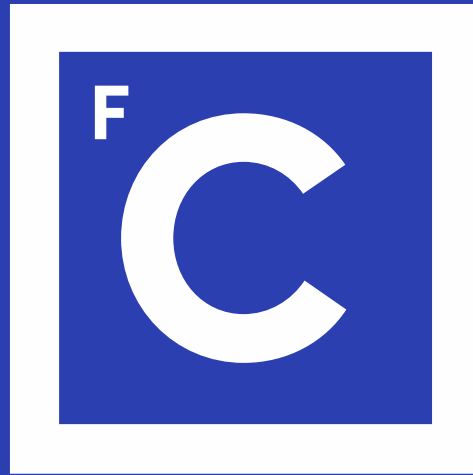




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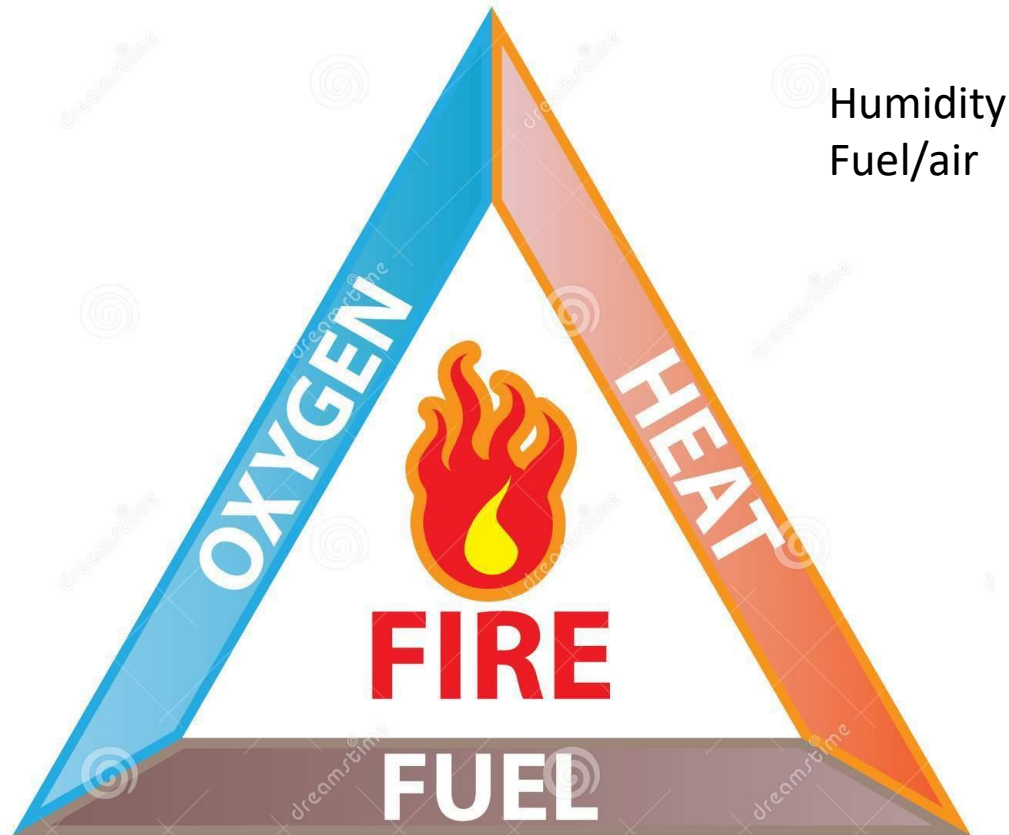
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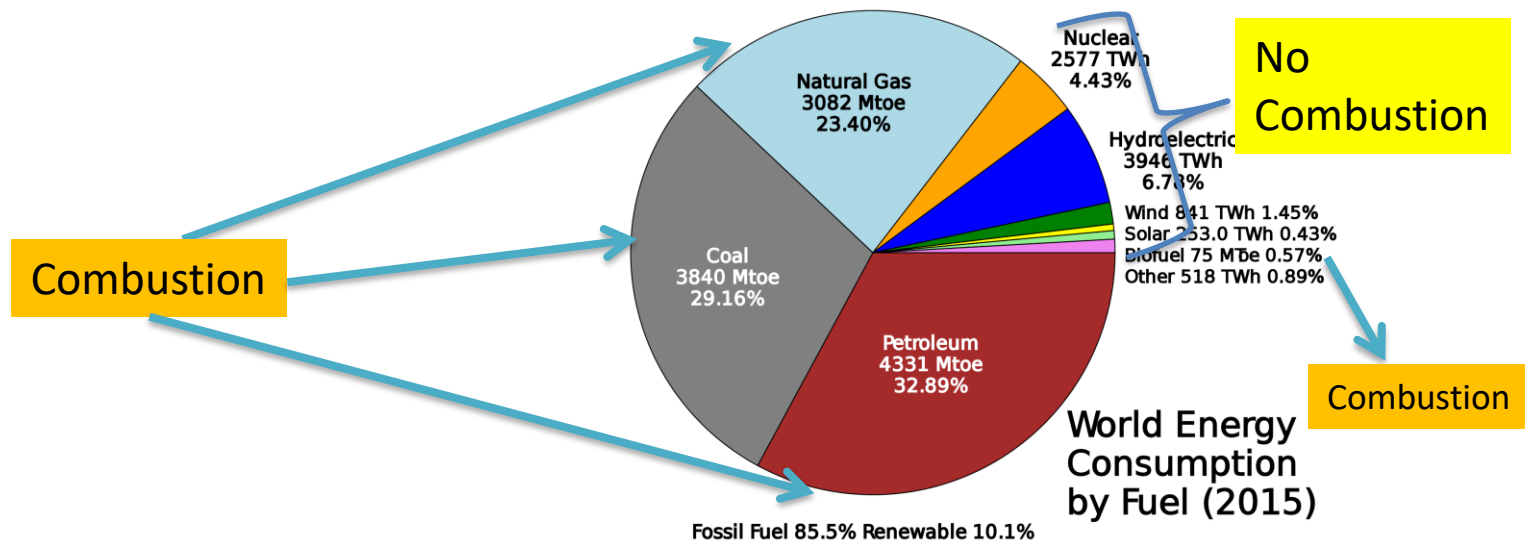


