Technical Data Book: Chapter 14 – Combustion

API TECHNICAL REPORT TDB-14
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SCOPE

Technical Report TDB-14 presents a comprehensive analysis of combustion, with an emphasis on the heats of combustion for various fuels such as pure compounds, refinery gases, liquid fuels, and coal. It offers detailed information including data sets, formulas, procedural guidance, and visual charts for quantifying gross and net heats of combustion, determining heat output from combustion processes, and assessing the calorific values of fuels. Additionally, the report features tables detailing the heats of combustion for specific pure compounds, along with classification data related to coal ranks.

Any references to other chapters within this document refer to the corresponding Technical Data Book Chapter which is published as API Technical Report TDB-x, where x is the chapter number.

14-0 Introduction

The heat of combustion of a substance is the heat evolved when that substance is converted to its final oxidation products by means of molecular oxygen. The following reaction represents the complete combustion of a hydrocarbon:

$$C_aH_b + \left(a + \frac{b}{4}\right) O_2 \rightarrow \frac{b}{2} H_2O + a(CO_2)$$

The standard heat of combustion is defined as the change in enthalpy resulting from the combustion of a substance, in the state that is normal at 77 °F and atmospheric pressure, beginning and ending at a temperature of 77 °F. The gross heat of combustion is the same as the standard heat of combustion except that the latter combustion begins and ends at 60 °F rather than 77 °F. The normal state of the water formed by the reaction is liquid in both cases.

The difference between the standard and the gross heats of combustion is the difference between the sensible heat changes of the products and the reactants from 60 °F to 77 °F. This sensible heat difference is usually negligible in comparison with the heats of combustion, so the gross and standard heats of combustion are approximately equal.

The net heat of combustion is the heat evolved in a combustion beginning and ending at 60 °F with products of gaseous water and carbon dioxide. Therefore,

$$\Delta H = Q - c\lambda_{H_2O} \qquad (14\text{-}0.1)$$

where:

ΔH	=	*net heat of combustion in Btu/lb-fuel*
Q	=	*gross heat of combustion in Btu/lb-fuel*
c	=	*pounds of water formed per pound of fuel consumed*
λ_{H_2O}	=	*heat of vaporization of water at 60 °F and at its vapor pressure in Btu/lb-fuel*

Pure Compounds

Net and gross heats of combustion are tabulated for many pure hydrocarbons in Tables 14A1.1 and 14A1.2. Procedure 14A1.3 may be used in determining the heats of combustion for mixed liquid fuels, including synthetic fuels and petroleum fractions.

Inasmuch as combustion reactions proceed with a decrease in enthalpy, the enthalpy change is negative in sign. However, the heat of combustion is defined as the heat evolved; therefore, the values for heat of combustion in this chapter and from the pure component property tables are positive. In all cases, complete combustion (to carbon dioxide) is assumed.

Refinery Gases and Fuel Oils

In most applications, the molecular oxygen necessary for combustion is supplied as air. To ensure complete combustion, excess air is commonly added. The following equation relates the heat available from combustion of a given fuel gas, when the flue gases exit at any temperature, *t*, to the gross heat of combustion and the composition of the flue gas. Excess air increases the negative term on the right-hand side of equation (14-0.2), thereby decreasing the available heat, ($H_t - H_{60}$):

$$(H_t - H_{60}) = Q - \sum_{i=1}^{n} d_i (H_t - H_{60})_i \qquad (14\text{-}0.2)$$

where:

$(H_t - H_{60})$	=	*heat available from combustion when the fuel is charged at 60 °F and the flue gases exit at t °F in Btu/lb-fuel*
$(H_t - H_{60})_i$	=	*total enthalpy change of flue gas component i from 60 °F to t °F in Btu/lb-fuel*
n	=	*total number of components in flue gas*
d_i	=	*pounds of flue gas component i per pound of fuel consumed*

For water, $(H_t - H_{60})_{H2O}$ contains both the sensible heat from 60 °F to *t* °F and the heat of vaporization. Equation (14-0.2) was used to develop Figures 14B1.1 through 14B1.7 for various refinery gases and fuel oils.

Equation (14-0.2) is a statement of the law of Hess: Enthalpy is a function of the state and not of the path used to reach the state. Therefore, the heat available from the combustion of a given fuel that is initially at 60 °F with a given amount of air is a function only of the flue gas temperature (i.e., the final state).

