THE COMPLETE ENERGY BALANCE

$$\frac{d}{dt}\left[m\left(U+\frac{u^2}{2g_c}+\frac{gz}{g_c}\right)\right] = \sum_{inlets}\left(H+\frac{u^2}{2g_c}+\frac{gz}{g_c}\right)^{in}\dot{m}^{in}$$

$$-\sum_{outlets}\left(H+\frac{u^2}{2g_c}+\frac{gz}{g_c}\right)^{out}\dot{m}^{out}+\sum_{surfaces}\underline{\dot{Q}}+\underline{\dot{W}}_{EC}+\underline{\dot{W}}_{S}$$

where $\dot{m}^{in}$ and $\dot{m}^{out}$ are absolute values of the flow rates

THE COMPLETE ENTROPY BALANCE

$$\frac{d\underline{S}}{dt} = \sum_{inlets} S^{in}\dot{m}^{in} - \sum_{outlets} S^{out}\dot{m}^{out} + \sum_{surfaces}\frac{\underline{\dot{Q}}}{T_{sys}} + \dot{S}_{gen}$$

where $\dot{m}^{in}$ and $\dot{m}^{out}$ are absolute values of the flow rates

USEFUL DERIVATIVES

Differential Property		Corresponding Maxwell Relation
$dU =$	$TdS - PdV \quad U(S, V)$	$-(\partial P/\partial S)_V = (\partial T/\partial V)_S$
$dH =$	$TdS + VdP \quad H(S, P)$	$(\partial V/\partial S)_P = (\partial T/\partial P)_S$
$dA =$	$-SdT - PdV \quad A(T, V)$	$(\partial P/\partial T)_V = (\partial S/\partial V)_T$
$dG =$	$-SdT + VdP \quad G(T, P)$	$-(\partial V/\partial T)_P = (\partial S/\partial P)_T$

Other useful derivative relations shown in Chapter 6

$$dS\,(T, P) = C_P/T\ dT - (\partial V/\partial T)_P\ dP \qquad 6.37$$

$$dS\,(T, V) = C_V/T\ dT + (\partial P/\partial T)_V\ dV \qquad 6.38$$

$$dS\,(V, P) = C_P(\partial T/\partial V)_P/T\ dV + C_V(\partial T/\partial P)_V/T\ dP \qquad 6.39$$

$$dH\,(T, P) = C_P\ dT + [V - T(\partial V/\partial T)_P]\ dP \qquad 6.40$$

$$dU\,(T, V) = C_V\ dT + [T(\partial P/\partial T)_V - P]\ dV \qquad 6.41$$

Software and supplementary information is available at http://chethermo.net

UNITS

Mass
1 kg = 1000 g = 0.001 metric ton = 2.20462 lb_m
1 lb_m = 16 oz = 5E-4 ton = 453.59 g = 0.45359 kg

Length
1 m = 100 cm = 1000 mm = 1E6 μm = 1E9 nm = 39.370 in = 3.2808 ft = 1.0936 yd
1 ft = 12 in = 0.30480 m = 30.480 cm
1 in = 2.5400 cm

Volume
1 m^3 = 1000 L = 1E6 cm^3 = 1E6 ml = 35.315 ft^3 = 264.17 gal
1 ft^3 = 1728.0 in^3 = 7.4805 gal = 0.028317 m^3 = 28.317 L = 28317 ml

Force
1 N = 1 kg-m/s^2 = 1E5 dynes = 1E5 g-cm/s^2 = 0.22481 lb_f
1 lb_f = 32.174 lb_m-ft/s^2 = 4.4482 N

Pressure
1 atm = 1.01325E5 N/m^2(Pa) = 1.01325 bar = 760 $mm_{Hg\ at\ 0°C}$ = 33.9 $ft_{H2O\ at\ 4°C}$
1 atm = 14.696 psia
1 bar = 0.1 MPa = 0.98692 atm = 14.504 psia = 750.06 $mm_{Hg\ at\ 0°C}$ = 10.197 $m_{H2O\ at\ 4°C}$