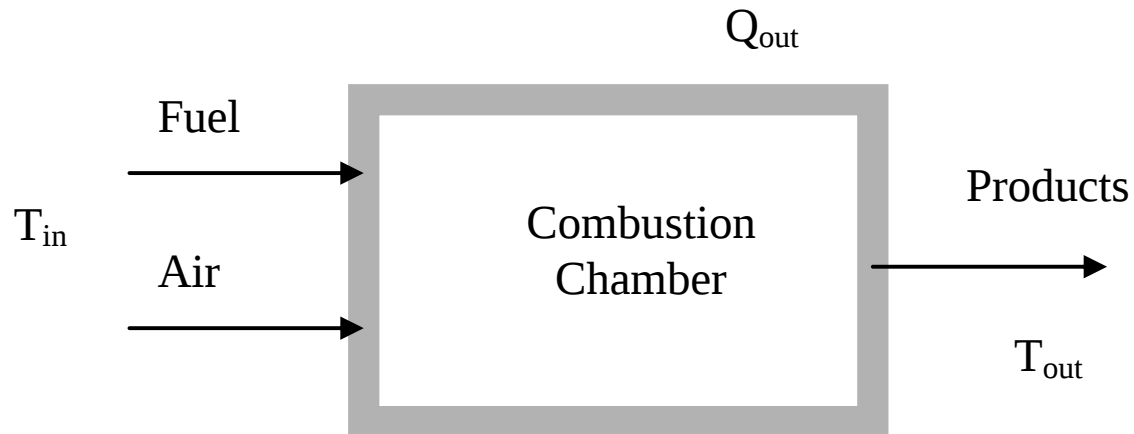
Technologies of combustion

Combustion definition

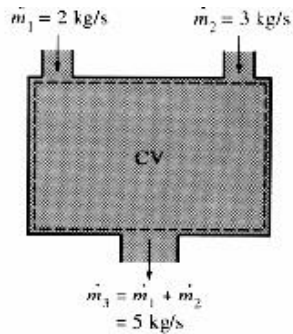
Combustion is essentially burning, fuels react with oxygen to release energy







(Massa que entra) – (Massa que sai) = (Variação total massa sistema)



Stationary regime

$$\sum_e \dot{m}_e - \sum_s \dot{m}_s = \frac{dm_{vc}}{dt}$$

$$\sum_e \dot{m}_e = \sum_s \dot{m}_s, \frac{dm_{vc}}{dt} = 0$$

Mass flow (kg/s)

Conservation of Energy

1st Law thermodynamics conservation of energy

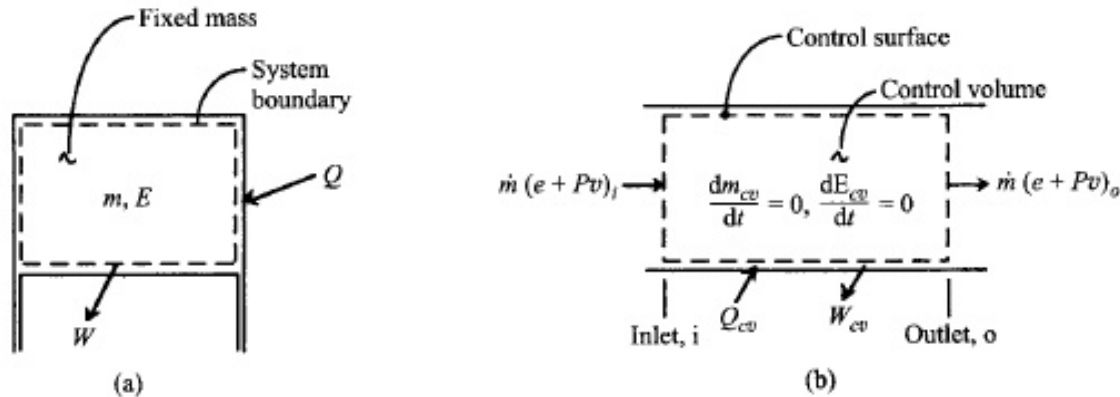
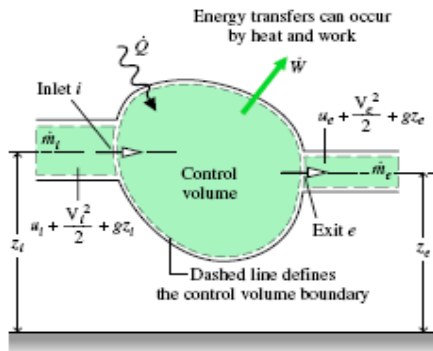


Figure 2.3 (a) Schematic of fixed-mass system with moving boundary above piston. (b) Control volume with fixed boundaries and steady flow.

- Closed system
- Open system

$$\Delta E = \Delta EP + \Delta EC + \Delta U = Q - W$$

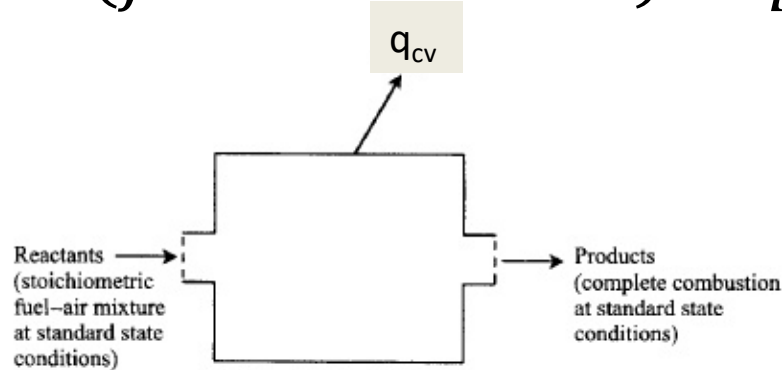


Usando definição de entalpia

$$\frac{dE_{cv}}{dt} = \dot{Q}_{cv} - \dot{W}_{cv} + \dot{m}_i \left(u_i + p_i v_i + \frac{V_i^2}{2} + gz_i \right) - \dot{m}_e \left(u_e + p_e v_e + \frac{V_e^2}{2} + gz_e \right)$$

$$\frac{dE_{cv}}{dt} = \dot{Q}_{cv} - \dot{W}_{cv} + \sum_i \dot{m}_i \left(h_i + \frac{V_i^2}{2} + gz_i \right) - \sum_e \dot{m}_e \left(h_e + \frac{V_e^2}{2} + gz_e \right)$$

reactants(fuel + oxidizer) → products



$$\dot{m}_i = \dot{m}_e \quad (\text{kg/s})$$

Figure 2.7 Steady-flow reactor used to determine enthalpy of combustion.

$$\dot{E}_{in} - \dot{E}_{out} = \Delta \dot{E}_{CV}$$

$$\dot{Q}_{net} + \underbrace{\sum \dot{m}_i \left(h_i + \cancel{\frac{\bar{V}_i^2}{2}} + \cancel{gz_i} \right)}_{\text{for each inlet}} - \underbrace{\sum \dot{m}_e \left(h_e + \cancel{\frac{\bar{V}_e^2}{2}} + \cancel{gz_e} \right)}_{\text{for each exit}} = \Delta \dot{E}_{CV} \quad (\text{J})$$

