those of E, cal/gmol.

[b] $CH_2(S)$ designates the singlet state of CH_2.

Fundamental gas flames

Premixed flame



M. Hupa 2000

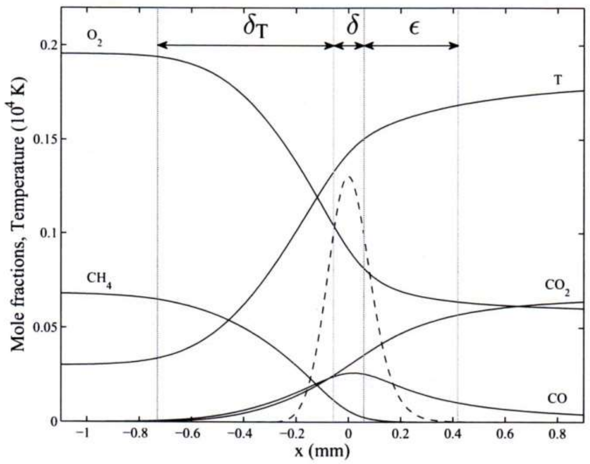
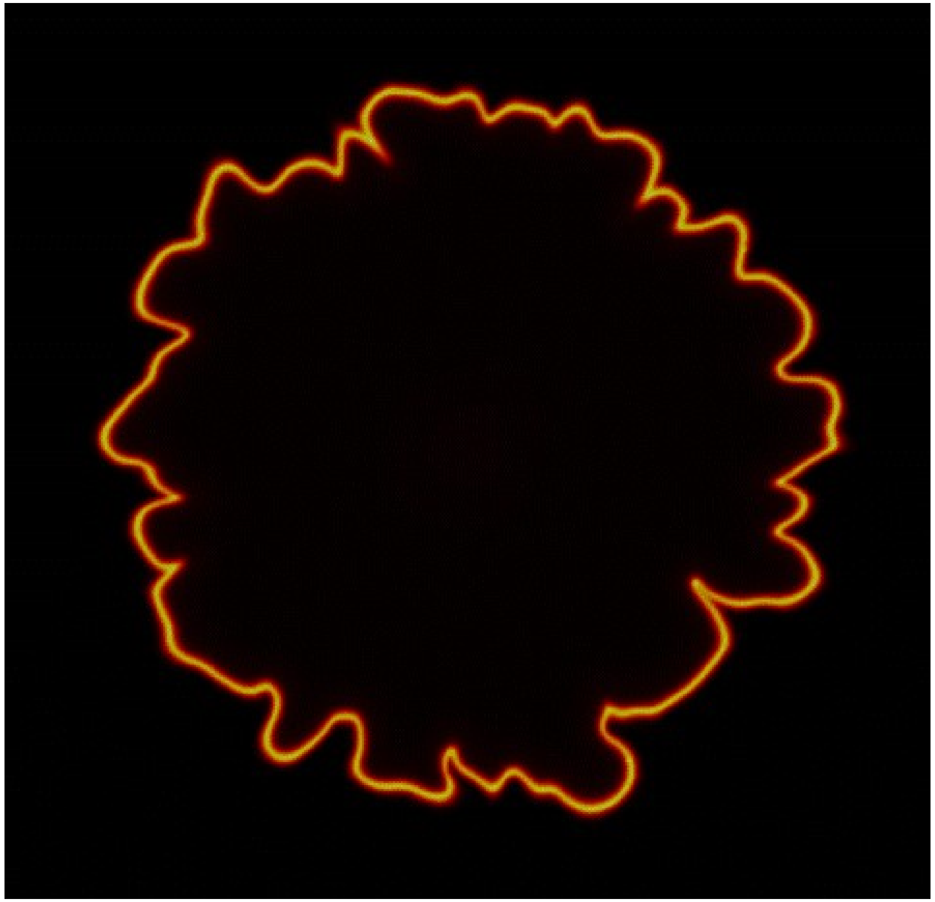


Figure 3.1: Structure of a lean methane/air flame (equivalence ratio Φ=0.6), including definition of different layers: inert preheating layer δ_T, reaction layer δ_r consisting of an inner layer with thickness δ and oxidation layer with thickness ϵ; dotted line indicates heat release profile.