Energy
1 J = 1 N-m = 1 MPa-cm^3 = 1 kgm^2/s^2 = 0.23901 cal = 0.73756 ft-lb_f
1 J = 1E7 ergs = 1E7 g-cm^2/s^2
1 kJ = 0.94781 Btu[see note 1] = 2.7778E-4 kW-h = 0.23901 food calorie

Power
1 W = 1 J/s = 0.2390 cal/s[see note 2] = 0.73756 ft-lb_f/s = 3.4121 Btu/h[see note 1]
1 hp = 550 ft-lb_f/s = 0.70726 Btu/s[see note 1] = 0.74570 kW

Gas Constant, R
= 8.31447 J/mole-K = 8.31447 cm^3-MPa/mole-K = 8.31447 m^3-Pa/mole-K
= 8,314.47 cm^3-kPa/mole-K = 83.1447 cm^3-bar/mole-K = 1.9859 Btu/lbmole-R[see note 1]
= 82.057 cm^3-atm/mole-K = 1.9872 cal/mole-K[see note 2] = 10.731 ft^3-psia/lbmole-R

Gravitational Constants at sea level
g = 9.8066 m/s^2 g/g_c = 9.8066 N/kg g_c = 1 (kg-m/s^2)/N
g = 32.174 ft/s^2 g/g_c = 1 lb_f/lb_m g_c = 32.174 ($1b_m$-ft/s^2)/$1b_f$

Faraday's Constant
F = 96,485 J/V

IUPAC Standard Conditions of Temperature and Pressure
T = 0°C = 273.15 K; P = 0.1 MPa; V(ideal gas) = 22711 cm^3/mole;
ρ(water) = 0.99984 g/cm^3 = 8.3441 lb_m/gal

1. The International Steam Table (IT) BTU.
2. The thermochemical calorie.

PROPERTIES OF SELECTED COMPOUNDS

Heat capacities are values for ***ideal gas at 298 K*** *and should be used for* ***order of magnitude calculations*** *only. See appendices for temperature-dependent formulas and constants.*