Table14-0.1 – Liquid and Gaseous Fuels

LIQUID FUELS			
Gravity (Degrees API)	**Sulfur (Percent by Weight)**	**Inerts (Percent by Weight)**	**Carbon-to-Hydrogen Weight Ratio**
0	2.95	1.15	8.80
5	2.35	1.00	8.55
10	1.80	0.95	8.06
15	1.35	0.85	7.69
20	1.00	0.75	7.65
25	0.70	0.70	7.17
30	0.40	0.65	6.79
35[a]	0.30	0.60	6.50

GASEOUS FUELS						
Actual Heat of Combustion						
Nominal High [b] Heating Value (Btu/ft^3 at 60°F)	**Gross (Btu/ft^3 at 60°F)**	**Gross (Btu/lb)**	**Net (Btu/lb)**	**Sulfur (Percent by Weight) [c]**	**Inert Gases (Percent by Weight) [d]**	**Molecular Weight of Hydrocarbon Portion**
1,000	1,037	21,800	19,700	4.72	5.38	16.5
1,200	1,248	21,600	--	3.88	4.42	20.4
1,400	1,458	21,500	--	3.32	3.78	24.3
1,600	1,669	21,300	19,400	2.90	3.30	28.2
1,800	1,879	21,000	--	2.52	2.88	32.1
2,000	2,090	20,800	--	2.29	2.61	36.1

a Above 35°API, the correction for impurities in Procedure 14A1.3 is negligible and the equations represent pure paraffins (carbon-to-hydrogen weight ratio is 12.0n/(2n + 2), where n is the number of carbon atoms in the hydrocarbon).

b The nominal high heating value is an approximate gross heat of combustion.

c Equivalent to 2.5 mole percent hydrogen sulfide.

d Equivalent to 1.25 mole percent carbon dioxide and 1.25 mole percent air.

Flue Gases

The enthalpies of common flue gas components are plotted in Figures 14C1.1 and 14C1.2. The enthalpy basis (enthalpy is zero for the ideal gas at 60 °F) is more convenient for combustion calculations than the basis used in the rest of this book. These enthalpies may be used in equation (14-0.2) with Table 14A1.1 heats of combustion to calculate the heat available from combustion as a function of temperature for pure hydrocarbons.

Figures 14B1.1 through 14B1.7 (see Table 14-0.1) were prepared for various liquid and gaseous fuels containing arbitrary amounts of impurities.

Most procedures include corrections to be used when the composition of the fuel differs appreciably from those previously tabulated.

The weight ratio of flue gas to fuel, for refinery gases and fuel oil, can be determined as a function of percent excess air by making a simple material balance. Equating the weight of the fuel minus the inerts plus air to the weight of the flue gas gives the following relation for fuel oil:

$$\frac{lb\ flue\ gas}{1\ lb\ fuel} = \frac{64.1x_{ws}}{32.1} + \frac{44.0(C/H)(1-x_{ws}-x_{wi})}{12.0(C/H+1)} + \frac{18.01(1-x_{ws}-x_{wi})}{2(C/H+1)} + \left[\frac{x_{ws}}{32.1} + \frac{(C/H)(1-x_{ws}-x_{wi})}{12.0(C/H+1)} + \frac{1-x_{ws}-x_{wi}}{4(C/H+1)}\right]\left[\frac{(79)(28.0)}{21} + \frac{(29.0)(\%\ Ex\ Air)}{21}\right] \quad (14\text{-}0.3)$$

where:

x_{ws}	=	*weight fraction of sulfur*
x_{wi}	=	*weight fraction of inerts*
C/H	=	*carbon-to-hydrogen weight ratio*
% Ex Air	=	*mole percent of excess air*

The mole percent of carbon dioxide in the flue gas may be obtained by a similar material balance. The percent carbon dioxide on a water-free basis is given as

$$\%CO_2 = \frac{(C/H)(1-x_{ws}-x_{wi})}{(12.0)(C/H+1)\left\{\begin{array}{l}\left(\frac{x_{ws}}{32.1} + \frac{(C/H)(1-x_{ws}-x_{wi})}{(12.0)(C/H+1)} + \left(\frac{79}{21} + \frac{\%\ Ex\ Air}{21}\right)\right) \\ \left[\frac{x_{ws}}{32.1} + \frac{(C/H)(1-x_{ws}-x_{wi})}{(12.0)(C/H+1)} + \frac{(1-x_{ws}-x_{wi})}{4(C/H+1)}\right]\end{array}\right\}} \quad (14\text{-}0.4)$$

For refinery gases, calculations normally account for the fact that inert gases (in this case, carbon dioxide, oxygen and nitrogen) appear in the flue gas. Equations (14-0.3) and (14-0.4) are based on data given by Maxwell (4) and assume average impurities as given in Table 14-0.1.

Coal

ASTM D 388 (1) gives the heating value ranges for the various grades of coal as reproduced in Table 14-0.2.

Procedure 14D1.1 is used to compute the gross and net calorific values of coal. These heating values are a function of the ultimate analysis and moisture percentage of the coal.

Table 14-0.2 – Classification of Coal by Rank

Class	Group	Agglomerating Character [a]	Fixed Carbon Limits% [b]		Volatile Matter Limits % [b]		Gross Calorific Value Limits Btu/lb [c]	
			≥	<	>	≤	≥	<
Anthracitic	Meta-anthracite	N	98	-	-	2	-	-
	Anthracite	N	92	98	2	8	-	-
	Semianthracite[d]	N	86	92	8	14	-	-
Bituminous	Low-volatile bituminous	CA [e]	78	86	14	22	-	-
	Medium-volatile bituminous	CA [e]	69	78	22	31	-	-
	High-volatile A bituminous	CA [e]	-	69	31	-	14,000 [f]	-
	High-volatile B bituminous	CA [e]	-	-	-	-	13,000 [f]	14,000
	High-volatile C bituminous	CA [e]	-	-	-	-	11,500	13,000
		A	-	-	-	-	10,500	11,500
Subbituminous	Subbituminous A	N	-	-	-	-	10,500	11,500
	Subbituminous B	N	-	-	-	-	9,500	10,500
	Subbituminous C	N	-	-	-	-	8,300	9,500
Lignitic	Lignite A	N	-	-	-	-	6,300	8,300
	Lignite B	N	-	-	-	-	-	6,300

a. A = agglomerating
CA = commonly agglomerating
N = non-agglomerating.

