

Lecture # 5

Chemical Thermodynamics 1

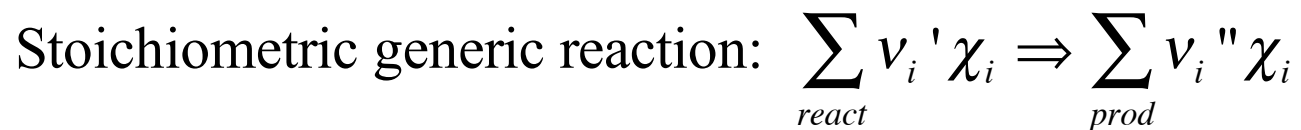
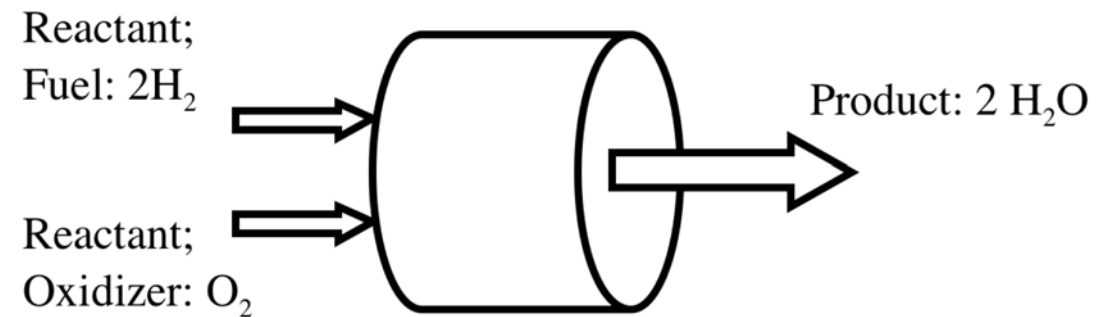
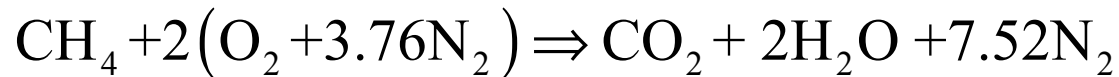
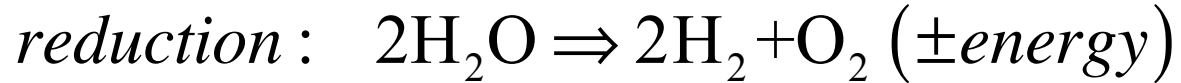
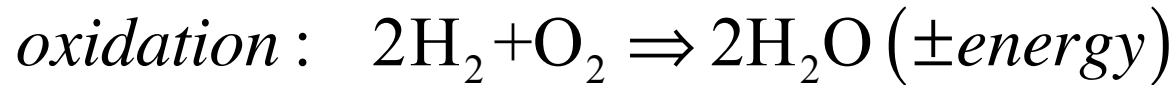
Ahmed Ghoniem

February 18, 2020

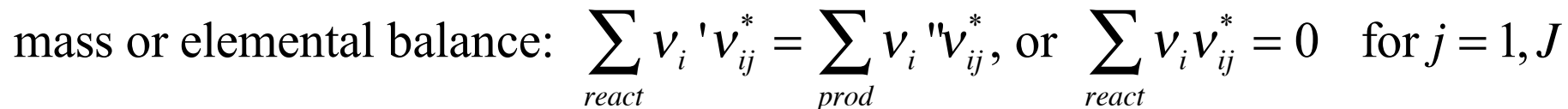
- Mass conservation in chemical reactions
- Energy conservation in chemical reactions
- Fuels and chemical energy carriers
- Combustion and Flame temperature.

Stoichiometry (element conservation) & Mass Conservation

Complete oxidation (burning) or reduction of “chemical energy carriers”:



v_i' and v_i'' are the stoichiometric coefficient satisfying conservation of element.



v_{ij}^* is the number of j atom in i molecule.

The molar stoichiometric air-fuel ratio:

$$\widehat{AF}_{ST} = \left(\frac{n_{air}}{n_{fuel}} \right)_{ST} = \left(\frac{n_{oxygen} + n_{nitrogen}}{n_{fuel}} \right)_{ST} = \frac{v'_{oxygen} + v'_{nitrogen}}{v'_{fuel}} \quad (\text{a mole has } N_a = 6.022 \cdot 10^{23} \text{ molecules})$$

for methane-air: $\widehat{AF}_{ST} = 2(1+3.76) = 9.52$

The mass-based stoichiometric air-fuel ratio $AF_{ST} = \left(\frac{m_{air}}{m_{fuel}} \right)_{ST} = \frac{v'_{oxygen} M_{oxygen} + v'_{nitrogen} M_{oxygen}}{v'_{fuel} M_{fuel}}$

For methane-air: $AF_{ST} = 2(32+3.76 \times 28)/(12+4) = 17.16$

For non stoichiometric reactions/combustion: $\widehat{AF} = \left(\frac{n_{air}}{n_{fuel}} \right) = \left(\frac{n_{oxygen} + n_{nitrogen}}{n_{fuel}} \right)$

The ratio between the actual and stoichiometric is: the excess air ratio is:

$$\lambda = \frac{AF}{AF_{ST}}, \quad \text{and the equivalence ratio: } \phi = \frac{1}{\lambda}$$

(Fuel) Lean and rich burn

Lean Burning, $\phi < 1$ (in many power plants, burners and diesel engines).

Likely to lead to complete combustion, low NOx formation (because of low T):



Rich Burning, $\phi > 1$, used in partial oxidation, fuel reforming and production of syngas, hydrogen, etc,

Example: partial oxidation (exothermic) for coal gasification/biochar: $\text{C} + \frac{1}{2}\text{O}_2 \Rightarrow \text{CO}$,

and methane partial oxidation $\text{CH}_4 + \frac{1}{2}\text{O}_2 \Rightarrow \text{CO} + 2\text{H}_2$

Not all reactions involve fuel oxygen!