F. Williams 1971

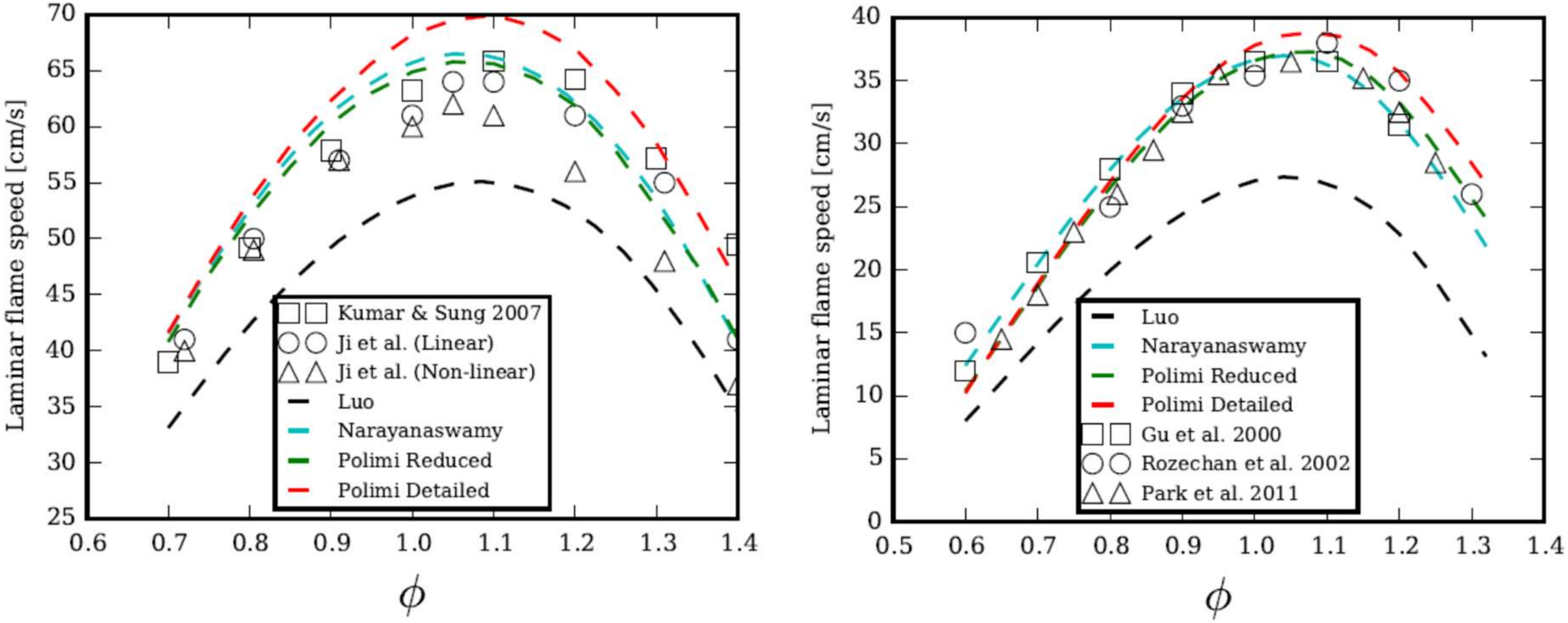
Flame speed in a premixed H_2 -case



M. Ghaderi Masouleh 2016

Flame front marked with hydroperoxyl (HO_2) radical

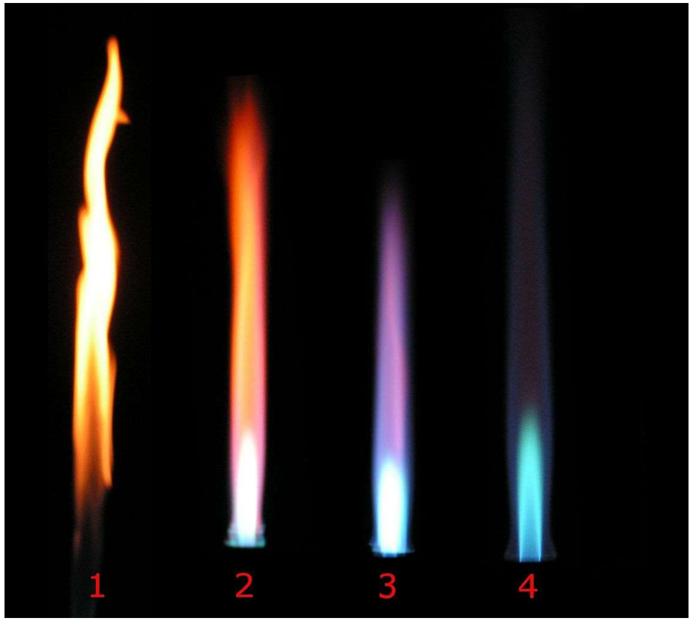
Laminar flame speed



n-dodecane/air, T=403K, P=1atm

methane/air, T=300K, P=0.1MPa

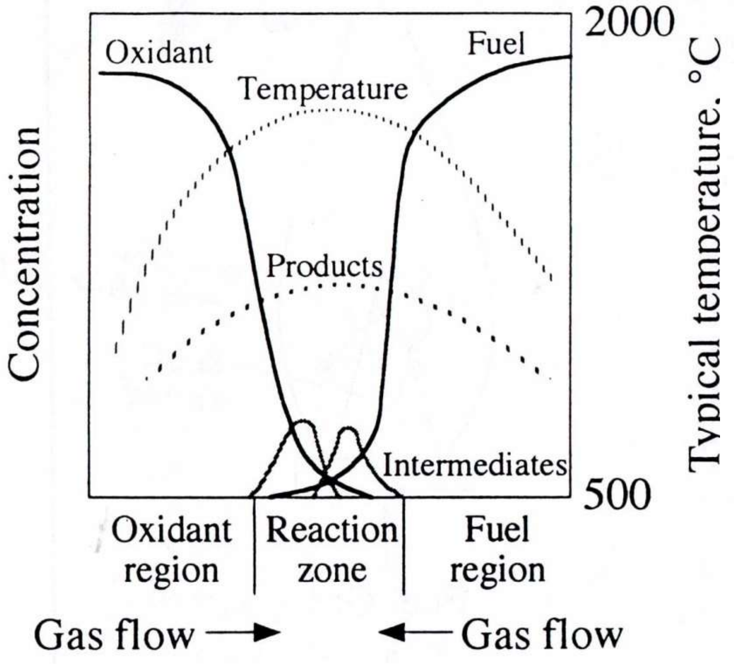
M. Ghaderi Masouleh et al., Fuel 2016



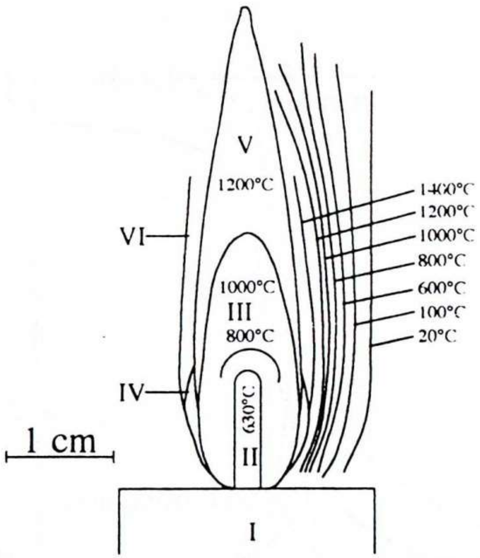
Diffusion ---- premixed combustion

Fundamental gas flames

Non-premixed flame



M. Hupa 2000



Relative temperatures in a candle flame from thermocouple measurements: I - Body of candle, II - Wick, III - Dark zone, IV - C_2 and Cl zone, V - Luminous zone, VI - Main reaction zone

Diffusion flame

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Non-premixed flame

A. Wehrfritz 2016

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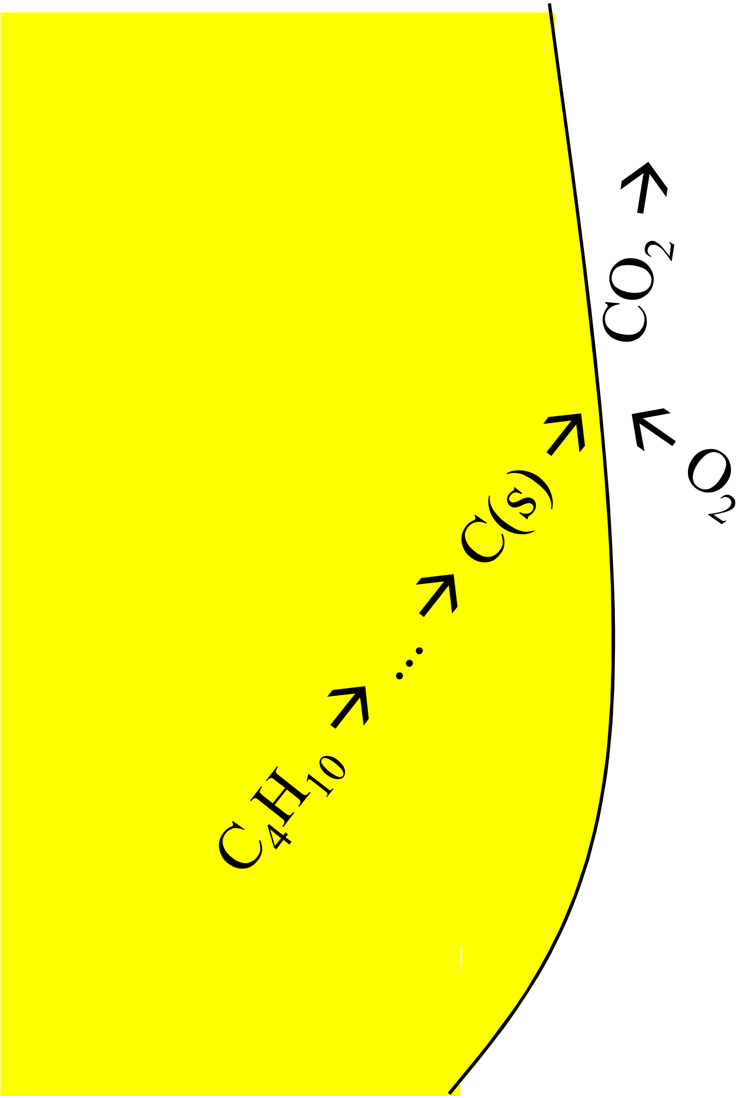
Diffusion flame chemistry



$C(s) + O_2 \rightarrow CO_2$

Properties of premixed and diffusion combustion processes

Premixed	**Diffusion**
-No soot	-Sooting flame
-Poor radiator	-Good raditive heat transfer
-Chemical reactions determine reaction rate	-Mixing determine reaction rate
-flame speed can be determined	-Cannot define burning velocity

-applications (stove, furnace..)
-safety issues

Discuss in pairs

Discuss with the person next to you for about 5 minutes the following topics

1. Think about the Bunsen burner, how does it operate ?
2. What does a premixed flame mean ? Where are fuel and air before combustion ? Where is the flame ? Is there is flame speed ? If yes, into what direction ?
3. What does a non-premixed flame mean ? Where are fuel and air before combustion ? Where is the flame ? Is there is flame speed ?

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Reaction scheme

- **Complete combustion**

$$C_xH_y + \left(x + \frac{y}{4}\right)O_2 + 3.77\left(x + \frac{y}{4}\right)N_2 \rightarrow$$

$$xCO_2 + \frac{y}{2}H_2O + 3.77\left(x + \frac{y}{4}\right)N_2$$

$$In \quad air \quad \frac{v_{N_2}}{v_{O_2}} = \frac{0.7905}{0.2095}$$

Additional material

Does it burn ?