b. Dry, mineral-matter-free basis.

c. Moist, mineral-matter-free basis, moist referring to coal containing its natural inherent moisture but not including visible water on the surface of the coal

d. If agglomerating, classify in low-volatile group of the bituminous class.

e. It is recognized that there may be non-agglomerating varieties in these groups of the bituminous class, and there are notable exceptions in the high-volatile C bituminous group.

f. Coals having 69 percent or more fixed carbon on the dry, mineral-matter-free basis are classified according to fixed carbon, regardless of calorific value.

Note: This table is adapted and republished by permission of ASTM from ASTM D 388, "Standard Classification of Coals by Rank," 1983 Annual Book of ASTM Standards, Volume 05.05. This classification does not include a few coals, principally nonbanded varieties that have unusual physical and chemical properties and come within the limits of fixed carbon or calorific value of the high-volatile bituminous and subbituminous ranks. All of these coals either contain less than 48 percent dry, mineral-matter-free fixed carbon or have more than 15,500 Btu/lb on the moist, mineral-matter- free basis.

Computer Methods

Procedure	Description
14A1.3	Heats of Combustion of Petroleum Fractions and Synthetic Fuels
14D1.1	Gross/Net Calorific Value of Coals

14A Heats of Combustion

Table 14A1.1 – Heats of Combustion of Pure Compounds (Btu/lb)

Compound	Gross Heat of Combustion at 60°F (Btu/lb) $-\Delta H_{c,60}$	Net Heat of Combustion at 60°F (Btu/lb) $-\Delta H_{c,60}$	Standard Heat of Combustion at 77°F (Btu/lb) $-\Delta H_{c,77}$
Nonhydrocarbons			
hydrogen (gas)	60,847	51,427	60,782
carbon monoxide (gas)	4,347	4,347	4,344
ammonia (gas)	8,831	1,155	8,818
hydrogen sulfide (gas)	7,091	6,533	7,087
carbonyl sulfide (gas)	3,923	3,923	3,924
carbon disulfide	6,075	6,075	6,077
sulfur dioxide (gas)	954	954	954
Paraffins			
methane (gas)	23,884	21,511	23,860
ethane (gas)	22,323	20,425	22,304
propane (gas)	21,643	19,917	21,625
n-butane (gas)	21,293	19,655	21,276
2-methylpropane (gas)	21,231	19,594	21,214
n-pentane	20,916	19,333	20,902
2-methylbutane	20,883	19,301	20,870
2.2-dimethylpropane (gas)	20,949	19,367	20,933
n-hexane	20,774	19,229	20,761
2-methylpentane	20,744	19,198	20,730
3-methylpentane	20,750	19,205	20,737
2,2-dimethylbutane	20,705	19,159	20,691
n-heptane	20,673	19,153	20,660
2-methylhexane	20,647	19,128	20,634
3-methylhexane	20,662	19,142	20,649
2,4-dimethylpentane	20,626	19,107	20,613
n-octane	20,593	19,094	20,580
2-methylheptane	20,577	19,078	20,564
2,2-dimethylhexane	20,547	19,047	20,534
2.2.4-trimethylpentane	20,558	19,059	20,545
n-nonane	20,536	19,052	20,524
n-decane	20,487	19,016	20,475
n-undecane	20,447	18,986	20,435
n-dodecane	20,415	18,962	20,403
n-tridecane	20,387	18,942	20,375
n-tetradecane	20,365	18,926	20,353
n-pentadecane	20,344	18,911	20,333
n-hexadecane	20,326	18,897	20,314
n-heptadecane	20,314	18,889	20,300
n-octadecane	20,194	18,773	20,181
n-nonadecane	20,212	18,795	20,200
n-eicosane	20,169	18,755	20,157

Table 14A1.1 – Heats of Combustion of Pure Compounds (Btu/lb) (Continued)