Reforming (endothermic) can also be steam gasification $\text{C} + \text{H}_2\text{O} \Rightarrow \text{CO} + \text{H}_2$

and methane reforming $\text{CH}_4 + \text{H}_2\text{O} \Rightarrow \text{CO} + 3\text{H}_2$

More hydrogen can be produced by the "water-gas shift": $\text{CO} + \text{H}_2\text{O} \Rightarrow \text{CO}_2 + \text{H}_2$

Thermodynamic Properties of Fuel Combustion at 25 C and 1 atm Pressure

Fuel	Chemical symbol	Molecular weight kg/kmol	FHV MJ/kg_fuel	A/F	$H_r - H_p$ MJ/kg_product	Δg MJ/kg_fuel	FHV MJ/kg_C
hydrogen	H ₂	2.016	119.96	34.28	3.4	117.63	NA
Carbon (graphite)	C _{solid}	12.01	32.764	11.51	2.619	32.834	32.764
Methane	CH ₄	16.04	50.040	17.23	2.745	51.016	66.844
Carbon monoxide	CO	28.01	10.104	2.467	2.914	9.186	23.564
Ethane	C ₂ H ₆	30.07	47.513	16.09	2.780	48.822	59.480
Methanol	CH ₄ O	32.04	20.142	6.47	2.696	22.034	53.739
Propane	C ₃ H ₈	44.10	46.334	15.67	2.779	47.795	56.708
Ethanol	C ₂ H ₆ O	46.07	27.728	9.000	2.773	28.903	53.181
Isobutane	C ₄ H ₁₀	58.12	45.576	15.46	2.769		53.142
Hexane	C ₆ H ₁₄	86.18	46.093	15.24	2.838		54.013
Octane	C ₈ H ₁₈	114.2	44.785	15.12	2.778		53.246
Decane	C ₁₀ H ₂₂	142.3	44,599	15.06	2.778		52.838
Dodecane	C ₁₂ H ₂₆	170.3	44.479	15.01	2.778		52.567
Hexadecane	C ₁₆ H ₃₄	226.4	44.303	14.95	2.778		52.208
Octadecane	C ₁₈ H ₃₈	254.5	44.257	14.93	2.778		52.102

FHV=LHV (water in the products in the vapor phase)

Δg is the Gibbs free energy of reaction (maximum work under isothermal reaction conditions).

Last column: the heating value/carbon = FHV*molecular weight of fuel/molecular weight of carbon.

Fossil/Organic/Hydrocarbon Fuels

COAL, OIL, NATURAL GAS.

OIL SHALE, TAR SANDS, PEAT.

“BIOMASS” .. Young, “renewable”.

- Formed due to the fossilization of *organic* matter, underground (although evidence of earth mantle inorganic (abiogenic) methane is rising).
- All formed of carbon and hydrogen, some with little oxygen, plus sulfur, mercury and other minerals, and non combustibles.
- Most require some form of processing: sulfur removal, grinding and washing, oil refining, gas desulfurization.

Energy Balance in Chemical Reactions

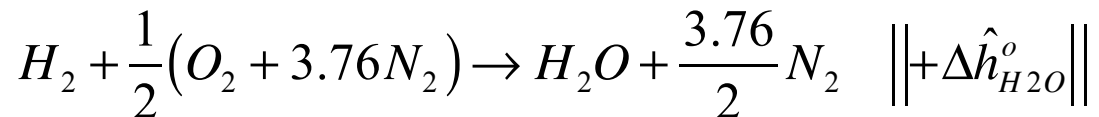
$$\frac{dE}{dt} = \dot{Q} - \dot{W} + \left(\sum_{react} \dot{m}_i (h_i + \mathbf{V}_i^2 + g_v z_i) - \sum_{prod} \dot{m}_i (h_i + \mathbf{V}_i^2 + g_v z_i) \right)$$

$$h_i = h_{i,thermal} + h_{i,chemical} = \int_{T^o}^T c_{p,i} dT + h_{i,chemical}^o$$

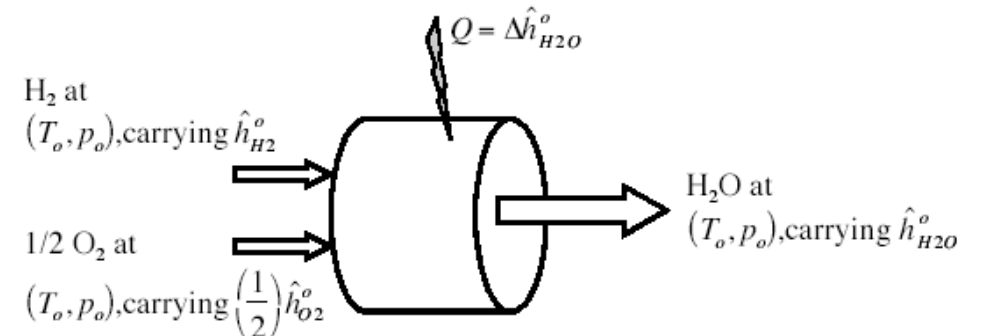
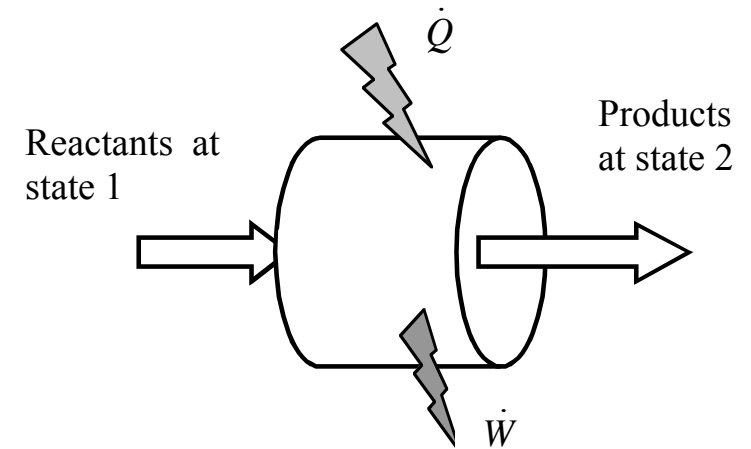
Steady, constant pressure and temperature, one mole of fuel:

$$Q = \sum_{prod} n_i \hat{h}_i - \sum_{react} n_i \hat{h}_i \quad (\equiv \text{heating value of the fuel})$$

- heat transfer out of the reaction, at constant p and T is *the enthalpy of reaction*.



$$\Delta\hat{h}_{fuel}^o = \sum_{prod} \nu_i'' \hat{h}_i^o - \sum_{react} \nu_i' \hat{h}_i^o, \quad \nu_i \text{ is the stoichiometric coefficient}$$



- Need to define a reference for the enthalpies.