- **Complete combustion with oxygen**

$$C_xH_yO_z+\left(x+\frac{y}{4}-\frac{z}{2}\right)O_2\rightarrow xCO_2+\frac{y}{2}H_2O$$

- **Compound is incombustible if** $\left(x+\frac{y}{4}-\frac{z}{2}\right)\leq 0$

$$\rightarrow\ z\geq 2x+\frac{1}{2}y$$

- **For example**
  - **CO_2** $z=2, x=1, y=0, \rightarrow 2\geq 2, \text{true, does not burn}$
  - **CO** $z=1, x=1, y=0, \rightarrow 1\geq 2, \text{false, burns}$

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Lambda

- **Lambda or Air factor**

$$\lambda = \frac{n_i}{n_{i,st}} \qquad \begin{cases} n_i = n_{O_2} + n_{N_2} \\ n_{i,st} = n_{O_2,st} + n_{N_2,st} \end{cases}$$

- **Because** $\begin{cases} n_{O_2} = x_{O_2} n_i \\ n_{O_{2,st}} = x_{O_2} n_{i,st} \end{cases}$ **, where** x_{O_2} **is oxygen mole fraction, Lambda can also be expressed as**

$$\lambda = \frac{n_{O_2}}{n_{O_2,st}}$$

- **Lambda can also be defined as**

$$\lambda = \frac{L}{L_{st}}$$

where L **is the available air / fuel ratio and** L_{st} **is the stoichiometric air / fuel ratio**

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Lambda

$$C_xH_y + \underset{\uparrow}{\lambda}\left(x + \frac{y}{4}\right)O_2 + \underset{\uparrow}{\lambda} \cdot 3.77\left(x + \frac{y}{4}\right)N_2 \rightarrow$$

$$xCO_2 + \frac{y}{2}H_2O + (\underset{\uparrow}{\lambda} - 1)\left(x + \frac{y}{4}\right)O_2 + \underset{\uparrow}{\lambda} \cdot 3.77\left(x + \frac{y}{4}\right)N_2$$

Practise writing reaction scheme

Write down reaction scheme for C2H2 (acetylene) with

- **Lambda=1**
- **Lambda=2**

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Example: If Lambda is not known

- **If you know your fuel and air amount, what is your Lambda ?**

1. Define the stoichiometric air consumption

-For very many hydrocarbons, it is close to L_{st} ~15
(-For methane it is a bit higher 17.1)

2. What is your available air / fuel ratio L ?

-30g of air and 1g of fuel → L = 30/1 = 30

3. Lambda is now

(assuming L_{st} = 15)

$$\lambda = \frac{30}{15} = 2$$

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Combustion Kinetics

- **Global reaction:**

$$CO + 1/2\, O_2 \rightarrow CO_2$$

- **Elementary reactions**

$$CO + O_2 \rightarrow CO_2 + O$$
$$CO + O + M \rightarrow CO_2 + M^*$$
$$O + O + M \rightarrow O_2 + M^*$$

M^* = has higher energy than M

- **Rate law (Law of mass action)**

$$aA + bB \rightarrow dD + eE \ldots \qquad \frac{d[A]}{dt} = -k[A]^a[B]^b$$

a, b, … are *reaction orders* respect to species A, B …

- **Elementary reaction rate**

$$\frac{d[CO]}{dt} = -k[CO][O_2]$$

Can be used only with elementary reactions

M = ”third body” – molecule brings (through collision) the energy needed to split the molecule, or takes away energy and stabilizes the combination of e.g. CO + O

Combustion Kinetics

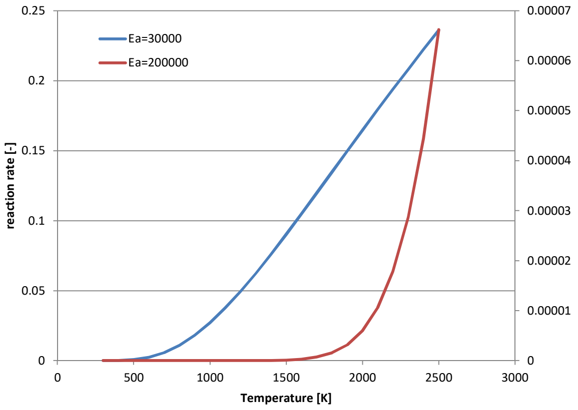
- Arrhenius' relation for <u>rate coefficient</u> ***k***

$$k = A \cdot e^{-E_a/RT}$$

A = **frequency factor (frequency of collision between molecules)**

E_a = **activation energy**

  - **Low activation energy E → low temperature sensitivity**
  - **High activation energy E → high temperature sensitivity**



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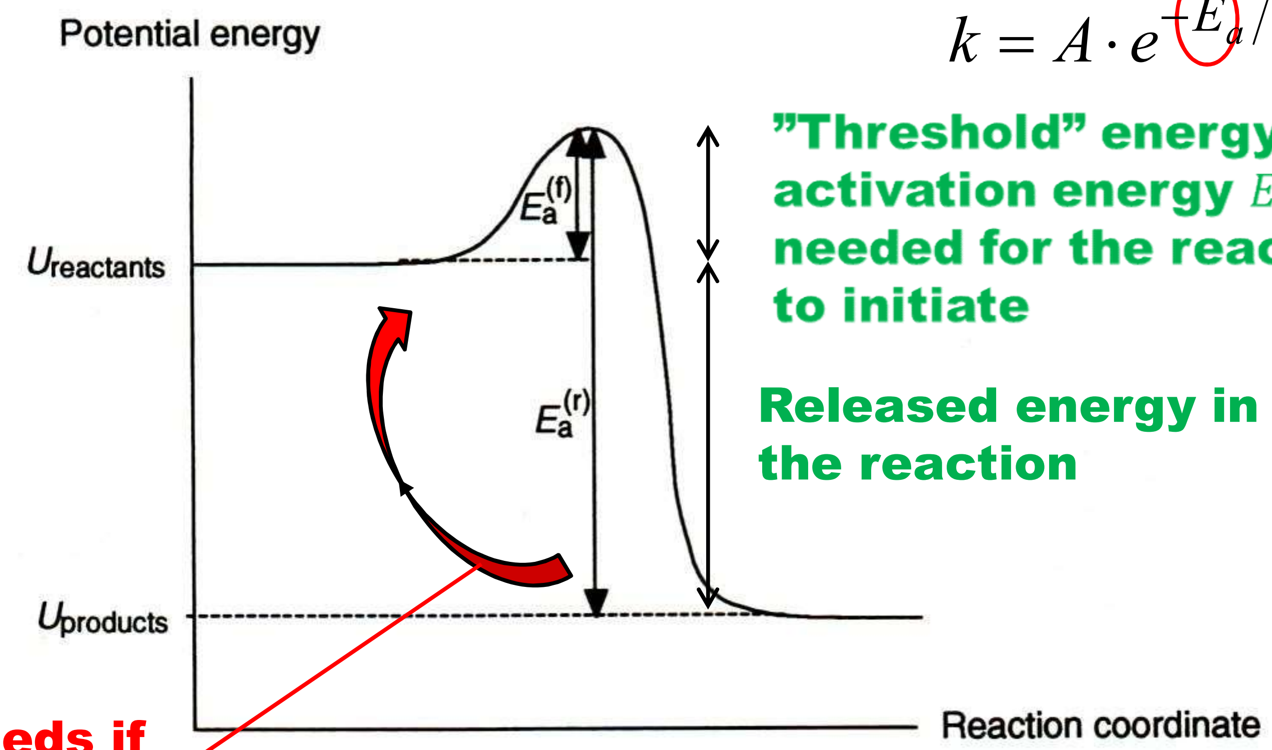
Energy diagram

$$k = A \cdot e^{-E_a/RT}$$



”Threshold” energy, i.e. activation energy E_a needed for the reaction to initiate

Released energy in the reaction

Reaction proceeds if enough heat from combustion is provided back in order to the cross the ”threshold” energy

Reactants → Products

Example: NO_x emissions
Thermal NO

- **Or Zeldovich-NO (1946)**

$$O + N_2 \xrightarrow{k_1} NO + N \qquad k_1 = 1.8 \cdot 10^{14} \exp\left(-318 kj\, mol^{-1} / (RT)\right)$$

$$N + O_2 \xrightarrow{k_2} NO + O \qquad k_2 = 9 \cdot 10^{9} \exp\left(-27 kj\, mol^{-1} / (RT)\right)$$

$$N + OH \xrightarrow{k_3} NO + H \qquad k_3 = 2.8 \cdot 10^{13}$$

Combustion, 1999, Warnatz, Maas, and Dibble

First reaction has high activation energy and hence it has relevant reaction rates only at high temperatures. It is also the rate limiting step of the mechanism (slowest reaction).