Compound	Gross Heat of Combustion at 60°F (Btu/lb) $-\Delta H_{c,60}$	Net Heat of Combustion at 60°F (Btu/lb) $-\Delta H_{c,60}$	Standard Heat of Combustion at 77°F (Btu/lb) $-\Delta H_{c,77}$
Napthenes			
cyclopentane	20,182	18,825	20,169
methylcyclopentane	20,121	18,764	20,108
ethylcyclopentane	20,609	19,253	20,597
1,1-dimethylcyclopentane	20,077	18,721	20,065
cis-1,2-dimethylcyclopentane	20,102	18,745	20,090
trans-1,2 dimethylcyclopentane	20,074	18,717	20,062
cis-1,3-dimethylcyclopentane	20,081	18,724	20,069
trans-1,3-dimethylcyclopentane	20,086	18,729	20,074
n-propylcyclopentane	20,100	18,743	20,088
n-butylcyclopentane	20,039	18,682	20,027
n-pentylcyclopentane	20,097	18,740	20,085
n-hexylcyclopentane	20,094	18,737	20,082
n-heptylcyclopentane	20,092	18,736	20,081
n-octylcyclopentane	20,090	18,734	20,079
n-nonylcyclopentane	20,089	18,733	20,078
n-decylcyclopentane	20,089	18,733	20,078
n-undecylcyclopentane	20,088	18,731	20,076
n-dodecylcyclopentane	20,087	18,731	20,076
n-tridecylcyclopentane	20,087	18,730	20,076
n-tetradecylcyclopentane	20,086	18,730	20,075
n-pentadecylcyclopentane	20,086	18,729	20,074
cyclohexane	20,028	18,672	20,016
methylcyclohexane	19,989	18,632	19,977
ethylcyclohexane	20,012	18,656	20,000
1,1-dimethylcyclohexane	19,987	18,630	19,975
cis-1.2-dimethylcyclohexane	20,013	1 8,657	20,001
trans-1,2-dimethylcyclohexane	19,988	1 8,632	19,976
cis-1,3-dimethylcyclohexane	19,970	18,614	19,958
trans1,3-dimethylcyclohexane	19,998	18,641	19,986
cis-1,4-dimethylcyclohexane	19,998	18,642	19,986
trans-1,4-dimethylcyclohexane	19,973	18,616	19,961
n-propylcyclohexane	20,014	18,658	20,002
n-butylcyclohexane	20,020	18,663	20,008
n-pentylcyclohexane	20,027	18,670	20,015
n-hexylcyclohexane	20,031	18,675	20,019
n-heptylcyclohexane	20,034	18,678	20,022
n-octylcyclohexane	20,037	18,680	20,025
n-nonylcyclohexane	20,040	18,683	20,028
n-decylcyclohexane	20,025	18,668	20,013
n-undecylcyclohexane	20,036	18,679	20,024
n-dodecylcyclohexane	20,047	18,690	20,036
n-tridecylcyclohexane	20,049	18,692	20,037
n-tetradecylcyclohexane	20,050	18,694	20,039

Table 14A1.1 – Heats of Combustion of Pure Compounds (Btu/lb) (Continued)

Compound	Gross Heat of Combustion at 60°F (Btu/lb) $-\Delta H_{c,60}$	Net Heat of Combustion at 60°F (Btu/lb) $-\Delta H_{c,60}$	Standard Heat of Combustion at 77°F (Btu/lb) $-\Delta H_{c,77}$
Olefins			
ethene (gas)	21,636	20,279	21,622
propene (gas)	21,030	19,673	21,016
1-butene (gas)	20,823	19,467	20,809
2-butene (gas)	20,771	19,414	20,757
trans-2-butene (gas)	20,743	19,386	20,729
2-methylpropene (gas)	20,696	19,340	20,683
1-pentene	20,538	19,182	20,527
1-hexene	20,454	19,097	20,443
2,3-dimethyl-2-butene	20,308	18,951	20,297
1-heptene	20,394	1 9,037	20,383
1-octene	20,349	18,992	20,338
1-nonene	20,317	18,960	20,306
1-decene	20,282	18,925	20,271
1-undecene	20,264	18,908	20,253
1-dodecene	20,249	18,892	20,238
1-tridecene	20,234	18,878	20,223
1-tetradecene	20,221	18,864	20,210
1-pentadecene	20,212	18,855	20,201
1-hexadecene	20,200	18,843	20,189
1-heptadecene	20,197	18,841	20,186
1-octadecene	20,188	18,832	20,177
1-nonadecene	20,176	18,820	20,165
1-eicosene	20,115	18,759	20,104
Diolefins and Acetylenes			
propadiene (gas)	20,853	19,902	20,844
1,2-butadiene (gas)	20,621	19,566	20,611
1,3-butadiene (gas)	20,199	19,144	20,189
ethyne (acetylene) (gas)	21,482	20,751	21,477
propyne (gas)	20,792	19,842	20,784
1-butyne (gas)	20,644	19,589	20,634
Aromatics			
benzene	17,985	17,254	17,980
methylbenzene	18,245	17,419	18,239
ethylbenzene	18,487	17,591	18,480
1.2-dimethylbenzene	18,438	17,542	18,431
1,3-dimethylbenzene	18,434	17,538	18,427
1,4-dimethylbenzene	18,439	17,543	18,432
n-propylbenzene	18,666	17,716	18,659
isopropyl benzene	18,659	17,709	18,651
1-methyl-2-ethylbenzene	18,641	17,691	18,633
1-methyl-3-elhylbenzene	18,635	17,685	18,627

Table 14A1.1 – Heats of Combustion of Pure Compounds (Btu/lb) (Continued)