Reference Enthalpy, Enthalpy of Formation

$$H = \sum_{i=1}^N m_i h_i(T, p_i) = \sum_{i=1}^N n_i \hat{h}_i(T, p_i)$$

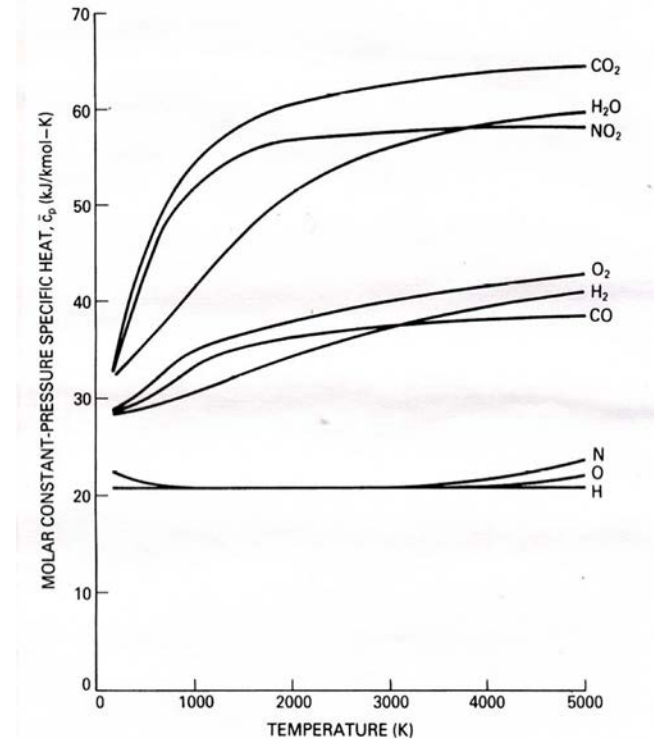
$$h_i = h_{f,i}^o + \int_{T^o}^T c_{p,i}(T) dT, \quad \text{and} \quad \hat{h}_i = \hat{h}_{f,i}^o + \int_{T^o}^T \hat{c}_{p,i}(T) dT$$

$$\hat{h}_f^o \equiv \Delta \hat{h}_f^o$$

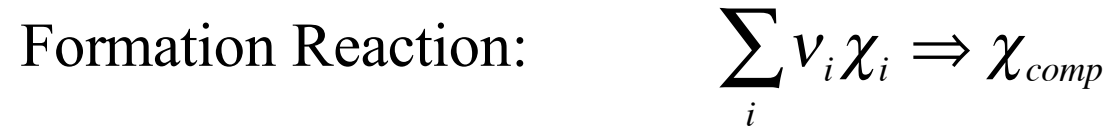
Reference Entropy

$$\begin{aligned} \hat{s} &= \sum_{i=1}^N X_i \hat{s}_i(T, p_i) \\ &= \sum_{i=1}^N X_i \left(\hat{s}_i^{oo} + \int_{T^o}^T \frac{\hat{c}_{p,i}(T)}{T} dT \right) - \mathfrak{R} \sum_{i=1}^N X_i \ln \frac{p_i}{p^o} \end{aligned}$$

$$\hat{s}_i^{oo} \equiv \Delta \hat{s}_f^o$$

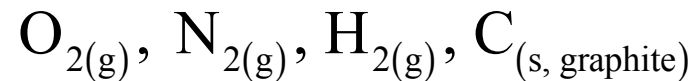


Enthalpy of Formation



$$\Delta \hat{h}_R^o = \hat{h}_{comp}^o - \sum_i \nu_i \hat{h}_i^o = \hat{h}_{comp}^o \text{ for formation reaction ...}$$

Enthalpy of reaction of stable molecules, in their phase at STP, is taken to be zero:



Energy of formation accounts for the net energy required to form or break bonds in a complex molecule.

Types of bonds: single, double, ... depending on the number of shared electrons. C has four bonds.

A saturated HC, like methane and methanol, use the four C bonds to attach another atom (H or C or a functional group (OH))

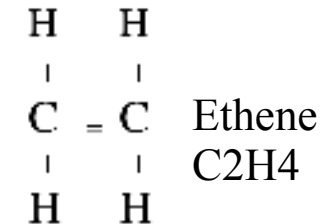
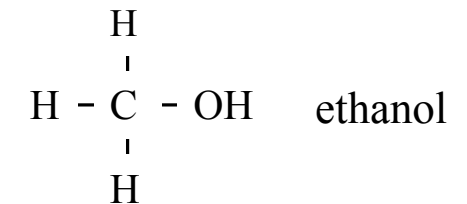
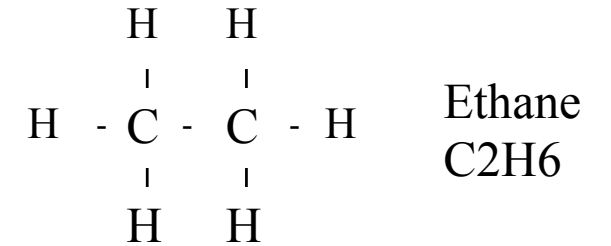
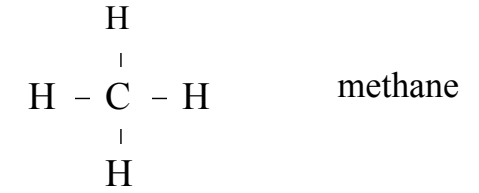
Unsaturated HC use multiple bond to connect C atoms

Single C-C bond 248 MJ/kmol
 Double C=C bond 615 MJ/kmol
 Triple 812 MJ/kmol

O-H bond 463 MJ/kmol
 Single O-O 139 MJ/kmol
 Double O=O 498 MJ/kmol

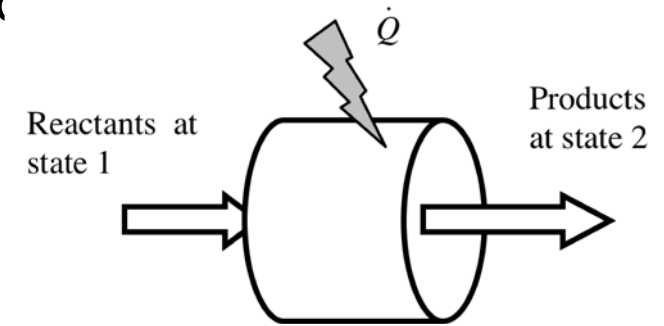
...