NO + NO2 = NOx
Nitric oxide + nitrogen dioxide = nitrogen oxides

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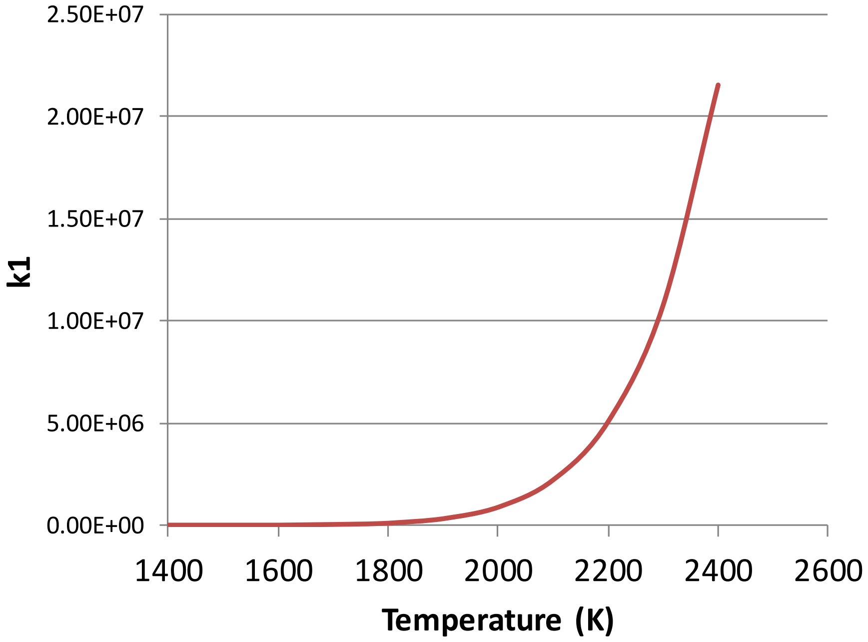
Example: Thermal NO



Temperature dependence of the rate coefficient k_1 in the Zeldovich mechanism.

Chemical bonds (in order to understand radicals)

- Chemical bonds are e.g. covalent, ionic, or metallic bond.
- In covalent bonds, atoms share electrones
- In chemical reactions, atoms try to reach noble gas electrone structure = octet structure (8 electrones)
- Hydrogen atom has 1 electrone, each atom shares 1 electrone

$$H:H$$

- Oxygen atom has 6 electrones in the outer electrone shell. Octet is reached when both share 2 electrones

$$\underset{\cdot\cdot}{\ddot{O}} :: \underset{\cdot\cdot}{\ddot{O}}$$

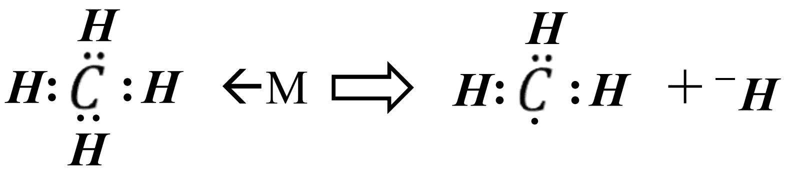
- Nitrogen has 5 electrones in the outer shell. Octet is reached when both share 3 electrones

$$:N ::: N:$$

- Covalent bond is relatively strong. Therefore, in order to break 2-atom gas molecules, such as hydrogen, oxygen, and nitrogen, high energy is required.

Radicals

1. **A radical has an unpaired electrone**



$$H:\underset{\underset{H}{\cdot\cdot}}{\overset{\overset{H}{\cdot\cdot}}{C}}:H \;\leftarrow M \;\Rightarrow\; H:\underset{\cdot}{\overset{\overset{H}{\cdot\cdot}}{C}}:H \;+\; {}^{-}H$$

2. **Structure is incomplete. Therefore, almost always when they collide they react.**
3. **Consequently, they are very reactive**

Examples of radicals:

-O, H, OH, HO_2, CH_3, CH_2, CH, C, NH_2, NH, N, CN

’Whole combustion chemistry is due to radicals’

Ignition (and radicals)

- **In applications where the combustion process is intermittent or periodic, like in internal combustion engines, ignition process becomes an important topic.**

- **With CH fuels ignition takes place only after a certain ignition delay time.**
- **During the ignition delay period, radical pool population is increasing but the fuel consumption rate and temperature increase are low**
- **Finally, the radical pool becomes large enough to consume a significant fraction of fuel, and rapid ignition takes place.**

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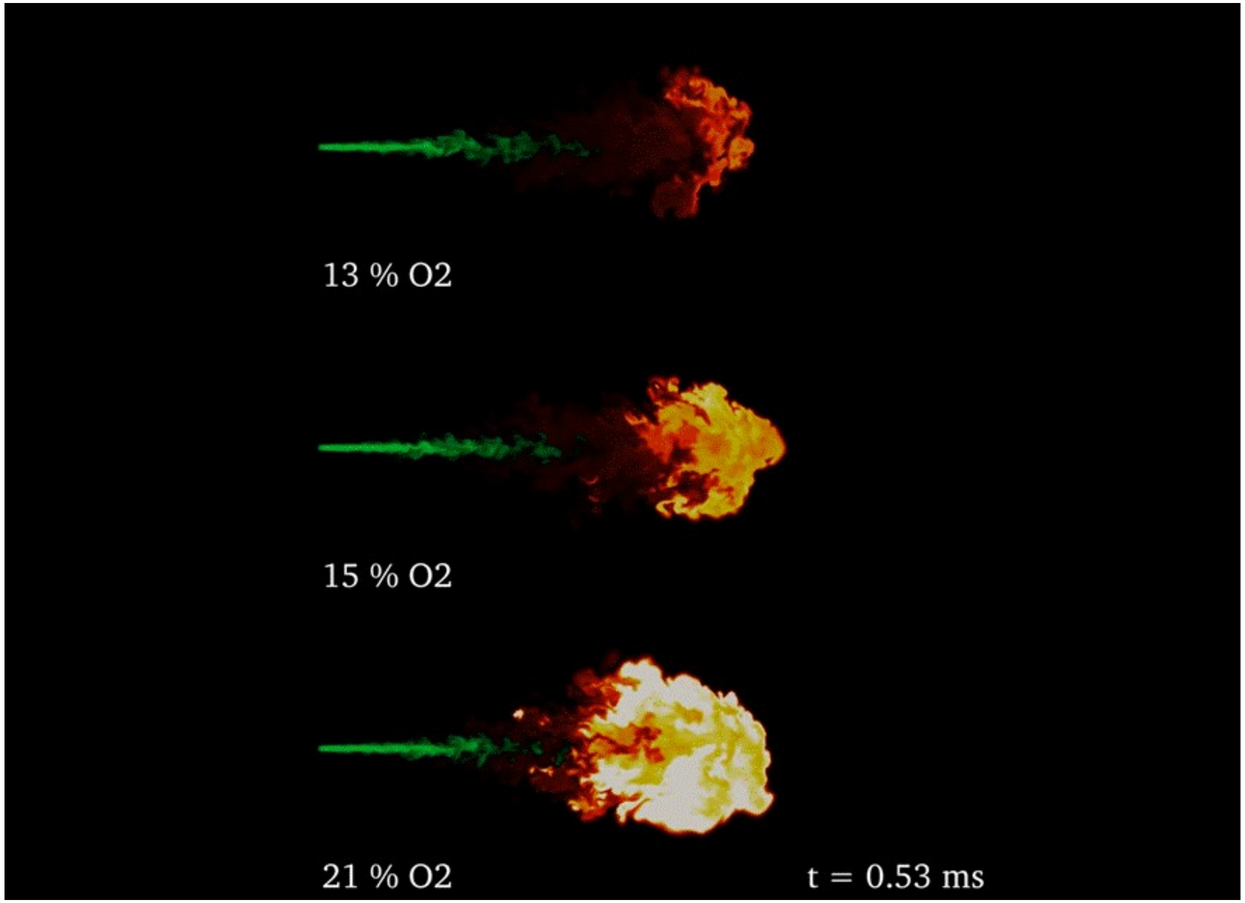
Ignition in a spray flame



