

Lecture 1

Combustion Theory

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1. Basic combustion reactions

- Calculating air fuel ratios
- Stoichiometric combustion,
- lean combustion and
- rich combustion
- Equivalence ratio & Excess air ratio

2. Term enthalpy (total energy associated)

- Absolute enthalpy
- Enthalpy of formation

3. Adiabatic Flame temperatures

Basic combustion reaction



- Air fuel mass ratios

$$\frac{m_{air}}{m_{fuel}} = \frac{a \cdot MW_{air}}{1 \cdot MW_{Fuel}}$$

- Stoichiometric combustion

$$b = 0$$

- Equivalence ratio

$$\Phi = \frac{(m_{air}/m_{fuel})_{stoic}}{(m_{air}/m_{fuel})} = \frac{a_{stoi}}{a}$$

- Fuel lean mixture ($\Phi < 1$); fuel rich combustion ($\Phi > 1$)

Exercise 1: 1 mole $C_{10}H_{22}$ combustion with 16 mole air

$$a_{stoi} = 15.5 \quad b = 0.5 \quad \Phi = 0.969$$

Basic combustion reaction



Known: 1 mole $C_{10}H_{22}$ combustion with 16 mole air

To obtain: a_{stoi}

b

Φ

Absolute Enthalpy and Enthalpy of Formation

$$\bar{h}_i(T) = \bar{h}_{f,i}^0(T_{ref}) + \Delta\bar{h}_{s,i}(T_{ref})$$

Absolute enthalpy
at temperature T

Enthalpy of formation at
standard reference state
($T_{ref} = 25^\circ\text{C}$, $P_{ref} = 1\text{atm}$)

Sensible enthalpy change
in going from T_{ref} to T

$$\Delta\bar{h}_{s,i}(T_{ref}) = \bar{h}_i(T) - \bar{h}_{f,i}^0(T_{ref})$$

Table A.2 Carbon dioxide (CO_2), MW = 44.011, enthalpy of formation @ 298 K (kJ/kmol) = -393,546

$T(\text{K})$	\bar{c}_p (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
200	32.387	-3,423	-393,483	199.876	-394,126
298	37.198	0	-393,546	213.736	-394,428
300	37.280	69	-393,547	213.966	-394,433
400	41.276	4,003	-393,617	225.257	-394,718

Table A.11 Oxygen (O_2), MW = 31.999, enthalpy of formation @ 298 K (kJ/kmol) = 0

$T(\text{K})$	\bar{c}_p (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
200	28.473	-2,836	0	193.518	0
298	29.315	0	0	205.043	0
300	29.331	54	0	205.224	0
400	30.210	3,031	0	213.782	0
500	31.114	6,097	0	220.620	0

The standard enthalpy of formation of a pure element is **zero**.

Absolute Enthalpy - mixtures

$$\bar{h}_i(T) = \bar{h}_{f,i}^0(T_{ref}) + \Delta\bar{h}_{s,i}(T_{ref})$$

For ideal-gas mixtures, mixture enthalpies are calculated:

$$\bar{h}_{mix} = \sum_i \chi_i \bar{h}_i$$

Mole basis (kJ/kmol)
 χ_i - mole fraction

$$h_{mix} = \sum_i Y_i h_i$$

Mass basis (kJ/kg)
 Y_i -mass fraction

Exercise 2:

A gas stream at 1 atm contains a mixture of CO, CO₂ and N₂ in which the CO mole fraction is 0.1 and the CO₂ mole fraction is 0.2. The gas-stream temperature is 1200K. Determine the absolute enthalpy of the mixture on both a mole basis (kJ/kmol) and a mass basis (kJ/kg).