Compound	Gross Heat of Combustion at 60°F (Btu/lb) $-\Delta H_{c,60}$	Net Heat of Combustion at 60°F (Btu/lb) $-\Delta H_{c,60}$	Standard Heat of Combustion at 77°F (Btu/lb) $-\Delta H_{c,77}$
Aromatics			
1-methyl-4-ethylbenzene	18,628	17,678	18,620
1.2.3-trimethylbenzene	18,600	17,650	18,593
1,2,4-trimethylbenzene	18,588	17,638	18,581
1,3,5-trimethylbenzene	18,578	17,628	18,570
n-butylbenzene	18,813	17,821	18,805
n-pentylbenzene	18,936	17,909	18,928
n-hexylbenzene	19,028	17,972	19,019
n-heptylbenzene	19,106	18,027	19,097
n-octylbenzene	19,177	18,077	19,167
n-nonylbenzene	19,234	18,116	19,225
n-decylbenzene	19,288	18,155	19,279
n-undecylbenzene	19,333	18,186	19,323
n-dodecylbenzene	19,378	18,220	19,368
n-tridecylbenzene	19,417	18,248	19,407
n-tetradecylbenzene	19,453	18,275	19,443

Table 14A1.2 – Heats of Combustion of Pure Compounds (Btu/ft^3)

Compound	Gross Heat of Combustion at 60°F (Btu/ft^3) $-\Delta H_{c,60}$	Net Heat of Combustion at 60°F (Btu/ft^3) $-\Delta H_{c,60}$
hydrogen	323.9	273.7
carbon monoxide	320.8	320.8
ammonia	396.3	321.1
hydrogen sulfide	636.8	586.7
carbonyl sulfide	621.1	621.1
carbon disulfide	1218.8	1218.8
sulfur dioxide	161.0	161.0
methane	1009.5	909.2
ethane	1768.8	1618.4
propane	2515.0	2314.4
n-butane	3260.9	3010.2
2-methylpropane	3251.4	3000.7
n-pentane	3976.5	3675.6
2-methylbutane	3970.3	3669.5
2,2-dimethylpropane	3982.8	3682.0
n-hexane	4717.6	4366.6
n-heptane	5458.2	5057.1
n-octane	6198.5	5747.2
cyclopentane	3729.5	3478.8
methylcyclopentane	4462.1	4161.2
ethylcyclopentane	5332.3	4981.3
n-propylcyclopentane	5943.6	5542.5
cyclohexane	4441.6	4140.7
methylcyclohexane	5171.8	4820.8
ethylcyclohexane	5917.7	5516.6
ethene	1599.2	1498.9
propene	2331.8	2181.4
1-butene	3078.8	2878.2
cis-2-butene	3071.0	2870.5
trans-2-butene	3066.9	2866.3
2-methylpropene	3060.0	2859.4
1-pentene	3795.4	3544.7
1-hexene	4535.9	4235.1
1-heptene	5276.6	4925.6
1-octene	6017.3	5616.1
propadiene	2201.2	2100.9
1,2-butadiene	2939.1	2788.7
1,3-butadiene	2879.0	2728.6
ethyne	1474.0	1423.9
propyne	2194.8	2094.5
1-butyne	2942.4	2791.9
benzene	3701.8	3551.4
methylbenzene	4429.7	4229.1
1,2-dimethylbenzene	5158.3	4907.6
1,3-dirnethylbenzene	5157.2	4906.5
1,4-dimethylbenzene	5158.6	4907.9

Procedure 14A1.3 – Heats of Combustion of Petroleum Fractions and Synthetic Fuels

Discussion

This procedure was last updated in 1983. The following equation is used to predict the gross heat of combustion of petroleum fractions and synthetic fuels:

$$-\Delta H^*_{c,60} = 17{,}672 + 66.6\,API - 0.316\,API^2 - 0.0014\,API^3 \qquad (14A1.3\text{-}1)$$

where:

$-\Delta H^*_{c,60}$ = *gross heat of combustion at 60 °F, in Btu/lb*

API = *API gravity*

If water is present in the fuel or if impurities are significantly different from those given in the Table 14-0.1, the following equation is used to correct for it:

$$-\Delta H_{c,60} = \left(-\Delta H^*_{c,60}\right) - 0.01\left(-\Delta H^*_{c,60}\right)(\%\,H_2O + \%S_e + \%\,inerts_e) + 40.5(\%\,S_e) \qquad (14A1.3\text{-}2)$$

where:

$-\Delta H_{c,60}$ = *corrected gross heat of combustion, in Btu/lb*

% H_2O = *weight percent of water in the fuel*

% S_e = *weight percent of sulfur in the fuel minus the average weight percent (given in Table 14-0.1)*

% $inerts_e$ = *weight percent of inerts in the fuel minus the average weight percent (given in Table 14-0.1)*

The net heat of combustion is obtained from equation (14A1.3-3).

$$-\Delta H^*_{c,60}\,(net) = 16{,}796 + 54.5\,API - 0.217\,API^2 - 0.0019\,API^3 \qquad (14A1.3\text{-}3)$$

where:

$-\Delta H^*_{c,60}\,(net)$ = *heat of combustion at 60 °F, in Btu/lb.*

$$-\Delta H_{c,60}\,(net) = \left[-\Delta H^*_{c,60}\,(net)\right] - 0.01\left[-\Delta H^*_{c,60}\,(net)\right](\%H_2O + \%S_e + \%\,Inerts_e) + 40.5\,(\%\,S_e) - 10.53\,(\%\,H_2O) \qquad (14A1.3\text{-}4)$$

where:

$-\Delta H_{c,60}$ *(net)* = *corrected net heat of combustion at 60 °F, in Btu/lb*

Procedure

Step 1: *Obtain the API gravity,impurities, and moisture weight percent of the petroleum fraction or synthetic fuel.*

Step 2: Use equations (14A1.3-1) and (14A1.3-2) to calculate the gross heat of combustion.