A. Wehrfritz 2016

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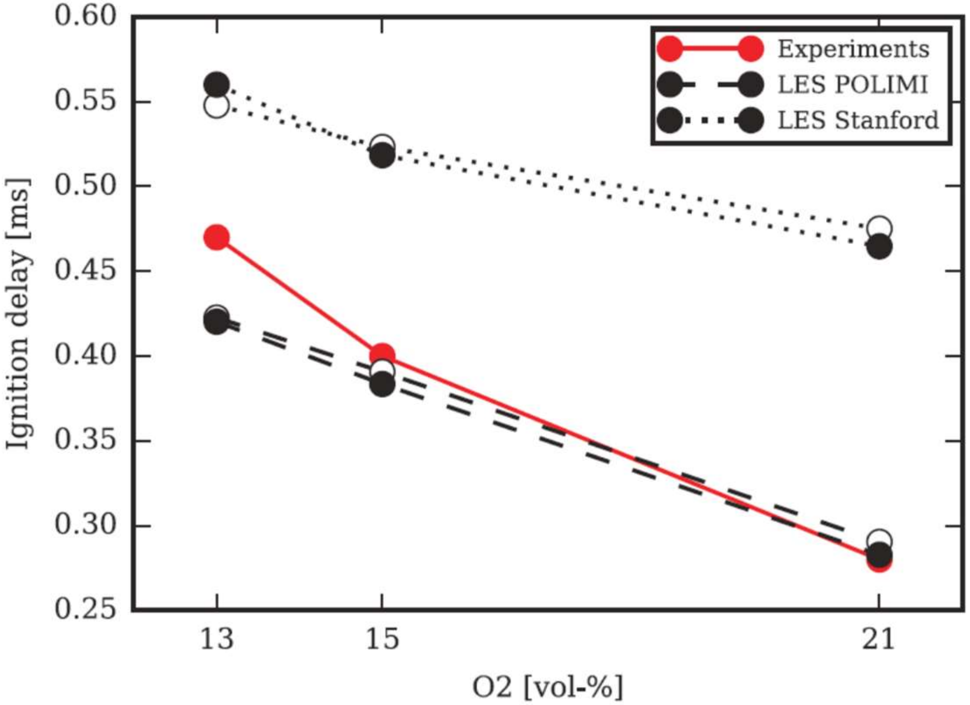
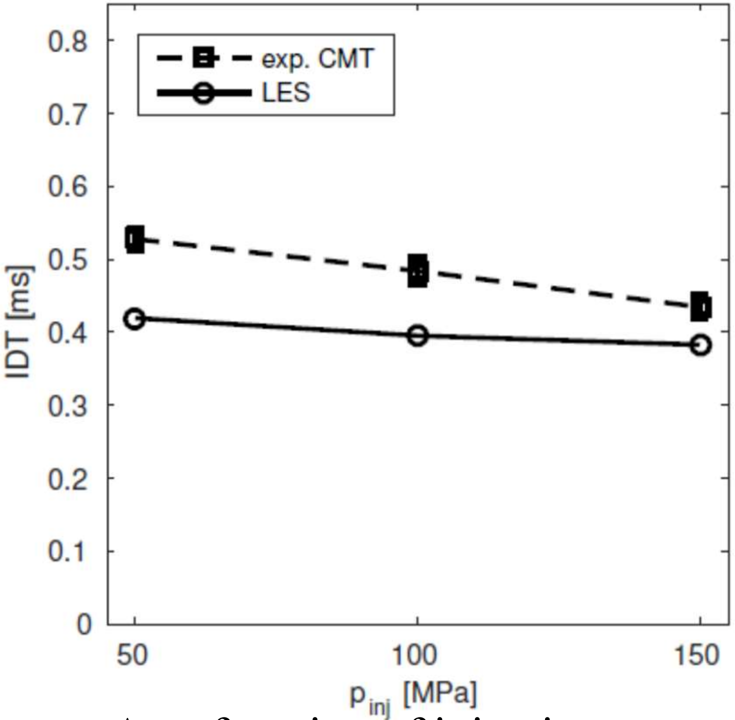
Ignition delay times in a spray flame



As a function of O_2 concentration



As a function of injection pressure

A. Wehrfritz et al. 2016

H. Kahila et al. 2017

Ignition and Radicals

(0) chain initiation:

$$CO + O_2 = CO_2 + \underline{O}$$

$$H_2 + M^* = \underline{H} + \underline{H} + M$$

$$CH_4 + M^* = \underline{CH_3} + \underline{H} + M$$

(1) chain carrying:

$$\underline{O} + O_2 + M = \underline{O_3} + M^*$$

$$\underline{H} + O_2 + M = \underline{HO_2} + M^*$$

(2) chain branching:

$$\underline{O_3} + CO + M^* = CO_2 + \underline{O} + \underline{O} + M$$

$$\underline{H} + O_2 = \underline{OH} + \underline{O}$$

(3) Chain terminating:

$$\underline{O} + \underline{O} + M = O_2 + M^*$$

$$\underline{H} + \underline{OH} + M = H_2O + M^*$$

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Hydrocarbon Oxidation

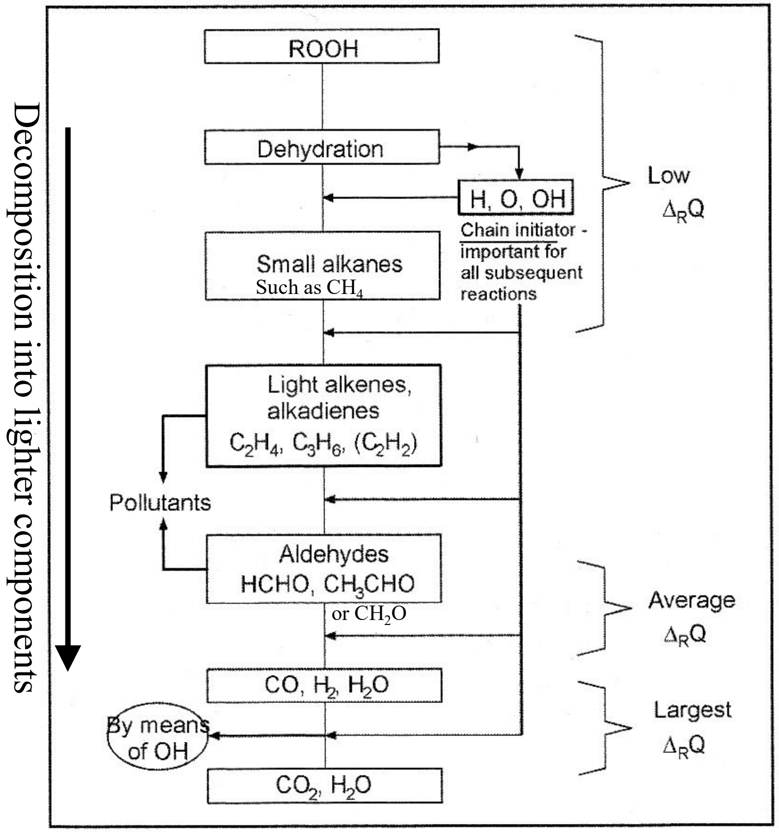
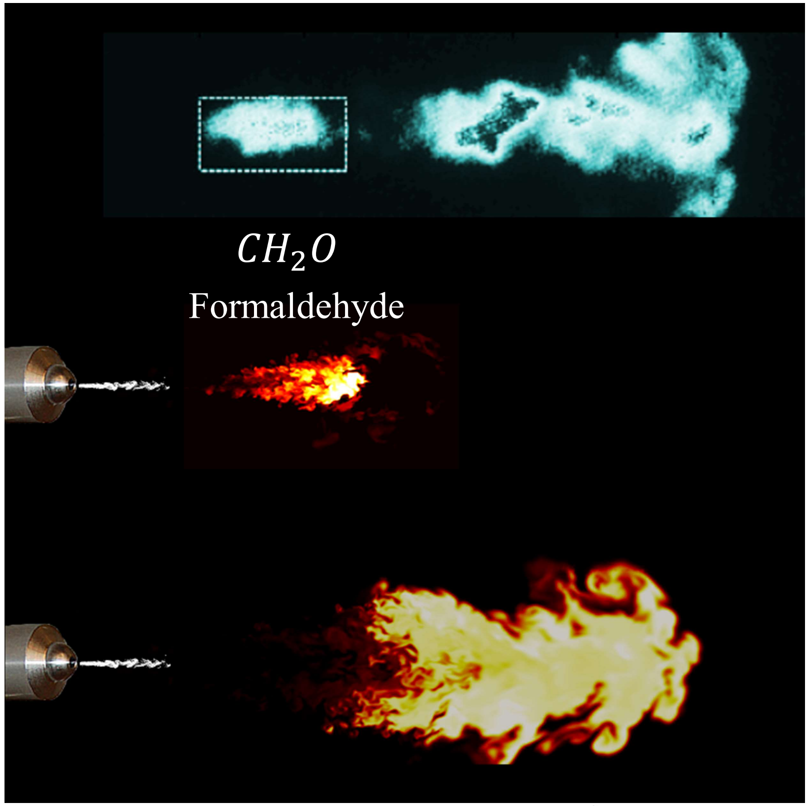


Fig. 14-5 Hydrocarbon oxidation process.