Exercise 2

For ideal-gas mixtures, mixture enthalpies are calculated:

$$\begin{aligned}\bar{h}_{mix} = \sum_i \chi_i \bar{h}_i &= \chi_{CO} \left[\bar{h}_{f,CO}^0 + (\bar{h}(T) - \bar{h}_{f,298}^0)_{CO} \right] \\ &\quad + \chi_{CO_2} \left[\bar{h}_{f,CO_2}^0 + (\bar{h}(T) - \bar{h}_{f,298}^0)_{CO_2} \right] \\ &\quad + \chi_{N_2} \left[\bar{h}_{f,N_2}^0 + (\bar{h}(T) - \bar{h}_{f,298}^0)_{N_2} \right]\end{aligned}$$

$$\begin{aligned}\bar{h}_{mix} &= 0.10[-110,541 + 28,440] \\ &\quad + 0.20[-393,546 + 44,488] \\ &\quad + 0.70[0 + 28,118] \\ &= -58,339.1 \text{ kJ/kmol}\end{aligned}$$

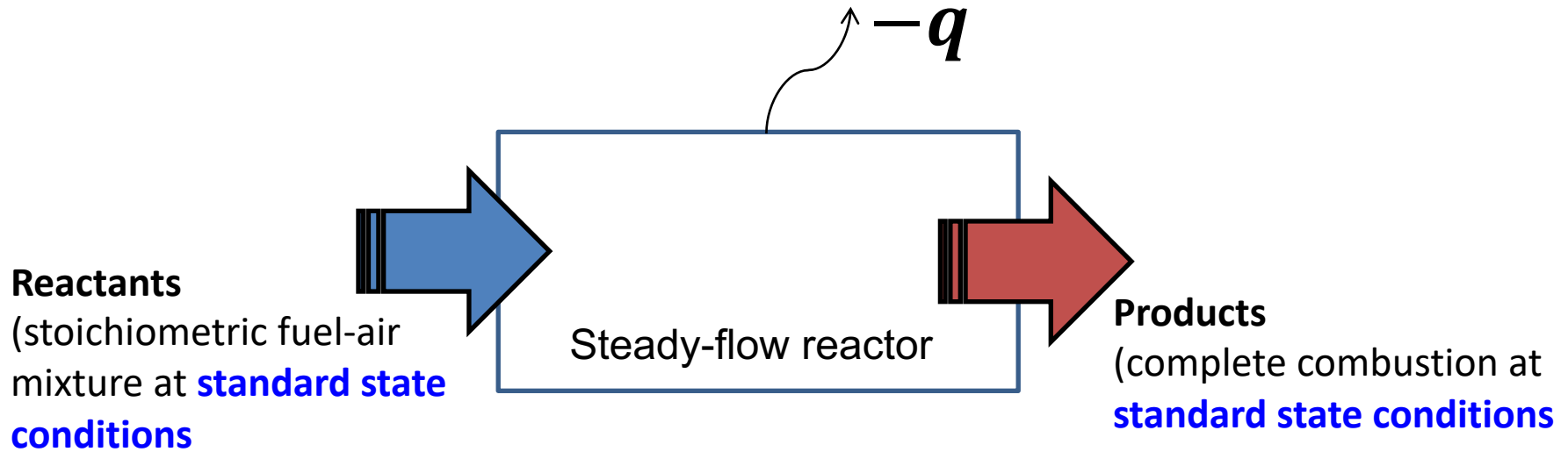
$$Y_{CO} = ?$$

$$Y_{CO_2} = ?$$

$$Y_{N_2} = ?$$

$$h_{mix} = ?$$

Enthalpy of combustion



$$\Delta h_R = H_{prod} - H_{reac} = -\Delta h_c$$

Enthalpy of combustion

Heat of combustion (heating value)

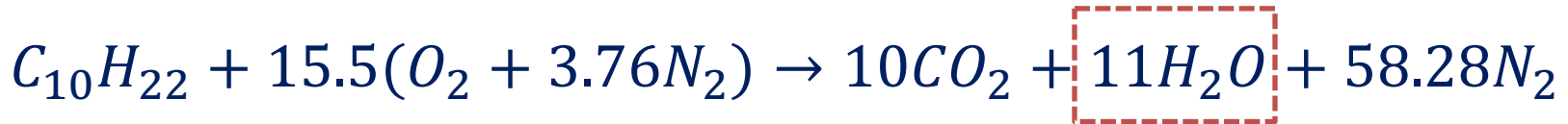
per-mole-of fuel (often applied to gaseous/liquid fuel)

per-mass-of fuel (often applied to solid fuel)