=0

Stationary regime

$$q_{cv} = h_{\text{reactants}} - h_{\text{products}} \quad (\text{J/kg})$$

$$\bar{R} = 8.314 \text{ kJ} / \text{kmol.K} \quad \text{Constante universal dos gases}$$

$$Z = \frac{pv}{RT} \quad \text{Factor de compressibilidade}$$

$$R = \frac{\bar{R}}{M} \quad \text{kJ/kg.K}$$

$Z=1$ é gas perfeito

$$pv = RT$$

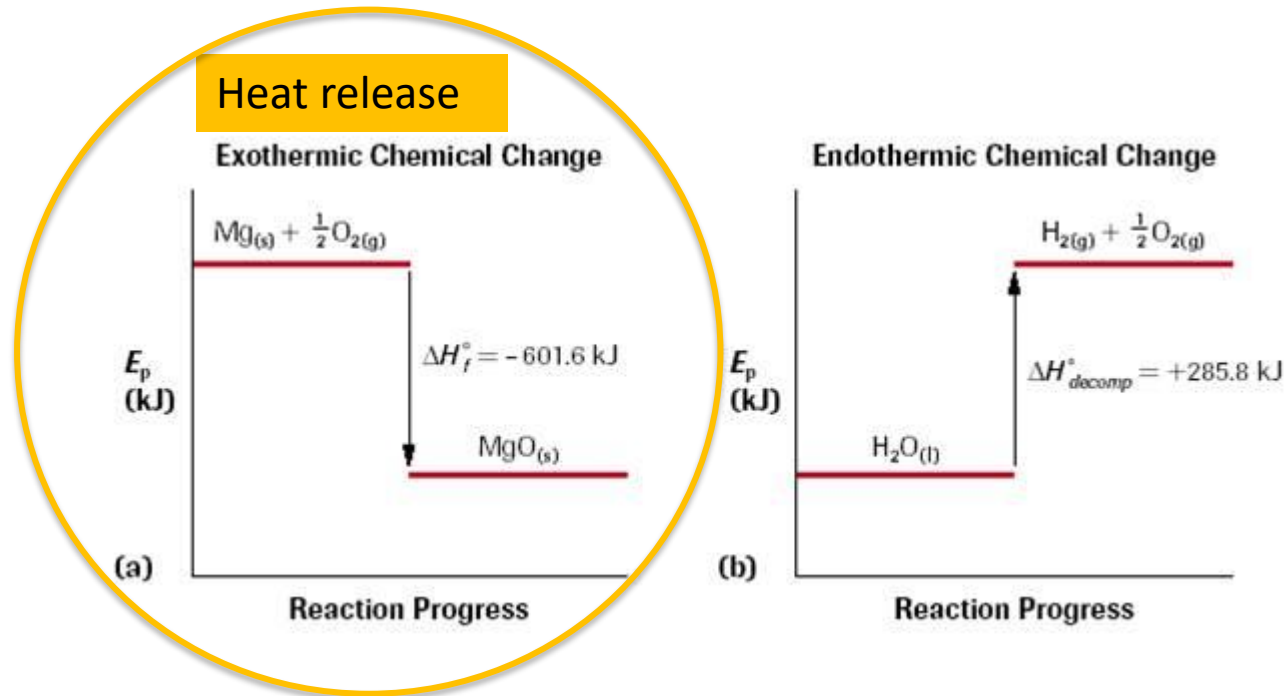
$$u = u(T)$$

$$h = h(T) = u(T) + RT$$

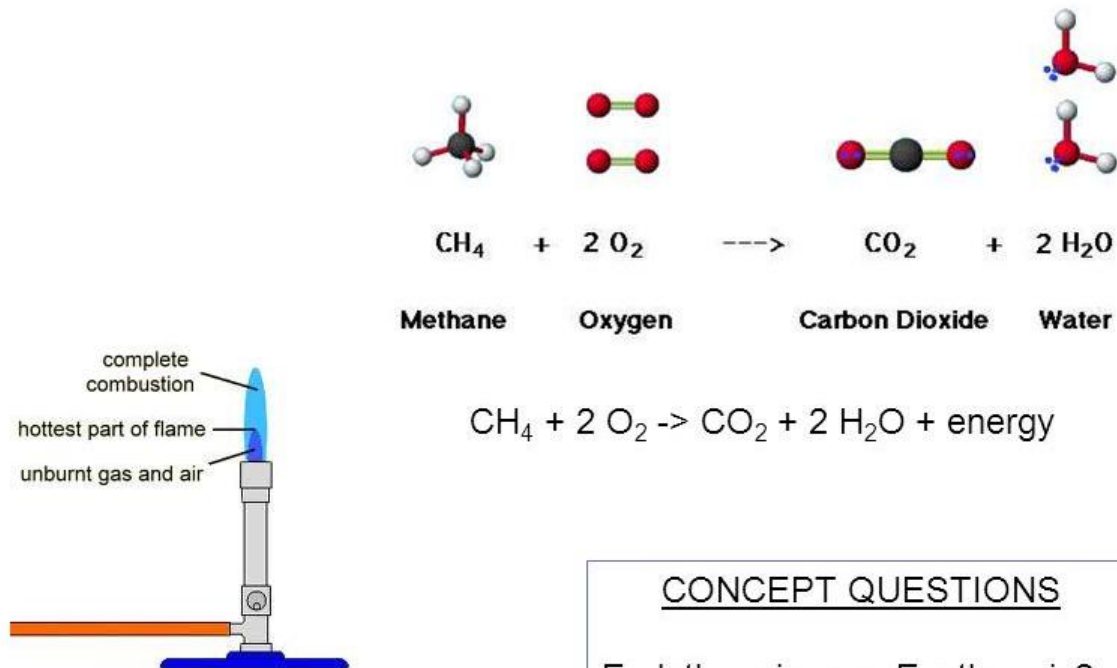
$$c_p(T) = c_v(T) + R$$

$$u(T_2) - u(T_1) = \int_{T_1}^{T_2} c_v(T) dT$$

$$h(T_2) - h(T_1) = \int_{T_1}^{T_2} c_p(T) dT$$



In combustion chemical bonds break, others form, but the energy balance is **exothermic**



CONCEPT QUESTIONS

Endothermic or Exothermic?

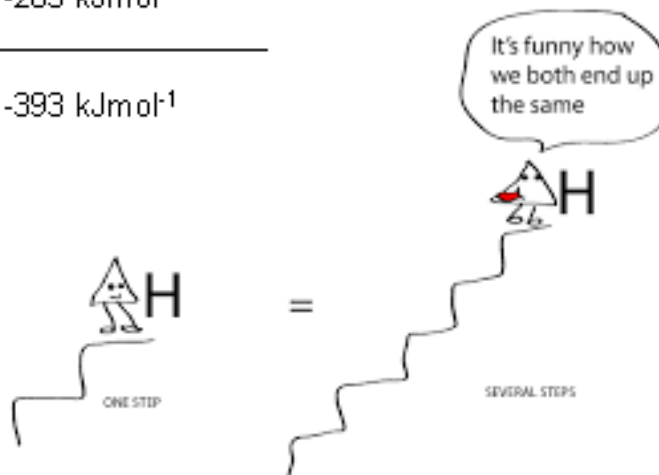
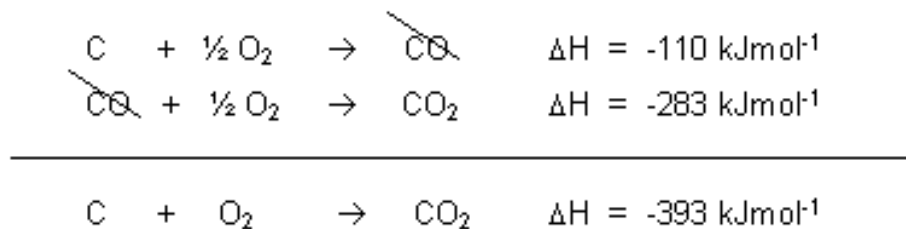
$+\Delta H$ or $-\Delta H$?