Experiment **CH_2O**

Simulation **CH_2O**

Simulation **Temperature**

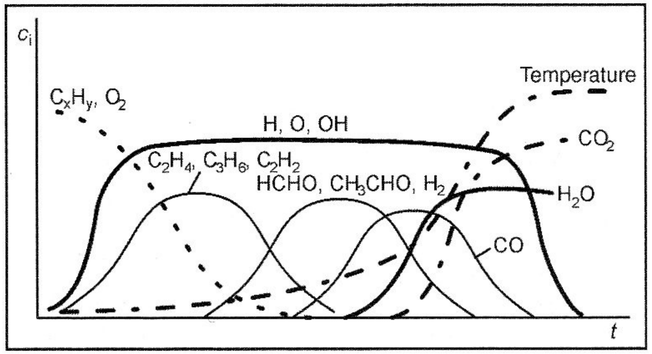
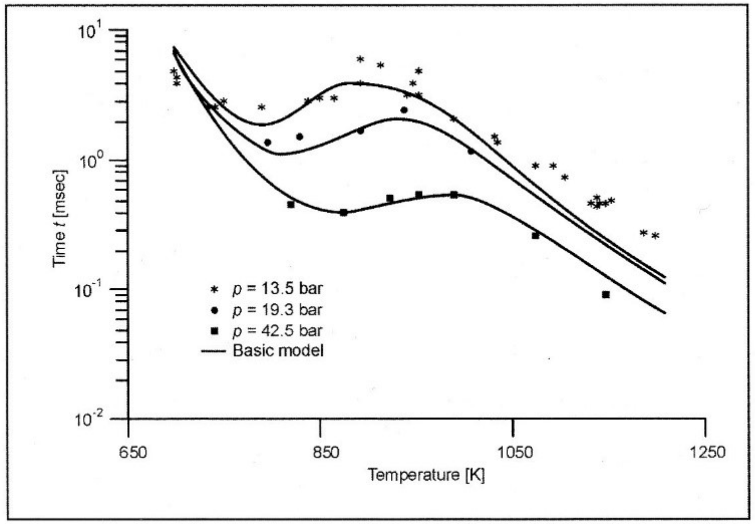


Fig. 14-7 Curve of temperature and concentration over time during hydrocarbon combustion.

Ignition



NTC –behavior
(Negative Temperature Coefficient)

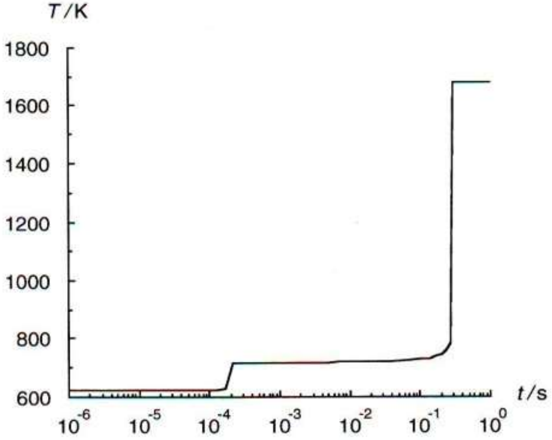


Fig. 16.6. Time behavior of the temperature in a two-stage ignition of a stoichiometric n-heptane-air mixture, p = 15 bar, T_0 = 625 K, adiabatic conditions (Esser 1990)

Two-stage ignition
(Warnatz, Maas, Dibble, 1999)

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Additional material

Ignition

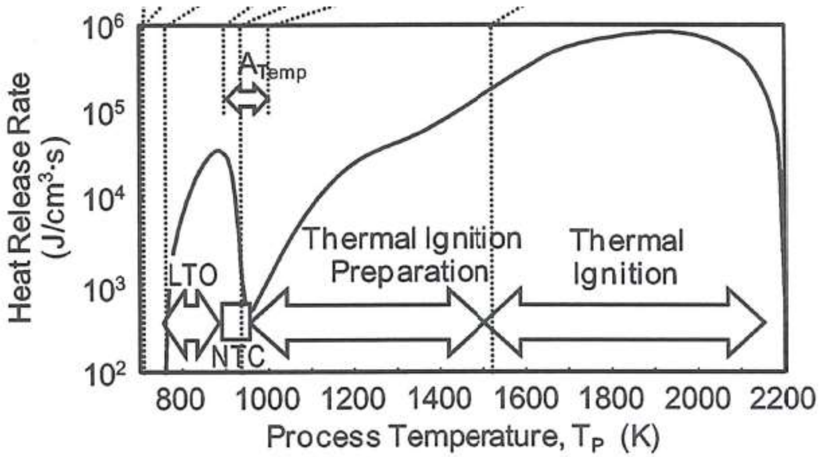


Figure 1 Reaction regimes (fuel: n-C_7H_{16}, initial temperature, T_0: 759 K, initial pressure, p_0: 2 MPa, equivalence ratio, ϕ: 0.5)

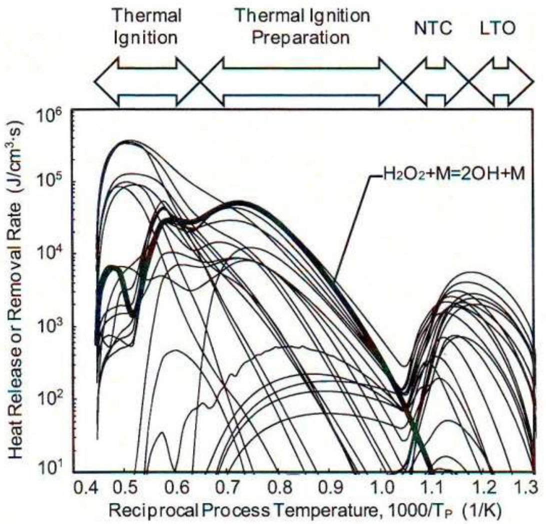


Figure 4 Absolute values of heat release or removal rates by major elementary reactions plotted against process temperature, T_P (fuel: n-C_7H_{16}, T_0: 759 K, p_0: 2 MPa, ϕ: 0.5)

Ando and Sakai, SAE 2009-01-0948

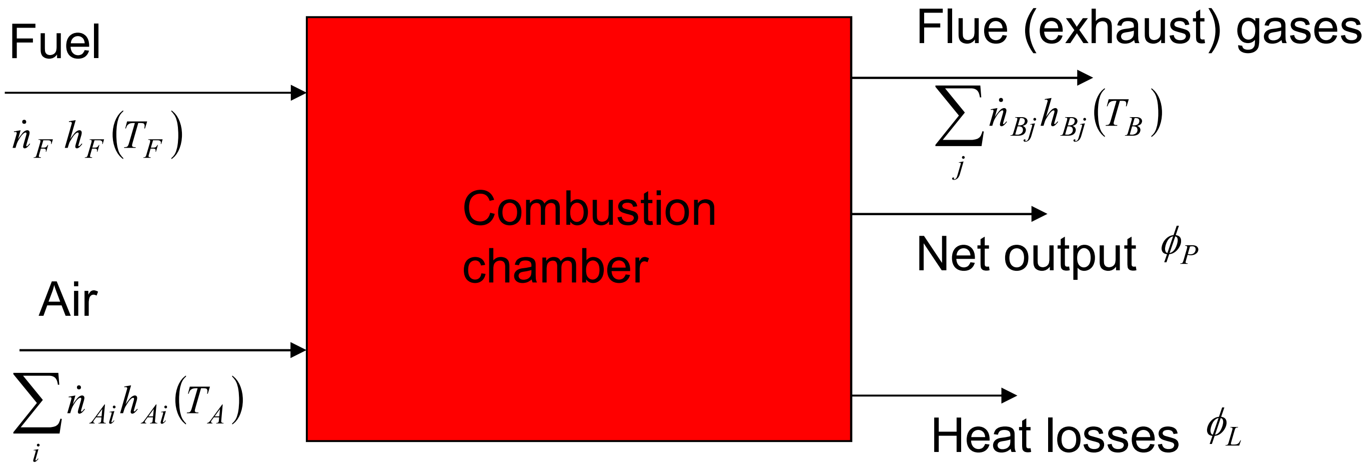
LTO = Low temperature oxidation

Another view: Different set of species responsible for low temperature and high temperature oxidation