Step 3: Calculate the net heat of combustion from equations (14A1.3-3) and (14A1.3-4).

Comments on Procedure 14A1.3

Purpose

Procedure 14A1.3 is a method to estimate heats of combustion of petroleum liquids and synthetic fuels.

Reliability

Gross heats of combustion estimated by this procedure have an average error of 180 Btu/lb-fuel. An average deviation of 205 Btu/lb-fuel was obtained for predicted net heat of combustion values.

Literature Sources

Equations (14A1.3-1) and (14A1.3-3) were developed using the figure given in Maxwell (4). Equations (14A1.3-2) and (14A1.3-4) were given reference (2).

Example

Determine the gross and net heats of combustion of an 11.3 °API fuel oil that contains 1.49 weight percent sulfur, 1.67 weight percent inerts and 0.30 weight percent water.

The average percent of sulfur in an 11.3 °API fuel on which equations (14A1.3-1) and (14A1.3-3) are based is 1.68 by interpolation from Table 14-0.1, so
% S_e = 1.49 - 1.68 = – 0.19. Similarly, the average inerts content for the basis fuel is 0.92, so % inerts_e =1.67 – 0.92 = 0.75.

The gross heat of combustion can now be calculated from equations (14A1.3-1) and (14A1.3-2).

$$-\Delta H^*_{c,60} = 17{,}672 + 66.6(11.3) - 0.316(11.3)^2 - 0.0014(11.3)^3$$
$$= 18{,}382$$
$$-\Delta H_{c,60} = 18{,}382 - (0.01)(18{,}382)(0.3 - 0.19 + 0.75) + 40.5(-0.19)$$
$$= 18{,}216 \text{ Btu/lb-fuel}$$

An experimental value is 18,088 Btu/lb-fuel.

From equations (14A1.3-3) and (14A1.3-4), the net heat of combustion is

$$-\Delta H^*_{c,60}\,(net) = 16{,}796 + 54.5(11.3) - 0.217(11.3)^2 - 0.0019(11.3)^3$$
$$= 17{,}381$$
$$-\Delta H_{c,60}\,(net) = 17{,}381 - 0.01(17{,}381)(0.30 - 0.19 + 0.75) + 40.5(-0.19) - 10.53(0.30)$$
$$= 17{,}221 \text{ Btu/lb-fuel}$$

An experimental value is 17,128 Btu/lb-fuel.