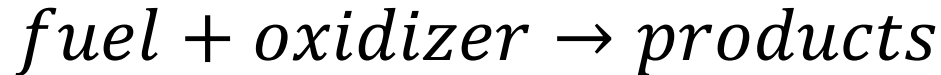
Heat release

Thermochemistry

HESS LAW

total enthalpy change during the complete course of a chemical reaction is the same whether the reaction is made in one step or in several steps





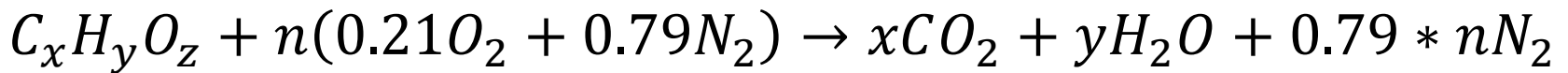
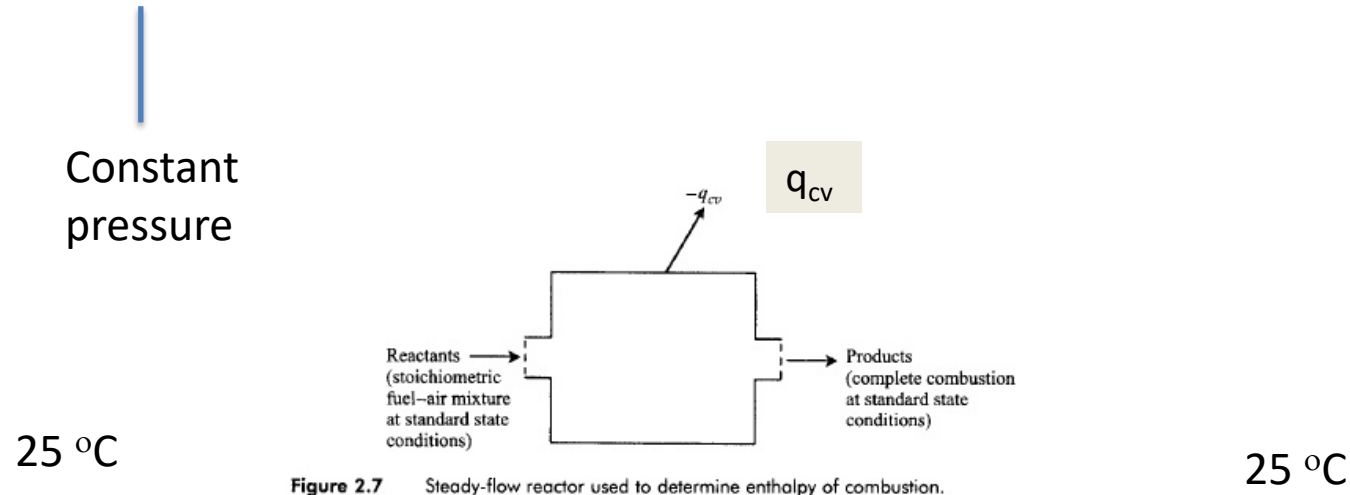
Standard reference state

$$\left\{ \begin{array}{l} T_{\text{ref}} = 25^{\circ}\text{C} \text{ (298.15 K)} \\ P_{\text{ref}} = 1 \text{ atm (101.325 kPa = 1 bar)} \\ h_{\text{ref}} = h_{f,i}^{\circ}(T_{\text{ref}}) = u + pv \text{ (J/kg)} \end{array} \right.$$

$$h_i(T) = h_{f,i}^{\circ}(T_{\text{ref}}) + \Delta h_{s,i}(T_{\text{ref}}) \quad (\text{J/kg})$$

- In words first equation says:
 - Absolute enthalpy at T is equal to sum of enthalpy of formation at standard reference state and sensible enthalpy change in going from T_{ref} to T

HEATING VALUE AND ENTHALPY OF REACTION



HHV = maximum heat release condensing water heat of vaporization (**2443 kJ/kg; 44010 kJ/kmol**)

LHV = q_{cv} in the reaction products is not recovered

Appendix A

Table A.2 Carbon dioxide (CO₂), MW = 44.011, enthalpy of formation @ 298 K
(kJ/kmol) = -393,546

$T(K)$	$\bar{c}_p$ (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
500	44.569	8,301	-393,712	234.833	-394,983
600	47.313	12,899	-393,844	243.209	-395,226
700	49.617	17,749	-394,013	250.680	-395,443
800	51.550	22,810	-394,213	257.436	-395,635
900	53.136	28,047	-394,433	263.603	-395,799
1,000	54.360	33,425	-394,659	269.268	-395,939
1,100	55.333	38,911	-394,875	274.495	-396,056
1,200	56.205	44,488	-395,083	279.348	-396,155
1,300	56.984	50,149	-395,287	283.878	-396,236
1,400	57.677	55,882	-395,488	288.127	-396,301
1,500	58.292	61,681	-395,691	292.128	-396,352
1,600	58.836	67,538	-395,897	295.908	-396,389
1,700	59.316	73,446	-396,110	299.489	-396,414
1,800	59.738	79,399	-396,332	302.892	-396,425
1,900	60.108	85,392	-396,564	306.132	-396,424
2,000	60.433	91,420	-396,808	309.223	-396,410

CO₂

Appendix A

Table A.2 Carbon dioxide (CO₂), MW = 44.011, enthalpy of formation @ 298 K (kJ/kmol) = -393,546