ID	Compound	T_c (K)	P_c (MPa)	ω	ρ g/cm^3	*MW*	C_P^{ig}/R	δ (J/cm^3)	α (J/cm^3)	β (J/cm^3)
Aliphatics										
1	METHANE	190.6	4.604	0.011	*0.29*	16	4.30	11.7	0	0
2	ETHANE	305.4	4.880	0.099	*0.43*	30	6.31	13.5	0	0
3	PROPANE	369.8	4.249	0.152	*0.58*	44	8.85	13.1	0	0
4	*n*-BUTANE	425.2	3.797	0.193	*0.60*	58	11.89	13.5	0	0
5	ISOBUTANE	408.1	3.648	0.177	*0.55*	58	11.70	12.5	0	0
7	*n*-PENTANE	469.7	3.369	0.249	0.62	72	14.45	14.3	0	0
8	ISOPENTANE	460.4	3.381	0.228	0.62	72	14.28	13.9	0	0
9	NEOPENTANE	433.8	3.199	0.196	0.60	72	14.62	13.1	0	0
11	*n*-HEXANE	507.4	3.012	0.305	0.66	86	17.21	14.9	0	0
17	*n*-HEPTANE	540.3	2.736	0.349	0.68	100	19.95	15.3	0	0
27	*n*-OCTANE	568.8	2.486	0.396	0.70	114	22.70	15.5	0	0
27	ISOOCTANE	544.0	2.570	0.303	0.70	114	22.50	14.1	0	0
46	*n*-NONANE	595.7	2.306	0.437	0.71	128	25.45	15.6	0	0
56	*n*-DECANE	618.5	2.123	0.484	0.73	142	28.22	15.7	0	0
64	*n*-DODECANE	658.2	1.824	0.575	0.75	170	33.71	15.9	0	0
66	*n*-TETRADECANE	696.9	1.438	0.570	0.76	198	39.22	16.1	0	0
68	*n*-HEXADECANE	720.6	1.419	0.747	0.77	226	44.54	16.2	0	0
Naphthenes										
104	CYCLOPENTANE	511.8	4.502	0.194	0.74	70	9.97	16.5	0	0
105	METHYLCYCLOPENTANE	532.8	3.785	0.230	0.74	84	13.21	16.1	0	0
137	CYCLOHEXANE	553.5	4.075	0.215	0.77	84	12.74	16.8	0	0
138	METHYLCYCLOHEXANE	572.2	3.471	0.235	0.77	98	16.25	16.1	0	0
153	DECALIN(cis)	703.6	3.200	0.279	0.89	138	20.04	17.6	0	0
Olefins and Acetylene										
201	ETHYLENE	282.4	5.032	0.085	*0.43*	28	5.26	13.5	0	0.40
202	PROPYLENE	364.8	4.613	0.142	*0.61*	42	7.69	13.2	0	0.40
207	1-BUTENE	419.6	4.020	0.187	*0.63*	56	10.31	13.7	0	0.40
204	ISOBUTENE	417.9	3.999	0.189	*0.59*	56	10.72	13.7	0	0.40
209	1-PENTENE	464.8	3.529	0.233	0.63	70	13.17	14.5	0	0.24
401	ACETYLENE	308.3	6.139	0.187	*0.50*	28	5.32	*18.68*	0.40	0.40
303	1,3-BUTADIENE	425.4	4.330	0.193	*0.65*	54	9.56	15.6	0	0.70
309	ISOPRENE	484	3.850	0.158	0.68	68	12.78	15.3	0	0.70
Aromatics										
501	BENZENE	562.2	4.898	0.211	0.87	78	9.82	18.7	0.63	2.24
502	TOLUENE	591.8	4.109	0.264	0.86	92	12.49	18.3	0.57	2.23
504	ETHYLBENZENE	617.2	3.609	0.304	0.86	106	15.44	18.0	0.23	1.83
505	*o*-XYLENE	630.4	3.734	0.313	0.88	106	16.03	18.4	0.10	1.80
506	*m*-XYLENE	617.1	3.541	0.326	0.86	106	15.35	18.1	0.19	1.84
507	*p*-XYLENE	616.3	3.511	0.326	0.86	106	15.26	17.9	0.27	1.87
510	CUMENE	631.2	3.209	0.338	0.86	121	18.25	17.4	0.20	2.57
558	BIPHENYL	789.3	3.847	0.366	0.99	154	19.52	19.3	0.50	4.00
563	DIPHENYLMETHANE	768	2.920	0.461	1.00	168	21.87	19.6	0.50	4.00
701	NAPHTHALENE	748.4	4.051	0.302	*0.98*	128	16.03	19.5	0.86	6.87
702	METHYLNAPHTHALENE	772	3.650	0.292	1.02	142	19.08	20.1	0.77	6.13
706	TETRALIN	720.2	3.300	0.286	0.97	132	18.63	19.3	0.60	4.82