O-OH 498 MJ/kmol
 H-O2 196 MJ/kmol



Substance	Formula	Δh_f° MJ/kmol	Δg_f° MJ/kmol	Δs_f° kJ/kmol K
Ammonia	NH ₃	-45.7	-16.2	-99.1
Argon	Ar	0	0	0
Benzene	C ₆ H ₆	83.0	129.7	-156.9
Carbon	C	0	0	0
Carbon dioxide	CO ₂	-393.8	-394.6	2.9
Carbon monoxide	CO	-110.6	-137.4	89.7
Ethane	C ₂ H ₆	-84.7	-33.0	-173.7
Ethanol	C ₂ H ₅ OH	-235.0	-168.4	-223.3
Ethylene	C ₂ H ₄	52.3	68.2	-53.1
Hydrogen	H ₂	0	0	0
Hydrogen (atomic)	H	218.0	203.3	49.4
Hydroxyl	OH	39.5	34.3	17.4
Isooctane	C ₈ H ₁₈	-224.3	13.7	-798.6
Methane	CH ₄	-74.9	-50.9	-80.6
Methanol	CH ₃ OH	-201.3	-162.6	-129.8
Nitrogen	N ₂	0	0	0
Nitrogen (atomic)	N	472.8	455.6	57.6
Nitrogen dioxide	NO ₂	33.9	52.0	-60.8
n-Octane	C ₈ H ₁₈	-208.6	16.4	-754.6
Oxygen	O ₂	0	0	0
Water	H ₂ O	-242.0	-228.8	-44.4

Enthalpy of Reaction, Steady, constant p, zero work, etc



Arbitrary mixture

$$Q = H_{out}(T_{out}) - H_{in}(T_{in}) = \sum_{prod} n_i \hat{h}_i - \sum_{react} n_i \hat{h}_i$$

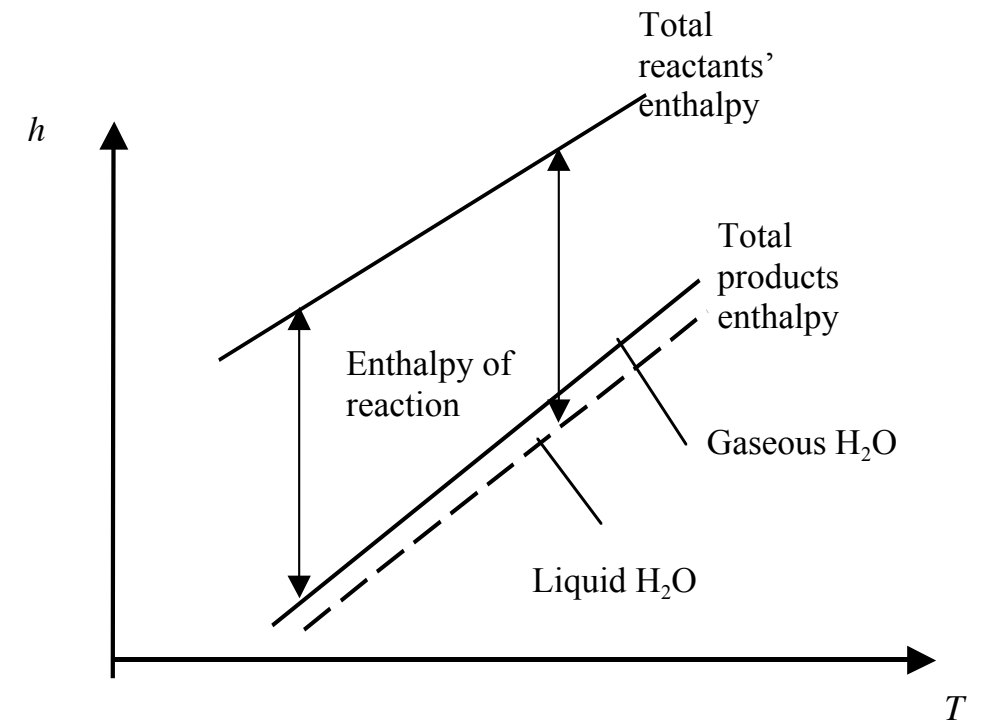
stoichiometric at STP (same T^o)

$$\Delta H_R^o = \sum_{prod} \nu_i'' \hat{h}_i^o - \sum_{react} \nu_i' \hat{h}_i^o$$

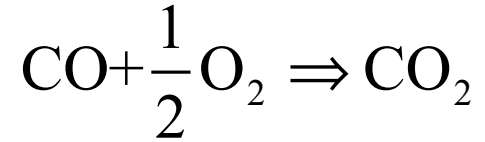
stoichiometric at arbitrary T

$$\Delta H_R(T) = \sum_{prod} \nu_i'' \hat{h}_i(T) - \sum_{react} \nu_i' \hat{h}_i(T) = \sum_{species} \nu_i \hat{h}_i(T)$$

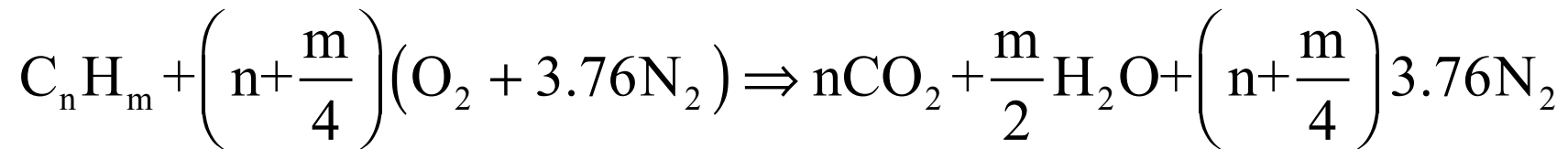
$$\nu_i = \nu_i'' - \nu_i'$$



Examples:



$$Q^o = \hat{h}_{\text{CO}_2}^o - \left(\hat{h}_{\text{CO}}^o + \frac{1}{2}\hat{h}_{\text{O}_2}^o \right) = -393 - (-110.6 + 0) = -282.5 \text{ kJ/gmol of CO}$$



$$\Delta \hat{H}_{R, \text{C}_n\text{H}_m}^o = n\hat{h}_{\text{CO}_2}^o + \frac{m}{2}\hat{h}_{\text{H}_2\text{O}}^o - \hat{h}_{\text{C}_n\text{H}_m}^o = \Delta \hat{h}_{R, \text{C}_n\text{H}_m}^o$$

For methane-air combustion, the "standard" enthalpy of reaction is:

$$\Delta \hat{h}_{\text{CH}_4}^o = -393.8 + 2(-242) - (-74.9) = -802.9 \text{ MJ/kgmol of methane}$$

Thermodynamic Properties of Fuel Combustion at 25 C and 1 atm Pressure

Fuel	Chemical symbol	Molecular weight kg/kmol	FHV MJ/kg_fuel	A/F	$H_r - H_p$ MJ/kg_product	D_g MJ/kg_fuel	FHV MJ/kg_C
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Carbon (graphite)	C _{solid}	12.01	32.764	11.51	2.619	32.834	32.764
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FHV=LHV (water in the products in the vapor phase)

D_g is the Gibbs free energy of reaction (maximum work under isothermal reaction conditions).