14B Heat Available from Combustion of Refinery Gases and Liquid Fuels

Figure 14B1.1 – Heat Available from Combustion: 1000 Btu/ft^3 Refinery Gas

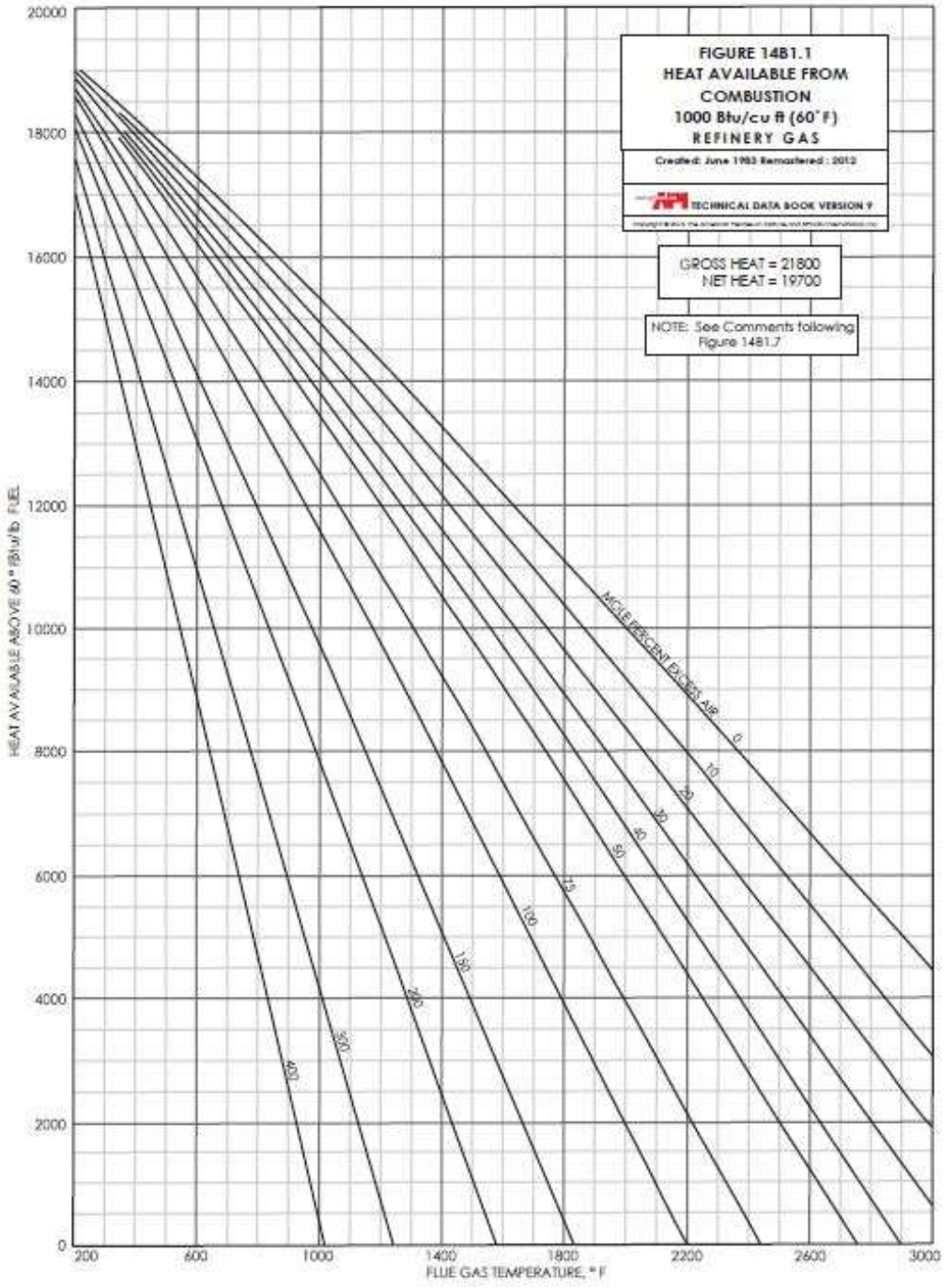


Figure 14B1.2 – Heat Available from Combustion: 1600 Btu/ft^3 Refinery Gas