$T(K)$	$\bar{c}_p$ (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)
2,000	60.433	91,420	-396,808	309.223	-396,410
2,100	60.717	97,477	-397,065	312.179	-396,384
2,200	60.966	103,562	-397,338	315.009	-396,346
2,300	61.185	109,670	-397,626	317.724	-396,294
2,400	61.378	115,798	-397,931	320.333	-396,230
2,500	61.548	121,944	-398,253	322.842	-396,152
2,600	61.701	128,107	-398,594	325.259	-396,061
2,700	61.839	134,284	-398,952	327.590	-395,957
2,800	61.965	140,474	-399,329	329.841	-395,840
2,900	62.083	146,677	-399,725	332.018	-395,708
3,000	62.194	152,891	-400,140	334.124	-395,562
3,100	62.301	159,116	-400,573	336.165	-395,403
3,200	62.406	165,351	-401,025	338.145	-395,229
3,300	62.510	171,597	-401,495	340.067	-395,041
3,400	62.614	177,853	-401,983	341.935	-394,838
3,500	62.718	184,120	-402,489	343.751	-394,620
3,600	62.825	190,397	-403,013	345.519	-394,388
3,700	62.932	196,685	-403,553	347.242	-394,141
3,800	63.041	202,983	-404,110	348.922	-393,879
3,900	63.151	209,293	-404,684	350.561	-393,602
4,000	63.261	215,613	-405,273	353.161	-393,311
4,100	63.369	221,945	-405,878	353.725	-393,004
4,200	63.474	228,287	-406,499	355.253	-392,683
4,300	63.575	234,640	-407,135	356.748	-392,346
4,400	63.669	241,002	-407,785	358.210	-391,995
4,500	63.753	247,373	-408,451	359.642	-391,629
4,600	63.825	253,752	-409,132	361.044	-391,247
4,700	63.881	260,138	-409,828	362.417	-390,851

CO₂

Appendix A

Table A.6 Water (H_2O), MW = 18.016, enthalpy of formation @ 298 K (kJ/kmol)
= -241,845; enthalpy of vaporization (kJ/kmol) = 44,010

$T(\text{K})$	$\bar{c}_p$ (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	32.255	-3,227	-240,838	175.602	-232,779
298	33.448	0	-241,845	188.715	-228,608
300	33.468	62	-241,865	188.922	-228,526
400	34.437	3,458	-242,858	198.686	-223,929
500	35.337	6,947	-243,822	206.467	-219,085
600	36.288	10,528	-244,753	212.992	-214,049
700	37.364	14,209	-245,638	218.665	-208,861
800	38.587	18,005	-246,461	223.733	-203,550
900	39.930	21,930	-247,209	228.354	-198,141
1,000	41.315	25,993	-247,879	232.633	-192,652
1,100	42.638	30,191	-248,475	236.634	-187,100
1,200	43.874	34,518	-249,005	240.397	-181,497
1,300	45.027	38,963	-249,477	243.955	-175,852
1,400	46.102	43,520	-249,895	247.332	-170,172
1,500	47.103	48,181	-250,267	250.547	-164,464
1,600	48.035	52,939	-250,597	253.617	-158,733
1,700	48.901	57,786	-250,890	256.556	-152,983
1,800	49.705	62,717	-251,151	259.374	-147,216
1,900	50.451	67,725	-251,384	262.081	-141,435
2,000	51.143	72,805	-251,594	264.687	-135,643

H_2O

Appendix A

Table A.6 Water (H_2O), MW = 18.016, enthalpy of formation @ 298 K (kJ/kmol)
 = -241,845; enthalpy of vaporization (kJ/kmol) = 44,010

$T(\text{K})$	$\bar{c}_p$ (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)
2,100	51.784	77,952	-251,783	267.198	-129,841
2,200	52.378	83,160	-251,955	269.621	-124,030
2,300	52.927	88,426	-252,113	271.961	-118,211
2,400	53.435	93,744	-252,261	274.225	-112,386
2,500	53.905	99,112	-252,399	276.416	-106,555
2,600	54.340	104,524	-252,532	278.539	-100,719
2,700	54.742	109,979	-252,659	280.597	-94,878
2,800	55.115	115,472	-252,785	282.595	-89,031
2,900	55.459	121,001	-252,909	284.535	-83,181
3,000	55.779	126,563	-253,034	286.420	-77,326
3,100	56.076	132,156	-253,161	288.254	-71,467
3,200	56.353	137,777	-253,290	290.039	-65,604
3,300	56.610	143,426	-253,423	291.777	-59,737
3,400	56.851	149,099	-253,561	293.471	-53,865
3,500	57.076	154,795	-253,704	295.122	-47,990
3,600	57.288	160,514	-253,852	296.733	-42,110
3,700	57.488	166,252	-254,007	298.305	-36,226
3,800	57.676	172,011	-254,169	299.841	-30,338
3,900	57.856	177,787	-254,338	301.341	-24,446
4,000	58.026	183,582	-254,515	302.808	-18,549
4,100	58.190	189,392	-254,699	304.243	-12,648
4,200	58.346	195,219	-254,892	305.647	-6,742
4,300	58.496	201,061	-255,093	307.022	-831
4,400	58.641	206,918	-255,303	308.368	5,085
4,500	58.781	212,790	-255,522	309.688	11,005
4,600	58.916	218,674	-255,751	310.981	16,930
4,700	59.047	224,573	-255,990	312.250	22,861

H_2O

Thermochemistry

Appendix A

Table A.7 Nitrogen (N_2), MW = 28.013, enthalpy of formation @ 298 K (kJ/kmol) = 0

$T(K)$	$\bar{c}_p$ (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	28.793	-2,841	0	179.959	0
298	29.071	0	0	191.511	0
300	29.075	54	0	191.691	0
400	29.319	2,973	0	200.088	0
500	29.636	5,920	0	206.662	0
600	30.086	8,905	0	212.103	0
700	30.684	11,942	0	216.784	0
800	31.394	15,046	0	220.927	0
900	32.131	18,222	0	224.667	0
1,000	32.762	21,468	0	228.087	0
1,100	33.258	24,770	0	231.233	0
1,200	33.707	28,118	0	234.146	0
1,300	34.113	31,510	0	236.861	0
1,400	34.477	34,939	0	239.402	0
1,500	34.805	38,404	0	241.792	0
1,600	35.099	41,899	0	244.048	0
1,700	35.361	45,423	0	246.184	0
1,800	35.595	48,971	0	248.212	0
1,900	35.803	52,541	0	250.142	0
2,000	35.988	56,130	0	251.983	0

N_2

Appendix A

Table A.7 Nitrogen (N_2), MW = 28.013, enthalpy of formation @ 298 K (kJ/kmol) = 0

$T(K)$	$\bar{c}_p$ (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)
2,100	36.152	59,738	0	253.743	0
2,200	36.298	63,360	0	255.429	0
2,300	36.428	66,997	0	257.045	0
2,400	36.543	70,645	0	258.598	0
2,500	36.645	74,305	0	260.092	0
2,600	36.737	77,974	0	261.531	0
2,700	36.820	81,652	0	262.919	0
2,800	36.895	85,338	0	264.259	0
2,900	36.964	89,031	0	265.555	0
3,000	37.028	92,730	0	266.810	0
3,100	37.088	96,436	0	268.025	0
3,200	37.144	100,148	0	269.203	0
3,300	37.198	103,865	0	270.347	0
3,400	37.251	107,587	0	271.458	0
3,500	37.302	111,315	0	272.539	0
3,600	37.352	115,048	0	273.590	0
3,700	37.402	118,786	0	274.614	0
3,800	37.452	122,528	0	275.612	0
3,900	37.501	126,276	0	276.586	0
4,000	37.549	130,028	0	277.536	0
4,100	37.597	133,786	0	278.464	0
4,200	37.643	137,548	0	279.370	0
4,300	37.688	141,314	0	280.257	0
4,400	37.730	145,085	0	281.123	0
4,500	37.768	148,860	0	281.972	0
4,600	37.803	152,639	0	282.802	0
4,700	37.832	156,420	0	283.616	0