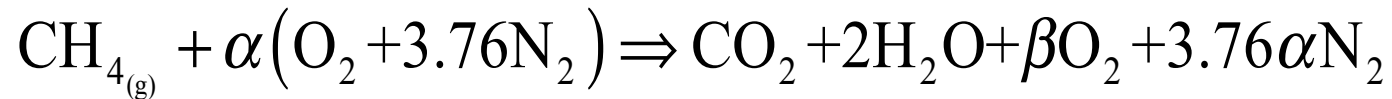
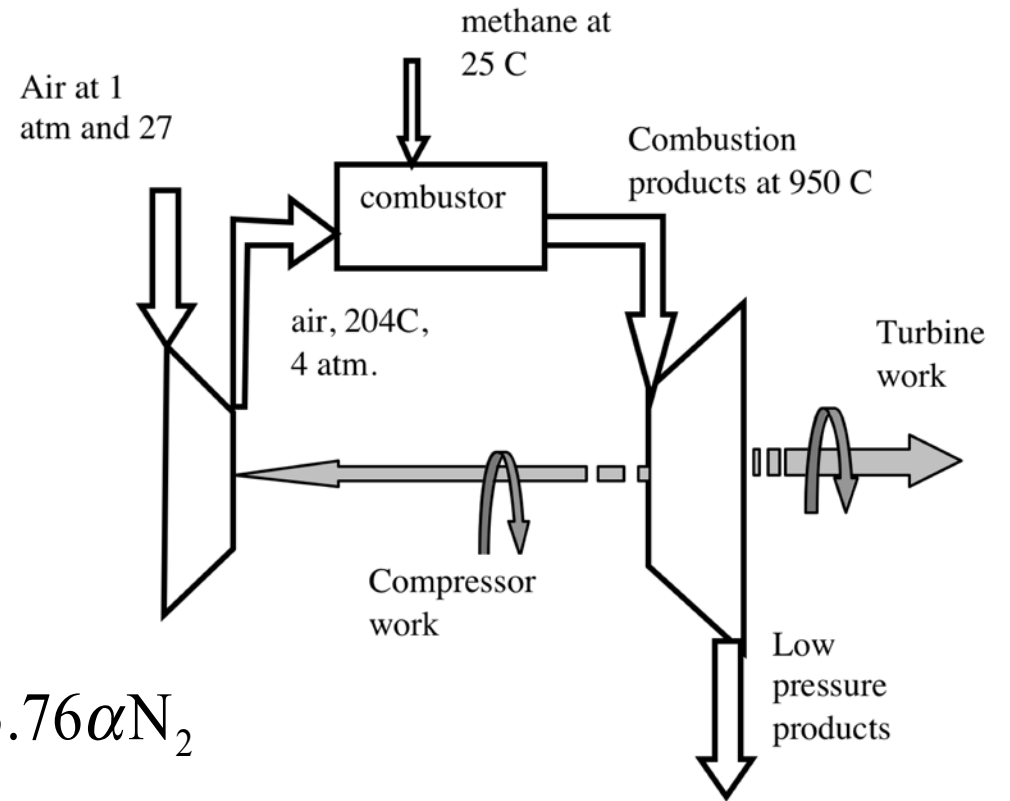
Last column: the heating value/carbon = FHV*molecular weight of fuel/molecular weight of carbon.

The Heating Value of a fuel is |enthalpy of reaction| per mole,
The table shows the LHV (water in vapor form).

HHV is obtained when water comes out in liquid form.

Fuel (phase)	LHV (kJ/mol)	HHV (kJ/mol)	$-\Delta G_R^{oo}(T^o, p^o)$ (kJ/mol)	$\hat{\xi}_{ch}^o$ (kJ/mol)
Hydrogen (g), H ₂	241.8	285.9	228.6	235.2
Carbon (s), C	393.5	393.5	394.4	410.5
<i>Paraffin (alkane) Family, C_n H_{2n+2}</i>				
Methane (g), CH ₄	802.3	890.4	818	830.2
Ethane (g), C ₂ H ₆	1427.9	1559.9	1467.5	1493.9
Propane (g), C ₃ H ₈	2044	2220	2108.4	2149
Butane (g), C ₄ H ₁₀	2658.5	2878.5	2747.8	2802.5
Pentane (g), C ₅ H ₁₂	3272.1	3536.1	3386.9	3455.8
Pentane (l), C ₅ H ₁₂	3245.5	3509.5	3385.8	3454.8
Hexane (g), C ₆ H ₁₄	3886.7	4194.8	4026.8	4110
Hexane (l), C ₆ H ₁₄	3855.1	4163.1	4022.8	4106
Heptane (g), C ₇ H ₁₆	4501.4	4853.5	4667	4764.3
Heptane (l), C ₇ H ₁₆	4464.9	4816.9	4660	4757.3
Octane (g), C ₈ H ₁₈	5116.2	5512.2	5307.1	5418.6
Octane (l), C ₈ H ₁₈	5074.6	5470.7	5297.2	5408.7

How much fuel is needed to raise the temperature of the products to 950 C, starting with air at 204 C and methane at 25C.



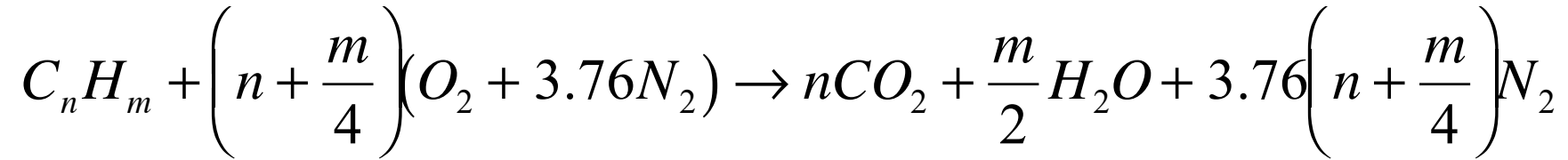
complete combustion: $\beta = \alpha - 2$

adiabatic combustion:

$$\hat{h}_{\text{CH}_4}^{27\text{C}} + \alpha(\hat{h}_{\text{O}_2}^{205\text{C}} + 3.76\hat{h}_{\text{N}_2}^{205\text{C}}) = \hat{h}_{\text{CO}_2}^{950\text{C}} + 2\hat{h}_{\text{H}_2\text{O}}^{950\text{C}} + (\alpha - 2)\hat{h}_{\text{O}_2}^{950\text{C}} + 3.76\alpha\hat{h}_{\text{N}_2}^{950\text{C}}$$

solve using enthalpy expressions: $\alpha = 7.428$ (for stoichiometric: $\alpha=2$)

Hydrocarbon Combustion in Air



- Hydrocarbons store energy in their chemical bonds. Highest energy storage per unit mass or unit volume (in liquid/solid forms).
- Chemical Energy is converted into thermal energy during combustion, or to other forms of chemical energy during refining and reforming (processes that may require energy).
- In complete, *stoichiometric* combustion of hydrocarbons, the products are water and carbon dioxide.