Adiabatic flame temperature

- Adiabatic flame temperature is the theoretical maximum temperature that can exist in a combustion system
- It is important to know what can be the maximum temperature
- This information can be useful when e.g. designing a new combustion device or e.g. when assessing the validity of simulation results

Energy balance of a combustion system



$$\phi_P + \phi_L = \dot{n}_F h_F(T_F) + \sum_i \dot{n}_{Ai} h_{Ai}(T_A) - \sum_j \dot{n}_{Bj} h_{Bj}(T_B) \qquad (1)$$

where e.g. h_F is the chemical enthalpy according to

$$h_F = \Delta H^{\circ}_{fF}(T_0) + c_{Fm}(T_F - T_0)$$

Additional material

Energy balance of a combustion system

- Definition of fuel heating value ($T_F = T_A = T_0$ and $\phi_L = 0$)

$$\phi_P = \dot{n}_F \, q \qquad\qquad q = \text{fuel heating value}$$

- We get from (1)

$$q = h_F(T_0) + \sum_i \frac{n_{Ai}}{n_F} h_{Ai}(T_0) - \sum_j \frac{n_{Bj}}{n_F} h_{Bj}(T_0) \qquad (2)$$

- The right side of eq. (1) can be arranged in equivalent form

$$\dot{n}_F h_F(T_F) + \sum_i \dot{n}_{Ai} h_{Ai}(T_A) - \sum_j \dot{n}_{Bj} h_{Bj}(T_B) = \dot{n}_F \left[h_F(T_0) + \sum_i \frac{n_{Ai}}{n_F} h_{Ai}(T_0) - \sum_j \frac{n_{Bj}}{n_F} h_{Bj}(T_0) \right]$$

$$+ n_F \left[\left(h_F(T_F) - h_F(T_0) \right) \right] + n_F \left[\sum_i \frac{n_{Ai}}{n_F} \left(h_{Ai}(T_A) - h_{Ai}(T_0) \right) - \sum_j \frac{n_{Bj}}{n_F} \left(h_{Bj}(T_B) - h_{Bj}(T_0) \right) \right]$$

- Putting this into (1) and taking into account (2) yields

Additional material

Energy balance of a combustion system

- Definition of fuel heating value ($T_F = T_A = T_0$ and $\phi_L = 0$)
- Manipulate the equation to get temperature differences, e.g. $h_F(T_F) - h_F(T_0)$
  We subtrack values and compensate this by adding the same value

$$\dot n_F h_F(T_F) + \sum_i \dot n_{Ai} h_{Ai}(T_A) - \sum_j \dot n_{Bj} h_{Bj}(T_B) = \dot n_F \left[h_F(T_0) + \sum_i \frac{n_{Ai}}{n_F} h_{Ai}(T_0) - \sum_j \frac{n_{Bj}}{n_F} h_{Bj}(T_0) \right]$$
$$+ n_F\left[\left(h_F(T_F) - h_F(T_0)\right)\right] + n_F\left[\sum_i \frac{n_{Ai}}{n_F}\left(h_{Ai}(T_A) - h_{Ai}(T_0)\right) - \sum_j \frac{n_{Bj}}{n_F}\left(h_{Bj}(T_B) - h_{Bj}(T_0)\right)\right]$$

- Putting this into (1) and taking into account (2) yields

Additional material

Energy balance of a combustion system

$$\dot{n}_F\, q + \dot{n}_F \underbrace{\left[h_F(T_F) - h_F(T_0)\right]}_{\text{Fuel pre-heating}} + \underbrace{\dot{n}_F \left[\sum_i \frac{n_{Ai}}{n_F}\left(h_{Ai}(T_A) - h_{Ai}(T_0)\right)\right]}_{\text{Air pre-heating}}$$

$$= \phi_P + \phi_L + \underbrace{\dot{n}_F \left[\sum_j \frac{n_{Bj}}{n_F}\left(h_{Bj}(T_B) - h_{Bj}(T_0)\right)\right]}_{\text{Exhaust gas losses}}$$

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Adiabatic flame temperature

- Energy balance for liquids and solid fuels

$$\dot{m}_F\, q + \dot{m}_F\left[h_F(T_F) - h_F(T_0)\right] + \dot{m}_F\left[\sum_i \frac{n_{Ai}}{m_F}\left(h_{Ai}(T_A) - h_{Ai}(T_0)\right)\right]$$

$$= \phi_P + \phi_L + \dot{m}_F\left[\sum_j \frac{n_{Bj}}{m_F}\left(h_{Bj}(T_B) - h_{Bj}(T_0)\right)\right]$$

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Adiabatic flame temperature

- Energy balance for liquids and solid fuels

$$\dot{m}_F\, q + \dot{m}_F\left[h_F(T_F) - h_F(T_0)\right] + \dot{m}_F\left[\sum_i \frac{n_{Ai}}{m_F}\left(h_{Ai}(T_A) - h_{Ai}(T_0)\right)\right]$$

$$= \underset{=0}{\cancel{\phi_P}} + \underset{=0}{\cancel{\phi_L}} + \underbrace{\dot{m}_F\left[\sum_j \frac{n_{Bj}}{m_F}\left(h_{Bj}(T_B) - h_{Bj}(T_0)\right)\right]}_{\text{All the fuel energy goes into the flue gases (savukaasut)}}$$

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Adiabatic flame temperature

- We obtain the equation for the adiabatic flame temperature

$$q+\left[h_F(T_F)-h_F(T_0)\right]+\sum_i \frac{n_{Ai}}{m_F}\left(h_{Ai}(T_A)-h_{Ai}(T_0)\right)$$

$$=\sum_j \frac{n_{Bj}}{m_F}\left(h_{Bj}\boxed{(T_{ad})}-h_{Bj}(T_0)\right)$$

- If fuel and air are at the reference temperature T_0

$$q=\sum_j \frac{n_{Bj}}{m_F}\left(h_{Bj}\boxed{(T_{ad})}-h_{Bj}(T_0)\right)$$

- Adiabatic flame temperature is the theoretical maximum temperature that can exist in a combustion system

Exercise

Calculate the adiabatic flame temperature for C_7H_{16}. Assume complete combustion to CO2 and H2O, and Lambda=1. The heating value of the fuel is 41.5 MJ/kg. Air and fuel are assumed to be at the reference temperature 273K before combustion. Hint: start with T_{ad} =2200K.

The procedure:

1. Write down the reaction scheme
2. Find out the coefficients $\frac{n_{Bj}}{m_F}$
3. Use the equation $q = \sum_j \frac{n_{Bj}}{m_F}\left(h_{Bj}(T_{ad}) - h_{Bj}(T_0)\right)$
4. Select first one temperature and select the according enthalpy values from the table. Then iterate to get the correct fuel heating value

Enthalpy table

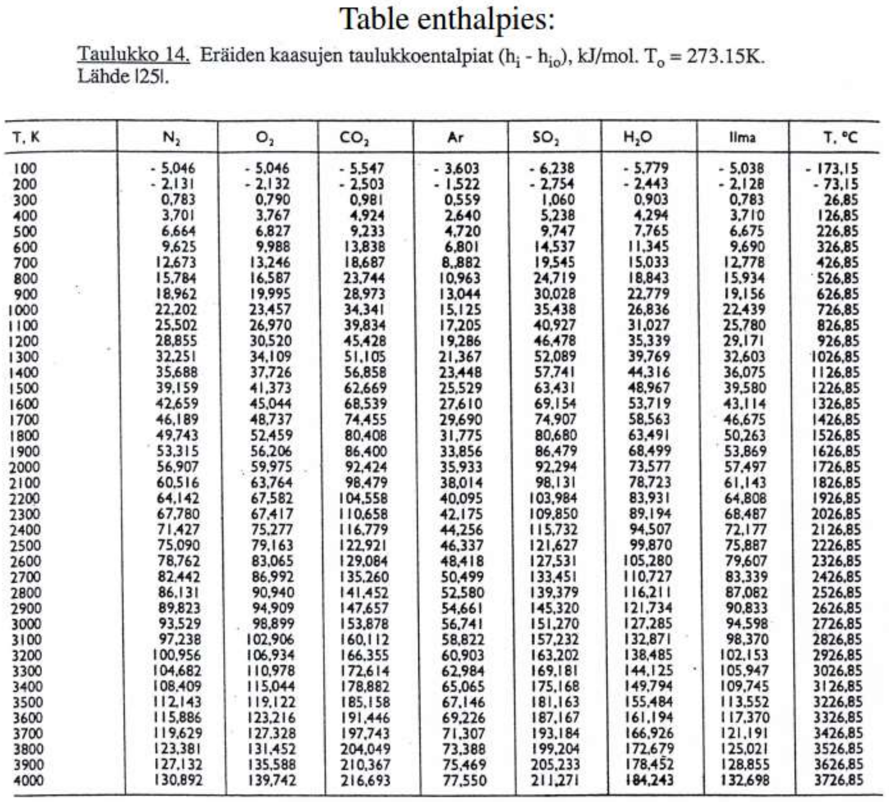

Table enthalpies:

Taulukko 14. Eräiden kaasujen taulukkoentalpiat ($h_i - h_{io}$), kJ/mol. $T_o = 273.15K$.
Lähde |25|.