N_2

Selected properties of hydrocarbon fuels: enthalpy of formation,^a Gibbs function of formation,^a entropy,^a and higher and lower heating values all at 298.15 K and 1 atm; boiling points^b and latent heat of vaporization^c at 1 atm; constant-pressure adiabatic flame temperature at 1 atm;^d liquid density^c

Formula	Fuel	Mol. wt. (kg/kmol)	$\bar{h}_f^\circ$ (kJ/kmol)	$\bar{g}_f^\circ$ (kJ/kmol)	s° (kJ/kmol-K)	HHV [†] (kJ/kg)	LHV [†] (kJ/kg)	Boiling pt. (°C)	h_{fg} (kJ/kg)	$T_{ad}^\dagger$ (K)	ρ_{liq}^* (kg/m ³)
CH ₄	Methane	16.043	-74,831	-50,794	186.188	55,528	50,016	-164	509	2226	300
C ₂ H ₂	Acetylene	26.038	226,748	209,200	200.819	49,923	48,225	-84	—	2539	—
C ₂ H ₄	Ethene	28.054	52,283	68,124	219.827	50,313	47,161	-103.7	—	2369	—
C ₂ H ₆	Ethane	30.069	-84,667	-32,886	229.492	51,901	47,489	-88.6	488	2259	370
C ₃ H ₆	Propane	42.080	20,414	62,718	266.939	48,936	45,784	-47.4	437	2334	514
C ₃ H ₈	Propane	44.096	-103,847	-23,489	269.910	50,368	46,357	-42.1	425	2267	500
C ₄ H ₈	1-Butene	56.107	1,172	72,036	307.440	48,471	45,319	-63	391	2322	595
C ₄ H ₁₀	<i>n</i> -Butane	58.123	-124,733	-15,707	310.034	49,546	45,742	-0.5	386	2270	579
C ₅ H ₁₀	1-Pentene	70.134	-20,920	78,605	347.607	48,152	45,000	30	358	2314	641
C ₅ H ₁₂	<i>n</i> -Pentane	72.150	-146,440	-8,201	348.402	49,032	45,355	36.1	358	2272	626
C ₆ H ₆	Benzene	78.113	82,927	129,658	269.199	42,277	40,579	80.1	393	2342	879
C ₆ H ₁₂	1-Hexene	84.161	-41,673	87,027	385.974	47,955	44,803	63.4	335	2308	673
C ₆ H ₁₄	<i>n</i> -Hexane	86.177	-167,193	209	386.811	48,696	45,105	69	335	2273	659
C ₇ H ₁₄	1-Heptene	98.188	-62,132	95,563	424.383	47,817	44,665	93.6	—	2305	—
C ₇ H ₁₆	<i>n</i> -Heptane	100.203	-187,820	8,745	425.262	48,456	44,926	98.4	316	2274	684
C ₈ H ₁₆	1-Octene	112.214	-82,927	104,140	462.792	47,712	44,560	121.3	—	2302	—
C ₈ H ₁₈	<i>n</i> -Octane	114.230	-208,447	17,322	463.671	48,275	44,791	125.7	300	2275	703
C ₉ H ₁₈	1-Nonene	126.241	-103,512	112,717	501.243	47,631	44,478	—	—	2300	—
C ₉ H ₂₀	<i>n</i> -Nonane	128.257	-229,032	25,857	502.080	48,134	44,686	150.8	295	2276	718
C ₁₀ H ₂₀	1-Decene	140.268	-124,139	121,294	539.652	47,565	44,413	170.6	—	2298	—
C ₁₀ H ₂₂	<i>n</i> -Decane	142.284	-249,659	34,434	540.531	48,020	44,602	174.1	277	2277	730
C ₁₁ H ₂₂	1-Undecene	154.295	-144,766	129,830	578.061	47,512	44,360	—	—	2296	—
C ₁₁ H ₂₄	<i>n</i> -Undecane	156.311	-270,286	43,012	578.940	47,926	44,532	195.9	265	2277	740

TABLE B.1 (continued)

Formula	Fuel	Mol. wt. (kg/kmol)	$\bar{h}_f^\circ$ (kJ/kmol)	$\bar{g}_f^\circ$ (kJ/kmol)	$\bar{s}^\circ$ (kJ/kmol-K)	HHV [†] (kJ/kg)	LHV [†] (kJ/kg)	Boiling pt. (°C)	h_{fg} (kJ/kg)	$T_{ad}^\dagger$ (K)	ρ_{liq}^* (kg/m ³)
C ₁₂ H ₂₄	1-Dodecene	168.322	-165,352	138,407	616.471	47,468	44,316	213.4	—	2295	—
C ₁₂ H ₂₆	n-Dodecane	170.337	-292,162	—	—	47,841	44,467	216.3	256	2277	749

[†] Based on gaseous fuel.

[‡] For stoichiometric combustion with air (79% N₂, 21% O₂).

* For liquids at 20°C or for gases at the boiling point of the liquified gas.

Sources:

^aRossini, F. D., *et al.*, *Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds*, Carnegie Press, Pittsburgh, 1953.

^bWeast, R. C. (ed.), *Handbook of Chemistry and Physics*, 56th Ed., CRC Press, Cleveland, 1976.

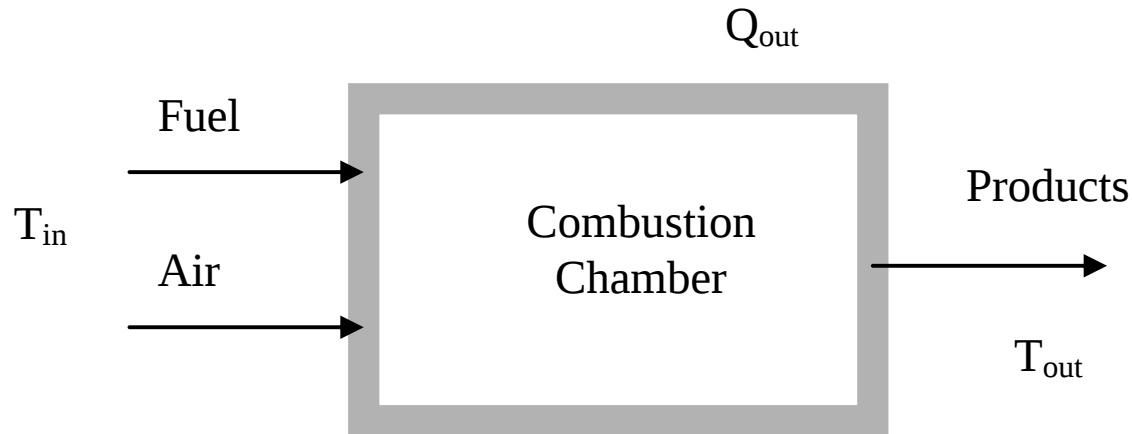
^cObert, E. F., *Internal Combustion Engines and Air Pollution*, Harper & Row, New York, 1973.