The table shows the LHV (water in vapor form), in MJ/kg fuel.

Commercial Fuels

Natural gas			36-42
Gasoline			47.4
Kerosene			46.4
No. 2 oil			45.5
No. 6 oil			42.5
Anthracite coal			32-34
Bituminous coal			28-36
Subbituminous coal			20-25
Lignite			14-18

Biomass Fuels

Wood (fir)			21
Grain			14
Manure			13

COAL

(fossilized vegetations)

lignite, subbituminous, bituminous, anthracite.

- Coal is carbon + hydrogen (CH_m , $m < 1$) + sulfur (up to 10% by weight) + nitrogen + oxygen + ash (non combustibles).
- Heating value per unit mass increases from lignite to anthracite, as the carbon ratio grow (and moisture, volatile matter including H_2 ratio, and sulfur decrease).
- Some sulfur can be washed away before combustion, but mostly is scrubbed from combustion products using limestone.
- In gasification, rich burning in oxygen and water forms syngas ($\text{CO}+\text{H}_2$), desulfurization before combustion or gas separation.

OIL

(or petroleum, liquid rock, fossilized marine life. algae)

- Made up of many organic compounds + hydrogen + nitrogen + sulfur. Sweet and sour refer to the amount of sulfur. CH_m , $1 < m < 2$.
- “Light oil” is generally composed of three hydrocarbon families:
 - Saturated hydrocarbons: normal alkanes (paraffins), $\text{C}_n\text{H}_{2n+2}$, with gas, $n = 1-4$, liquid, $n = 5-15$, and solids, $n > 15$.
 - Unsaturated hydrocarbons, and aromatics like benzene, C_6H_6 , toluene, C_7H_8 and naphthalene, C_{10}H_8 .
 - Resin and asphaltenes, heavier hydrocarbons rich in nitrogen, oxygen, sulfur and vanadium.
- Refining: distillation (separation of lighter components), catalytic cracking (heating) and reforming (with steam or hydrogen). Products are typically refinery gas, LPG, gasoline (mostly octane C_8H_{18}), aviation fuels (JPx), diesels, heating and lube oils

A Large Demand for Hydrogen is due to the Declining Quality of Available Crude Oil

ORNL DWG 2001-107R2

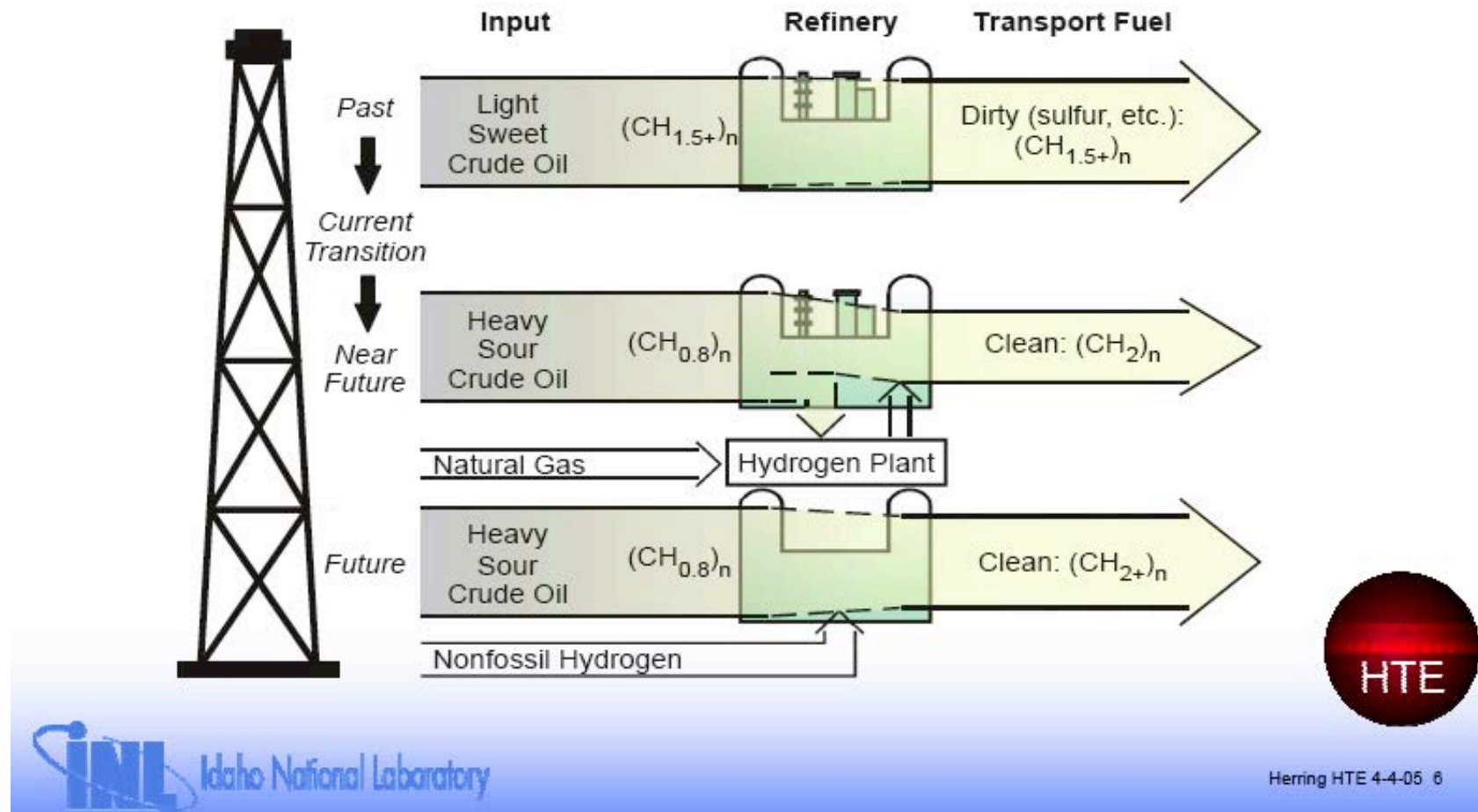


Image courtesy of Idaho National Laboratory, DOE.