Enthalpy of combustion

Exercise 3

Determine the upper and lower heating values at 298K of gaseous *n*-decane ($C_{10}H_{22}$), per kilo-mole of fuel and per kilogram of fuel.



$$H_{reac} = H_{C_{10}H_{22}} + H_{air}$$

$$H_{prod} = H_{CO_2} + H_{H_2O} + H_{N_2}$$

Note:

- The numerical value of H_{prod} depends on whether the H_2O in the products is liquid or gaseous. Here **you could consider H_2O as gaseous product firstly.**
- The sensible enthalpies for all species involved are **zero** as we desire Δh_c at the reference state (298K)
- Also, the enthalpies of formation of the O_2 and N_2 are **zero** at 298K.

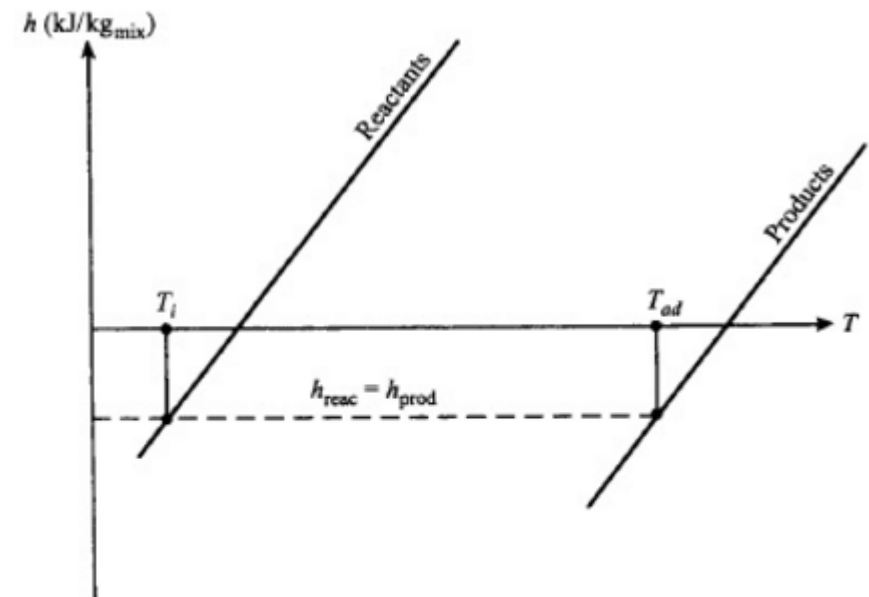
Adiabatic flame temperature @ constant pressure

Fuel-air mixture burns adiabatically:

$$H_{\text{reac}}(T_i, P) = H_{\text{prod}}(T_{\text{ad}}, P)$$

$$\bar{h}_i(T_{\text{ad}}) - \bar{h}_{f,i}^0(T_{\text{ref}}) = \int_{298}^{T_{\text{ad}}} \bar{c}_{P,i} dT$$