^dCalculated using HPFLAME (Appendix F).

Thermochemistry



Fuel	Chemical formula	LHV (MJ/kg)	Density (kg/L)	LHV (MJ/L)	CO ₂ (kg/L)	CO ₂ (g/MJ)
Gasolina	$C_n H_{1.87n}$	44	0.72-0.78	31.7	2.28	66.6-72.1
Gasóleo	$C_n H_{1.8n}$	42.5	0.84-0.88	35.7	2.68	75.0
Etanol	$C_2 H_6 O$	26.9	0.785	21.1	1.50	71.1
Biodiesel	$C_n H_{2n} O_2$	37.1	0.88	32.6	2.47-2.80	75.8-85.8
Gás natural	$\sim CH_4$	50	0.72 (kg/m ³)*	36.0 (MJ/m ³)	1.98 (kg/m ³)	55.0
GPL	$\sim C_3 H_8$	46.4	0.51 (2 kg/m ³)*	23.7	1.53	64.7



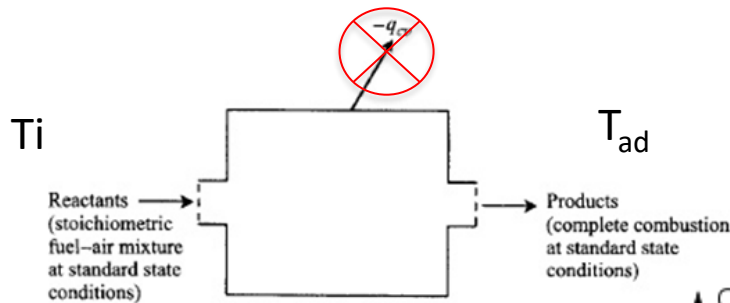
- Maximum heat release, max Q_{out} : $T_{out}=T_{in}$
- Maximum flame temperature, adiabatic combustion chamber, T_{ad} :

$H_{reag}(T_{in})=H_{prod}(T_{ad})$ (constant pressure, e.g. Diesel engine, gas turbine, furnace)

$H_{reag}(T_{in})=H_{prod}(T_{ad})-R(n_{prod}T_{ad}-n_{reag}T_{in})$ (constant volume, e.g. gasoline engine)

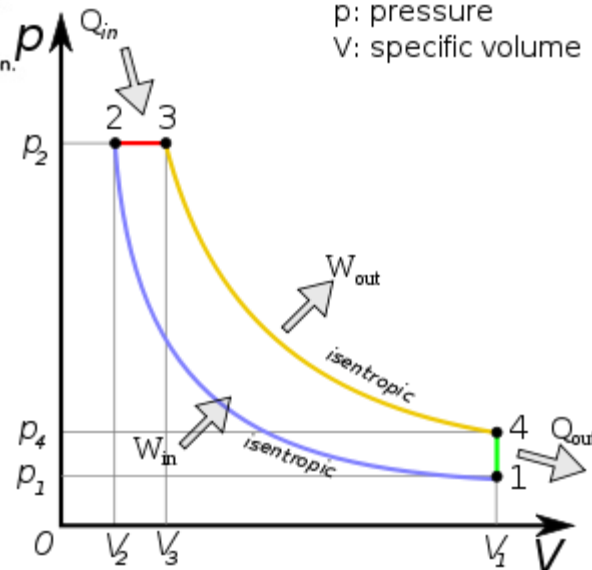
Adiabatic flame temperature = T_{ad}

Constant pressure



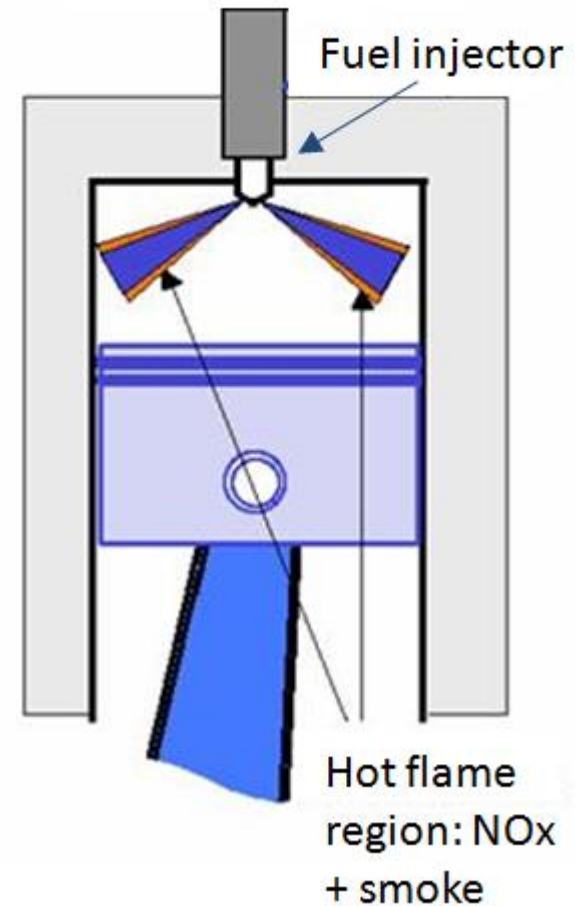
Steady-flow reactor used to determine enthalpy of combustion.