Non-Conventional “Heavy” Oil

(all require intensive processing)

Oil Shale:

impermeable hard rock containing (organic, non petroleum) *kerogen* (pre-oil), which pyrolyzes into oil + (organic, petroleum) *bitumen* that liquefies with heating.

Tar and Tar Sands:

a mixture of sand and *bitumen* (coal-like), the bitumen is extracted by heating and steam, and it can be refined into oil components.

After slowing down in 2016, U.S. shale oil is expected to ramp up again in 2017, continuing a decade-long surge. Constructed by Lucas Davis (UC Berkeley) using EIA data.



Courtesy of [Lindsey G](#) on [Wikimedia](#). License: CC BY.

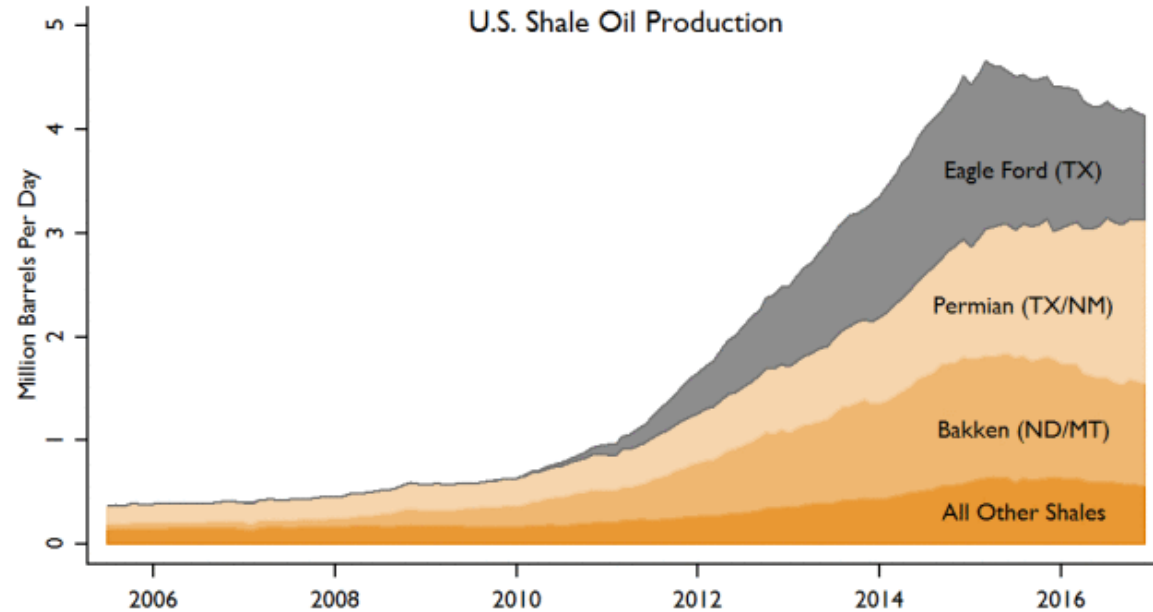


Figure courtesy of Lucas Davis, UC Berkeley. Used with permission.

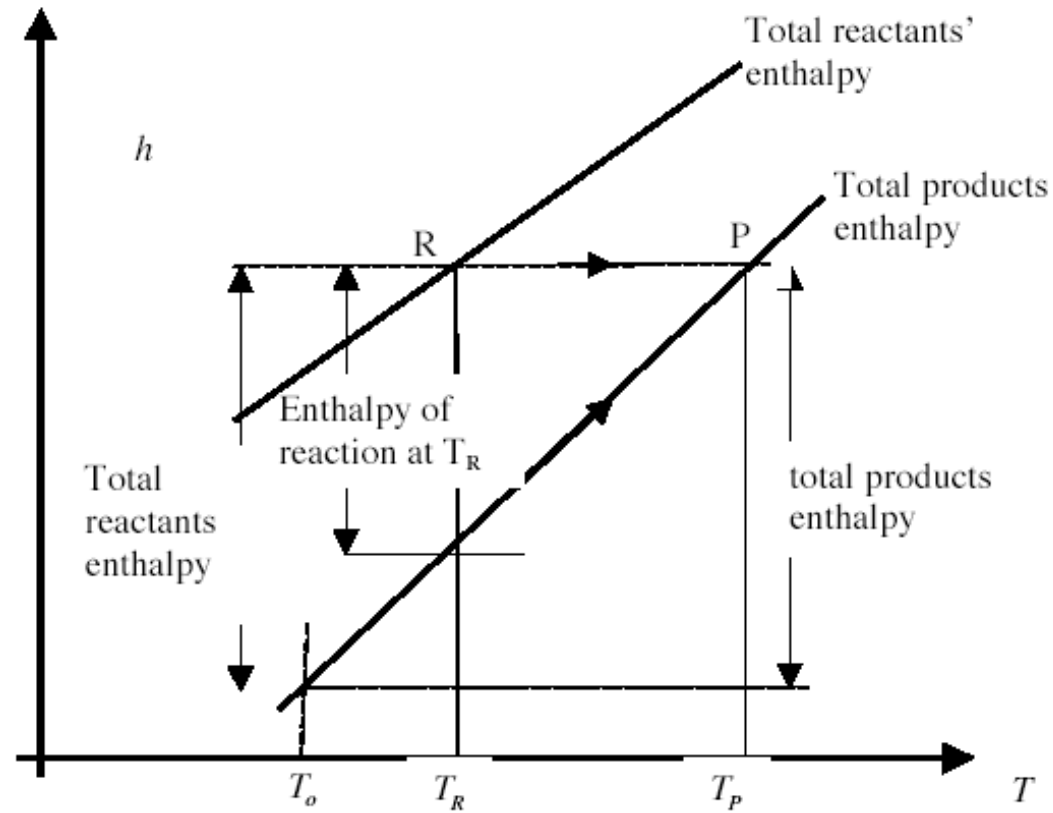
U.S. oil production in 2015 reached its highest level in decades, driven large increases in production from shale oil. Ford, Permian, and Bakken, but other areas have grown rapidly as well, and shale oil now represents almost half of all U.S. production.