T, K	N_2	O_2	CO_2	Ar	SO_2	H_2O	Ilma	T, °C
100	- 5,046	- 5,046	- 5,547	- 3,603	- 6,238	- 5,779	- 5,038	- 173,15
200	- 2,131	- 2,132	- 2,503	- 1,522	- 2,754	- 2,443	- 2,128	- 73,15
300	0,783	0,790	0,981	0,559	1,060	0,903	0,783	26,85
400	3,701	3,767	4,924	2,640	5,238	4,294	3,710	126,85
500	6,664	6,827	9,233	4,720	9,747	7,765	6,675	226,85
600	9,625	9,988	13,838	6,801	14,537	11,345	9,690	326,85
700	12,673	13,246	18,687	8,882	19,545	15,033	12,778	426,85
800	15,784	16,587	23,744	10,963	24,719	18,843	15,934	526,85
900	18,962	19,995	28,973	13,044	30,028	22,779	19,156	626,85
1000	22,202	23,457	34,341	15,125	35,438	26,836	22,439	726,85
1100	25,502	26,970	39,834	17,205	40,927	31,027	25,780	826,85
1200	28,855	30,520	45,428	19,286	46,478	35,339	29,171	926,85
1300	32,251	34,109	51,105	21,367	52,089	39,769	32,603	1026,85
1400	35,688	37,726	56,858	23,448	57,741	44,316	36,075	1126,85
1500	39,159	41,373	62,669	25,529	63,431	48,967	39,580	1226,85
1600	42,659	45,044	68,539	27,610	69,154	53,719	43,114	1326,85
1700	46,189	48,737	74,455	29,690	74,907	58,563	46,675	1426,85
1800	49,743	52,459	80,408	31,775	80,680	63,491	50,263	1526,85
1900	53,315	56,206	86,400	33,856	86,479	68,499	53,869	1626,85
2000	56,907	59,975	92,424	35,933	92,294	73,577	57,497	1726,85
2100	60,516	63,764	98,479	38,014	98,131	78,723	61,143	1826,85
2200	64,142	67,582	104,558	40,095	103,984	83,931	64,808	1926,85
2300	67,780	67,417	110,658	42,175	109,850	89,194	68,487	2026,85
2400	71,427	75,277	116,779	44,256	115,732	94,507	72,177	2126,85
2500	75,090	79,163	122,921	46,337	121,627	99,870	75,887	2226,85
2600	78,762	83,065	129,084	48,418	127,531	105,280	79,607	2326,85
2700	82,442	86,992	135,260	50,499	133,451	110,727	83,339	2426,85
2800	86,131	90,940	141,452	52,580	139,379	116,211	87,082	2526,85
2900	89,823	94,909	147,657	54,661	145,320	121,734	90,833	2626,85
3000	93,529	98,899	153,878	56,741	151,270	127,285	94,598	2726,85
3100	97,238	102,906	160,112	58,822	157,232	132,871	98,370	2826,85
3200	100,956	106,934	166,355	60,903	163,202	138,485	102,153	2926,85
3300	104,682	110,978	172,614	62,984	169,181	144,125	105,947	3026,85
3400	108,409	115,044	178,882	65,065	175,168	149,794	109,745	3126,85
3500	112,143	119,122	185,158	67,146	181,163	155,484	113,552	3226,85
3600	115,886	123,216	191,446	69,226	187,167	161,194	117,370	3326,85
3700	119,629	127,328	197,743	71,307	193,184	166,926	121,191	3426,85
3800	123,381	131,452	204,049	73,388	199,204	172,679	125,021	3526,85
3900	127,132	135,588	210,367	75,469	205,233	178,452	128,855	3626,85
4000	130,892	139,742	216,693	77,550	211,271	184,243	132,698	3726,85

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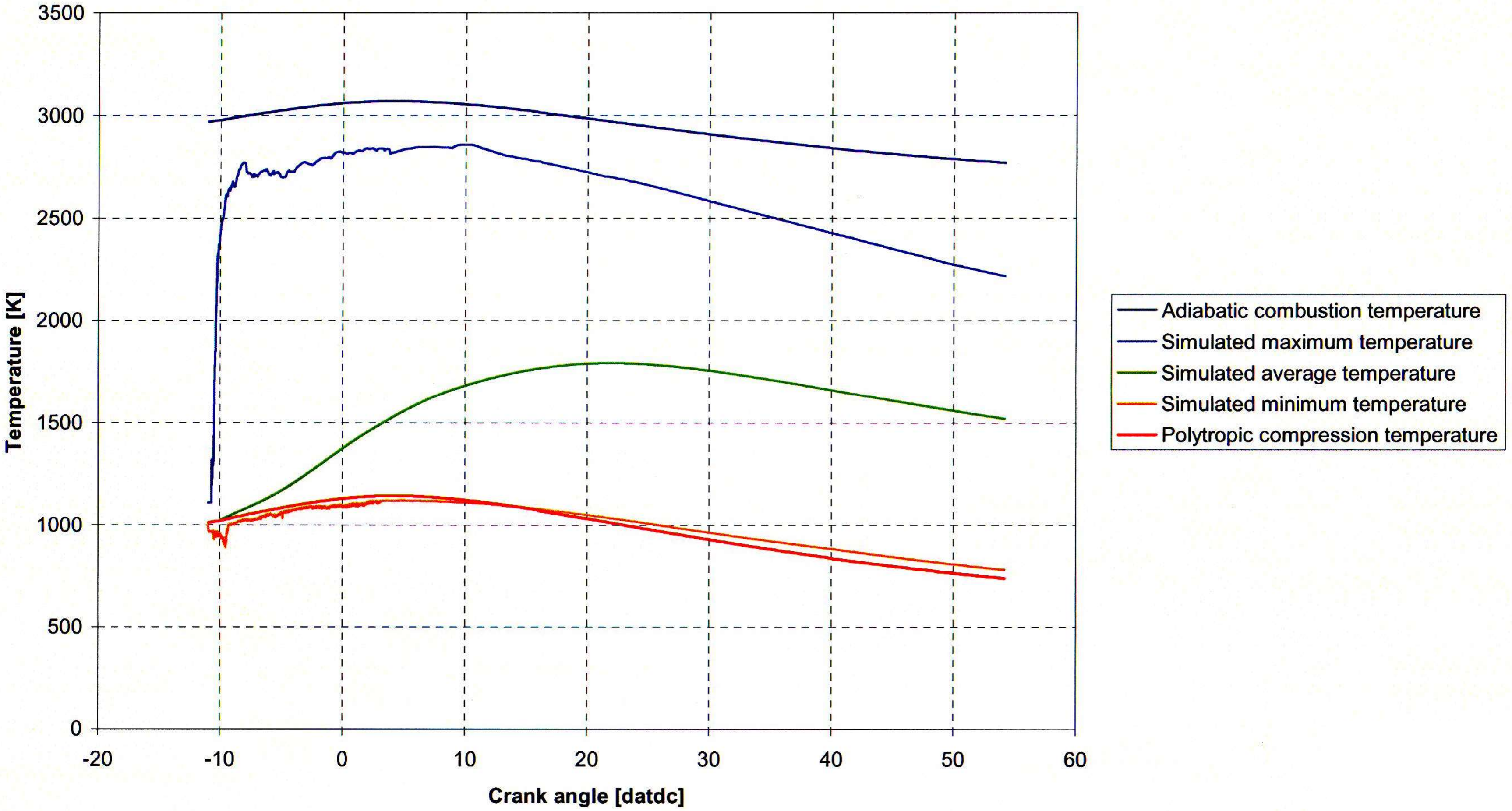
Engine process with very high adiabatic flame temperature



http://elearning.cerfacs.fr/combustion/illustrations/whatisaflame/index.php