ID	Compound	T_c (K)	P_c (MPa)	ω	ρ g/cm^3	MW	C_P^{ig}/R	δ (J/cm^3)	α (J/cm^3)	β (J/cm^3)
Oxygenates										
1101	METHANOL	512.6	8.096	0.566	0.79	32	5.28	29.6	17.43	14.49
1102	ETHANOL	516.4	6.384	0.637	0.79	46	7.88	26.1	12.58	13.29
1102	PROPANOL	536.7	5.170	0.628	0.80	60	10.50	24.5	11.97	10.35
1104	ISOPROPANOL	508.3	4.764	0.669	0.78	60	10.69	23.4	9.23	11.86
1105	1-BUTANOL	562.9	4.412	0.594	0.81	74	13.13	23.4	8.44	11.01
1107	ISOBUTANOL	547.7	4.295	0.589	0.80	74	13.03	22.9	3.99	3.99
1479	THF	501.1	5.190	0.217	0.88	72	16.85	19.0	0.00	10.43
1402	DIETHYL ETHER	466.7	3.590	0.281	0.71	74	13.53	15.4	0.00	6.61
1444	ETHYLENE OXIDE	469	7.100	0.200	*0.89*	44	5.80	21.7	1.17	9.38
1052	METHYL ETHYL KETONE	535.6	4.100	0.329	0.80	72	12.56	18.9	0.00	9.70
Halocarbons										
1601	FREON-12(CCl2F2)	385	4.070	0.176	*1.49*	120.8	8.71	15.0		
2650	FREON-134a(C2H2F4)	374.2	4.06	0.327	*1.37*	102	10.20	16.6		
1504	VINYL CHLORIDE	420	5.68	0.1001	*0.97*	62.4	6.46	17.8	1.10	2.19
1502	METHYL CHLORIDE	416.3	6.590	0.156	*1.01*	50.4	4.90	19.7	3.42	1.14
1521	CHLOROFORM(CHCl3)	536.4	5.400	0.216	1.48	119.2	7.92	18.9	5.80	0.12
1501	CARBON TETRACL(CCl4)	556.4	4.500	0.194	1.58	153.6	10.10	17.5	1.25	0.64
1551	CHLOROBENZENE	632.4	4.460	0.249	1.10	112.4	11.73	19.3	0.00	2.50
Gases										
914	ARGON	150.9	4.898	−0.004	*0.70*	40	2.499	10.8	0	0
922	BROMINE	584.2	10.335	0.119	3.10	160	4.363	23.6	0	0
918	CHLORINE	417.2	7.711	0.069	1.56	71	4.088	20.1	0	0
913	HELIUM-4	5.2	0.228	0.000	*0.12*	4	2.501	*1.22*	0	0
920	KRYPTON	209.4	5.502	0.001	*1.29*	84	2.502	13.1	0	0
919	NEON	44.4	2.653	−0.041	*1.20*	20	2.502	*9.44*	0	0
959	XENON	289.7	5.840	0.012	*2.95*	131	2.502	*15.91*	0	0
912	NITRIC OXIDE	180.2	6.485	0.585	*1.28*	30	3.588	*23.12*	0	0
899	NITROUS OXIDE	309.6	7.245	0.142	*1.22*	44	4.633	*20.31*	0	0
910	SULFUR DIOXIDE	430.8	7.884	0.245	*1.46*	64	4.796	12.3	3.16	3.16
911	SULFUR TRIOXIDE	490.9	8.207	0.422	*1.90*	80	6.111	31.1	0	0
901	OXYGEN	154.6	5.043	0.022	*0.97*	32	3.529	8.2	0	0
902	HYDROGEN	33.3	1.297	−0.215	*0.20*	2	3.507	*2.0*	0	0
905	NITROGEN	126.1	3.394	0.040	*0.88*	28	3.500	5.3	0	0
908	CARBON MONOXIDE	132.9	3.499	0.066	*0.88*	28	3.505	6.3	0	0
909	CARBON DIOXIDE	304.2	7.382	0.228	*1.18*	44	4.456	14.6	1.87	0
Nasty gases										
1922	HYDROGEN SULFIDE	373.5	8.937	0.081	*0.95*	34	4.115	18.0	3.19	3.19
1938	CARBON DISULFIDE	552	7.800	0.115	*1.26*	76	4.109	20.4	0.59	0.33
1904	HYDROGEN CHLORIDE	324.6	8.200	0.120	*1.19*	36.5	3.551	22.0	22.0*	0
1771	HYDROGEN CYANIDE	456.8	5.320	0.407	*0.68*	27	4.330	24.8	3.00	3.00
Miscellaneous compounds										
1051	ACETONE	508.2	4.701	0.306	0.79	58	8.96	19.6	0.00	11.14
1772	ACETONITRILE	545.5	4.833	0.353	0.78	44	6.28	24.1	3.49	8.98
1252	ACETIC ACID	592.7	5.786	0.462	1.04	60	15.01	19.0	24.03	7.50
1911	AMMONIA	406.6	11.270	0.252	0.68	17	4.29	29.2	2.11	8.44
1921	WATER	647.3	22.120	0.344	1.00	18	4.04	47.9	50.13	15.06

References: API Technical Data Book (1988), and Reid, R.C., Prausnitz, J.M., and Sherwood, T.K., The Properties of Liquids and Gases, 3rd Edition, 1977. McGraw-Hill:New York. For a more complete list, see the spreadsheet in props.xlsx or the MATLAB props folder. Italics designate estimated or effective values.