$\Delta H = 0$ for constant pressure



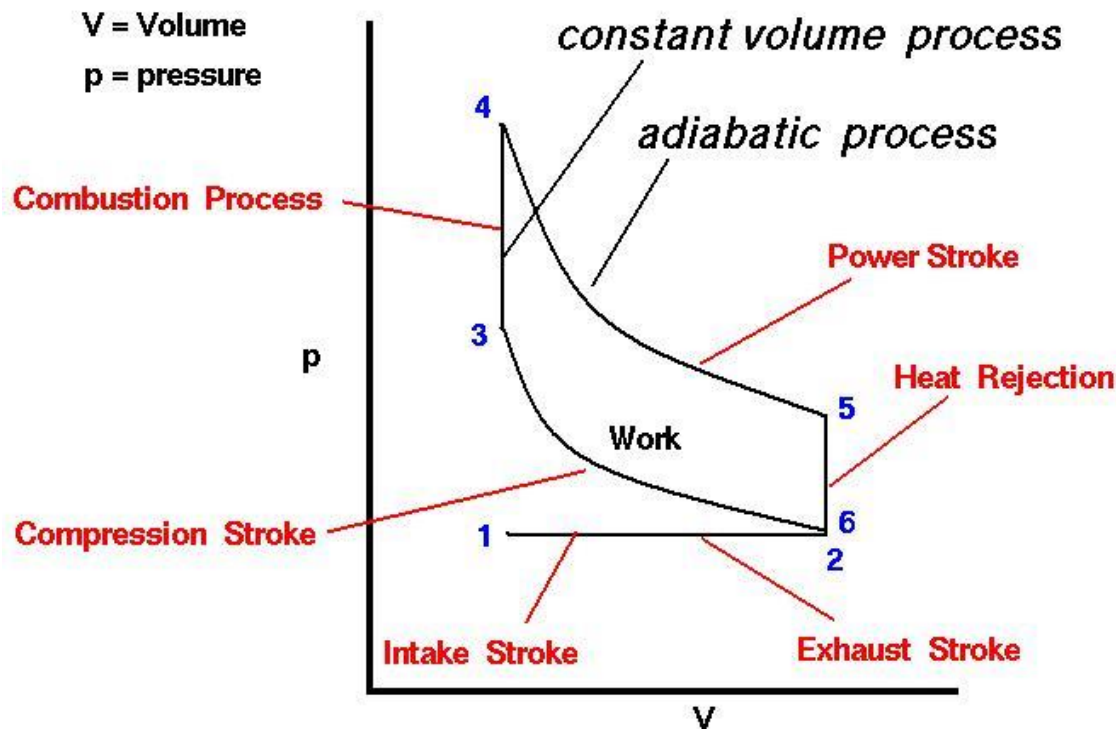
p : pressure
 V : specific volume

Diesel Engine
(compression ignition)

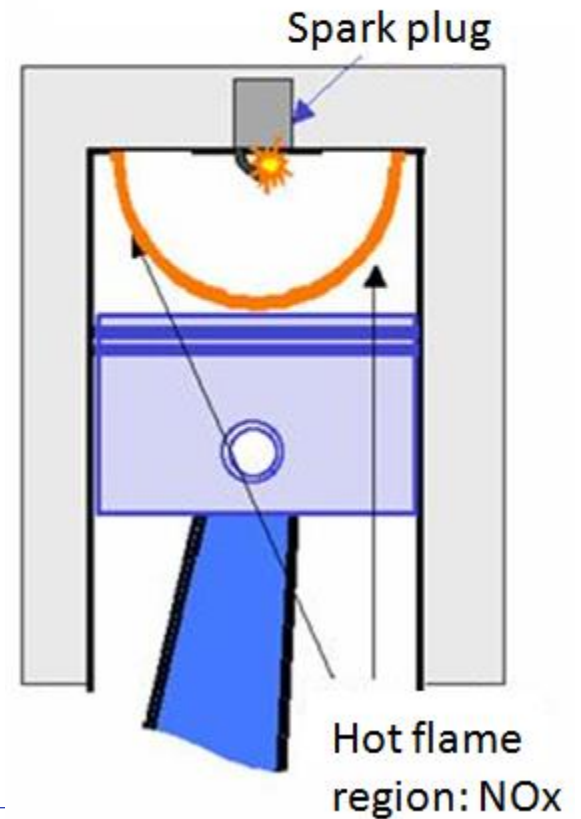


Adiabatic flame temperature = T_{ad}

Constant volume



Gasoline Engine (spark ignition)

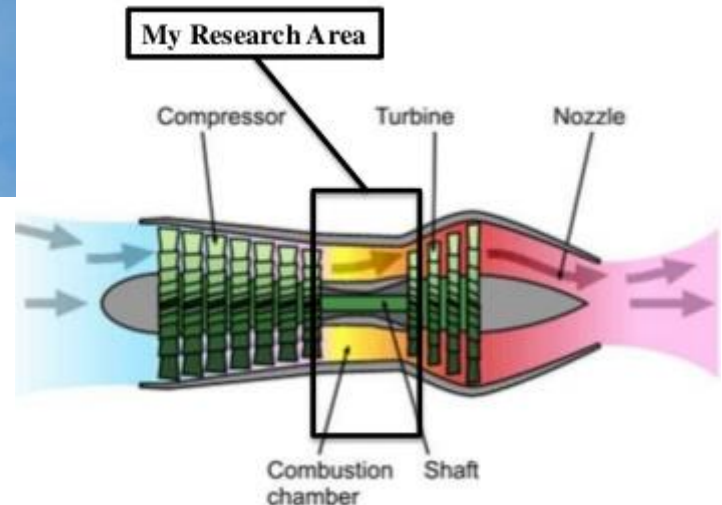


Thermochemistry

P#3 Determine the reference enthalpy of combustion of methane, CH_4 , with air with $\lambda=1$. what is the lower and higher heating value for methane combustion?

Thermochemistry

P#4 A small, low-emission, stationary gas-turbine engine (see Fig. 2.4) operates at full load (3950 kW) at an equivalence ratio of 0.286 with an air flowrate of 15.9 kg/s. The equivalent composition of the fuel (natural gas) is $C_{1.16}H_{4.32}$. Determine the fuel mass flowrate and the operating air–fuel ratio for the engine.



Thermochemistry

P#5 Determine the upper and lower heating values at 298 K of gaseous n-decane, $C_{10}H_{22}$, per mol of fuel and per kg of fuel, and (A/F)_{st} (molar and mass basis). If the enthalpy of vaporization of n-decane is 359 kJ/kg_{fuel} at 298 K, what are the upper and lower heating values of liquid n-decane?

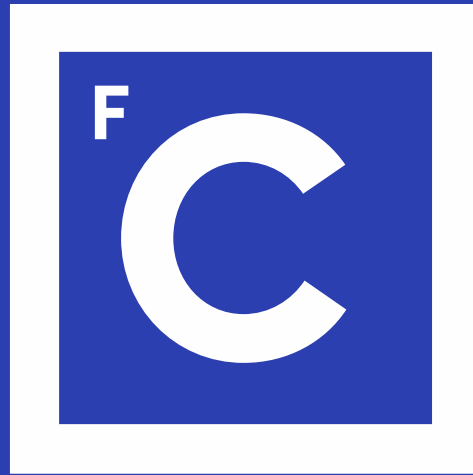
Thermochemistry

P#6 Estimate the constant-pressure adiabatic flame temperature for the combustion of a stoichiometric CH₄-air mixture. The pressure is 1 atm and the initial reactant temperature is 298 K. Make the necessary assumptions.

Thermochemistry

P#7 Estimate the constant-volume adiabatic flame temperature for the combustion of a stoichiometric CH₄-air mixture. The initial pressure is 1 atm and the initial reactant temperature is 298 K. Make the necessary assumptions.

Thanks



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