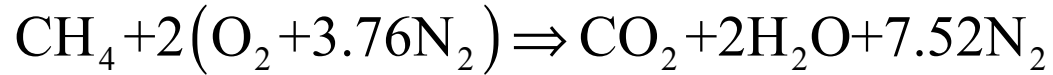
NATURAL GAS

- Mostly methane, CH_4 , ethane C_2H_6 , some propane, C_3H_8 , and little butane, C_4H_8 , with small fractions of higher hydrocarbons, may contain sulfur, oxygen, CO_2 at small quantities.
- Requires least processing.
- Biogenic Gas: near surface, difficult to exploit.
- **Methane hydrides/hydrates**, found in deep oceans, and permafrost, encapsulated in water (estimated to exceed 2 orders of magnitude of proven gas reserves) in ice like structures.
- Shale gas, like shale oil.
- Abiogenic gas, deep underground, non organic

Adiabatic Flame Temperature

$$\sum_{react} n_i \hat{h}_i(T_r) = \sum_{prod} n_i \hat{h}_i(T_p)$$





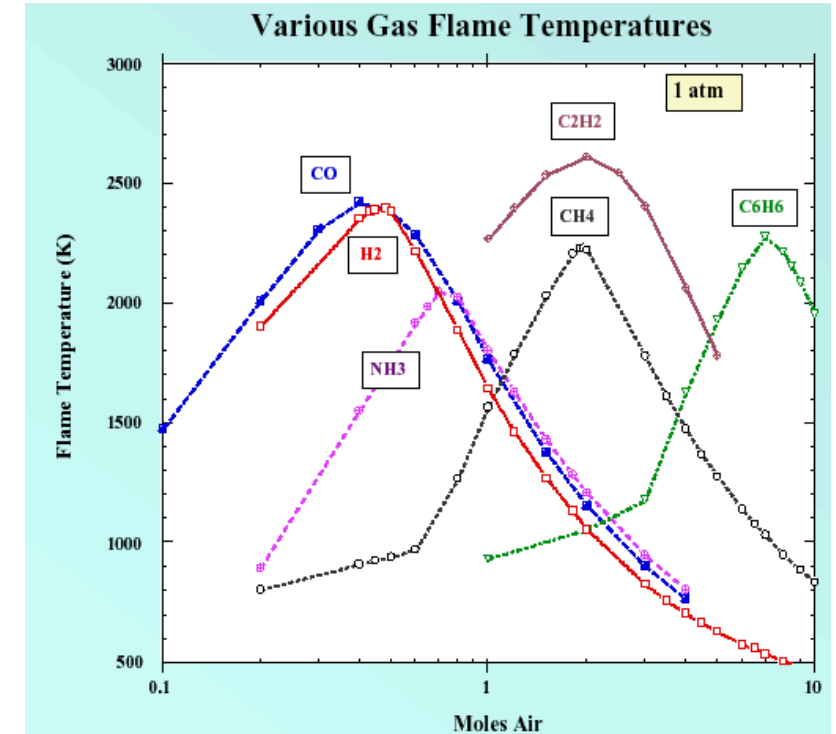
starting with $T = 298 \text{ K}$

$$\sum_{\text{react}} \nu_i \hat{h}_i(298) = \hat{h}_{\text{methane}}^o = -74,831 \text{ kJ/kgmole}$$

$$\hat{h}_{\text{CO}_2}(T_p) + 2\hat{h}_{\text{H}_2\text{O}}(T_p) + 7.52\hat{h}_{\text{N}_2}(T_p) = \sum_{i=1}^3 n_i \hat{h}_i^o + \sum_{i=1}^3 n_i \int_{T_o}^{T_p} \hat{c}_{p,i} dT$$

By iteration: $T = 2340 \text{ K}$.

The adiabatic flame temperature is highest at conditions slightly richer than stoichiometric (because of dissociation). Most fuels peak around 2300-2400 K, hydrogen's and CO are higher, and acetylene is the highest. *Lean* and *rich* burn, or lower and higher equivalence ratios, lead to lower flame temperature, with the latter containing fuel fragments. Oxy-combustion is much higher.



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Combustion in a Closed Volume

$$\begin{aligned}
 Q - W &= \Delta U = U_p - U_r \\
 &= H_p - H_r - \left((pV)_p - (pV)_r \right) \\
 &= \sum_{prod} n_i \hat{h}_i(T_p) - \sum_{react} n_i \hat{h}_i(T_r) - \left(n_p \mathcal{R}T_p - n_r \mathcal{R}T_r \right)
 \end{aligned}$$

“Standard” Internal Energy of Reaction

$$\begin{aligned}
 \Delta \hat{U}_R^o &= \sum_{prod} \nu_i \hat{h}_i(T^0) - \sum_{react} \nu_i \hat{h}_i(T^0) - (\nu_p - \nu_r) \mathcal{R}T^0 \\
 &= \Delta \hat{H}_R^o - (\nu_p - \nu_r) \mathcal{R}T^0
 \end{aligned}$$

$$\nu_p = \sum \nu'', \quad \nu_r = \sum \nu'$$

The complete combustion of various hydrocarbons in a **perfectly insulated constant-volume combustion chamber**, stoichiometric mixture with dry air starting at 298 C and 1 atm. from Gyftopoulos and Beretta

Fuel	Formula	T_b K	p_b atm
Hydrogen	H ₂	2870.8	8.33
Carbon	C	2677.9	7.58
Methane	CH ₄	2655.4	9.02
Acetylene	C ₂ H ₂	3009.7	10.00
Ethylene	C ₂ H ₄	2811.0	9.63
Ethane	C ₂ H ₆	2691.1	9.42
Propane	C ₃ H ₈	2698.7	9.56
<i>n</i> -Butane	C ₄ H ₁₀	2702.7	9.64
Benzene	C ₆ H ₆	2767.6	9.61
<i>n</i> -Heptane	C ₇ H ₁₆	2707.6	9.75
<i>n</i> -Octane	C ₈ H ₁₈	2706.9	9.76
Octane	C ₈ H ₁₈	2702.6	9.74

Efficiency

Combustion: $(\eta_{comb})_I = \frac{\sum_{prod} n_i \hat{h}_i - \sum_{react} n_i \hat{h}_i}{-\hat{h}_{R,f}} = \frac{Q_H}{HV_{fuel}} < 1$, (incomplete combustion; heat losses)

For engines and FC (chemical engines: $\eta_{fuel-utiliz} = \frac{\dot{W}_{net}}{\dot{m}_{fuel} HV_{fuel}}$

OR: $\eta_{fuel-utiliz} = \frac{W_{net}}{W_{max}} \frac{W_{max}}{Q_H} \frac{Q_H}{HV_{fuel}} = \eta_{II} \cdot \eta_{car} \cdot \eta_{comb}$

For fuel production: $(\eta_{reform})_I = \frac{\text{Energies Out}}{\text{Energies In}} = \frac{\text{Chemical Energy Out}}{\text{Chemical Energy In}} = \frac{(\dot{n}_f \Delta \hat{h}_f)_{out}}{\sum_{in} (\dot{n}_f \Delta \hat{h}_f)}$

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2.60J Fundamentals of Advanced Energy Conversion
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