Sensible enthalpy



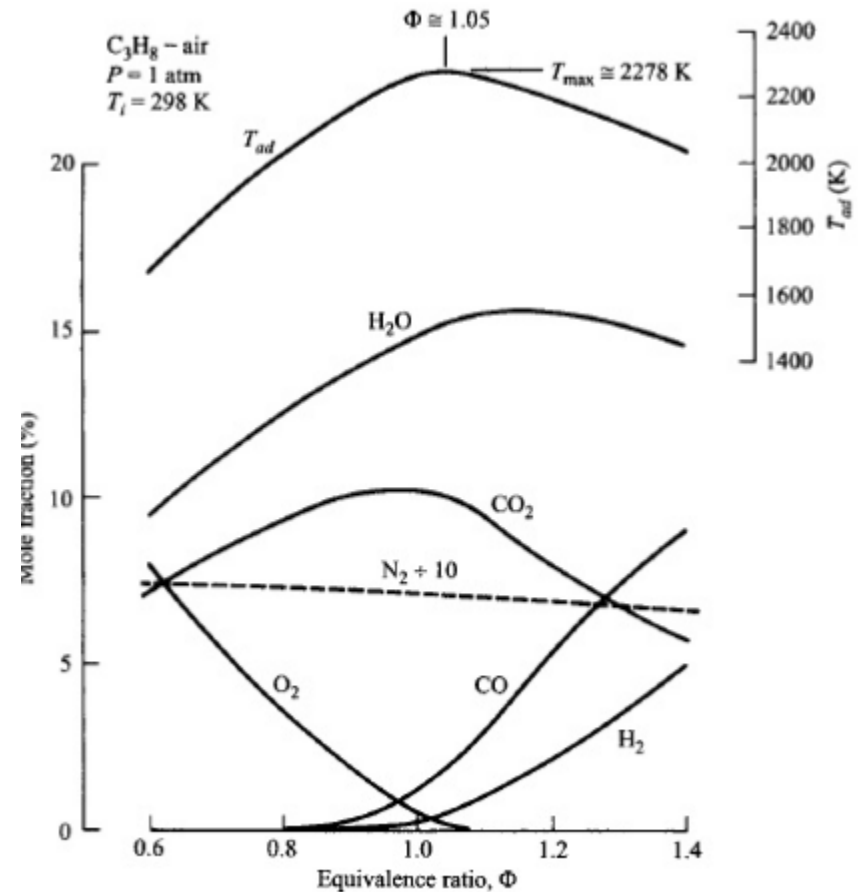
Exercise

Estimate the constant-pressure adiabatic flame temperature for the combustion of stoichiometric CH₄-air mixture. The pressure is 1atm and the initial reactant temperature is 298K. Assumptions: (1) Complete combustion, the product mixture consists of only CO₂, H₂O and N₂; (2) The product mixture enthalpy is estimated using constant specific heats evaluated at 1200K ($\approx 0.5(T_i + T_{\text{ad}})$), with a first guess of T_{ad} to be ca. 2100K.

Discussions on adiabatic flame temperature

(text book 'An Introduction to Combustion : Concepts and Applications' – Chapter 2)

- How we could improve the accuracy of the calculated adiabatic flame temperature?
- What to consider for the calculation of adiabatic flame temperature when the equivalence ratio is less than or above one?
- How pressure affects ?



Equilibrium adiabatic flame temperature and major product species for propane-air combustion at 1 atm.

Summary

- Combustion fundamentals
- Absolute enthalpy and sensible enthalpy
- Enthalpy of combustion
- Constant-pressure adiabatic flame temperature

Nomenclature

a	Molar oxygen–fuel ratio (kmol/kmol)
\bar{c}_p	Constant-pressure specific heat (J/kmol-K)
h_f^o, \bar{h}_f^o	Enthalpy of formation (J/kg or J/kmol)
H, h, \bar{h}	Enthalpy (J or J/kg or J/kmol)
Δh_c	Enthalpy of reaction (J or J/kg or J/kmol)
$\Delta H_R, \Delta h, \Delta \bar{h}_R$	Heat of combustion (heating value) (J/kg)
m	Mass (kg)
MW	Molecular weight (kg/kmol)
T	Temperature (K)
Y	Mass fraction (kg/kg)

Greek Symbols

ϕ	Equivalence ratio
χ	Mole fraction

Subscripts

ad	Adiabatic
f	Formation
i	i th species
mix	Mixture
$prod$	Product
$reac$	Reactant
ref	Reference
s	Sensible
$stoic$	Stoichiometric

Superscripts

o	Denotes standard-state pressure ($P^o = 1 \text{ atm}$)
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Other Notation

$[X]$	Molar concentration of X (kmol/m ³)
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