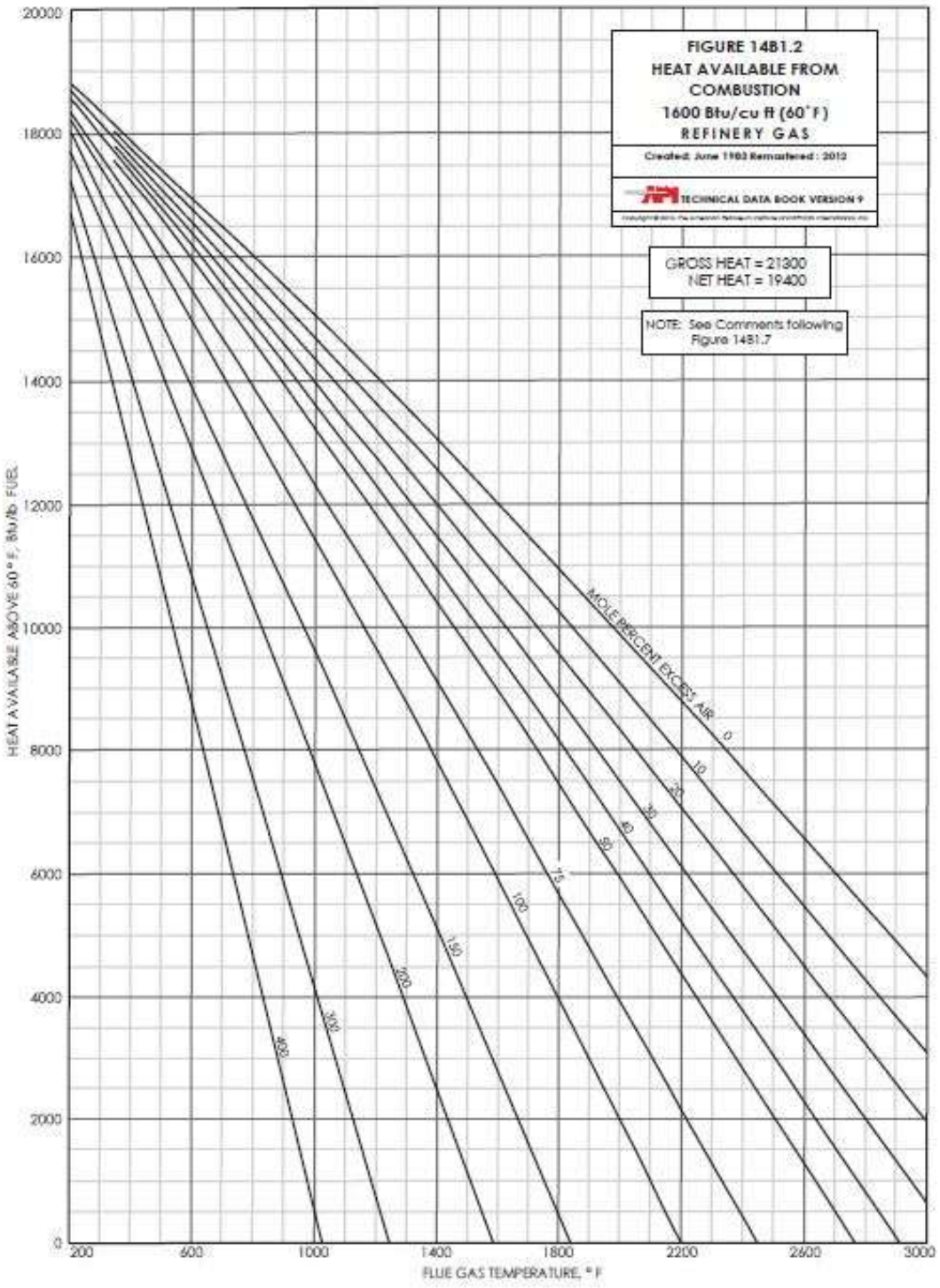


Figure 14B1.3 – Heat Available from Combustion: 0 API Fuel Oil

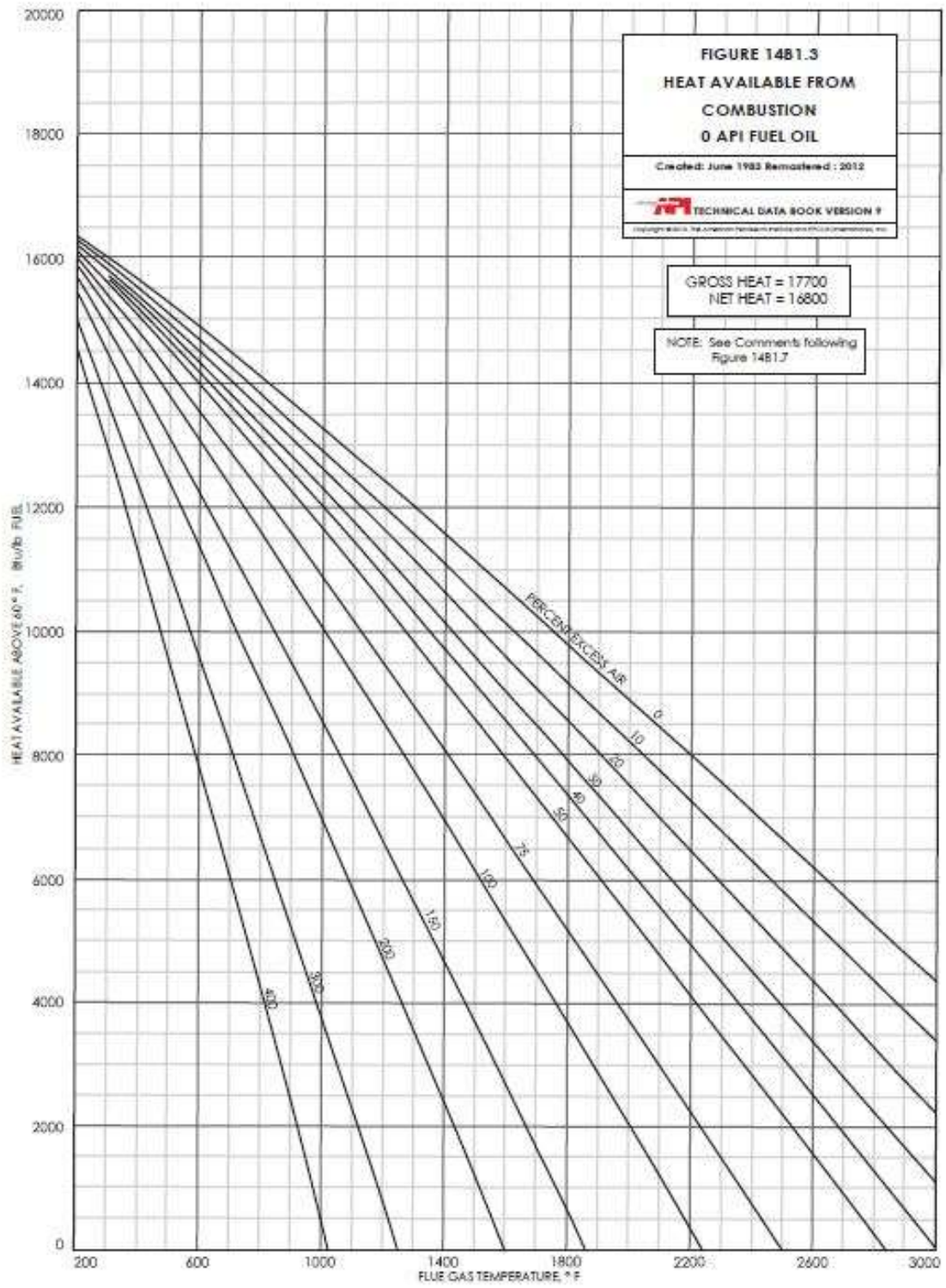


Figure 14B1.4 – Heat Available from Combustion: 5 API Fuel Oil

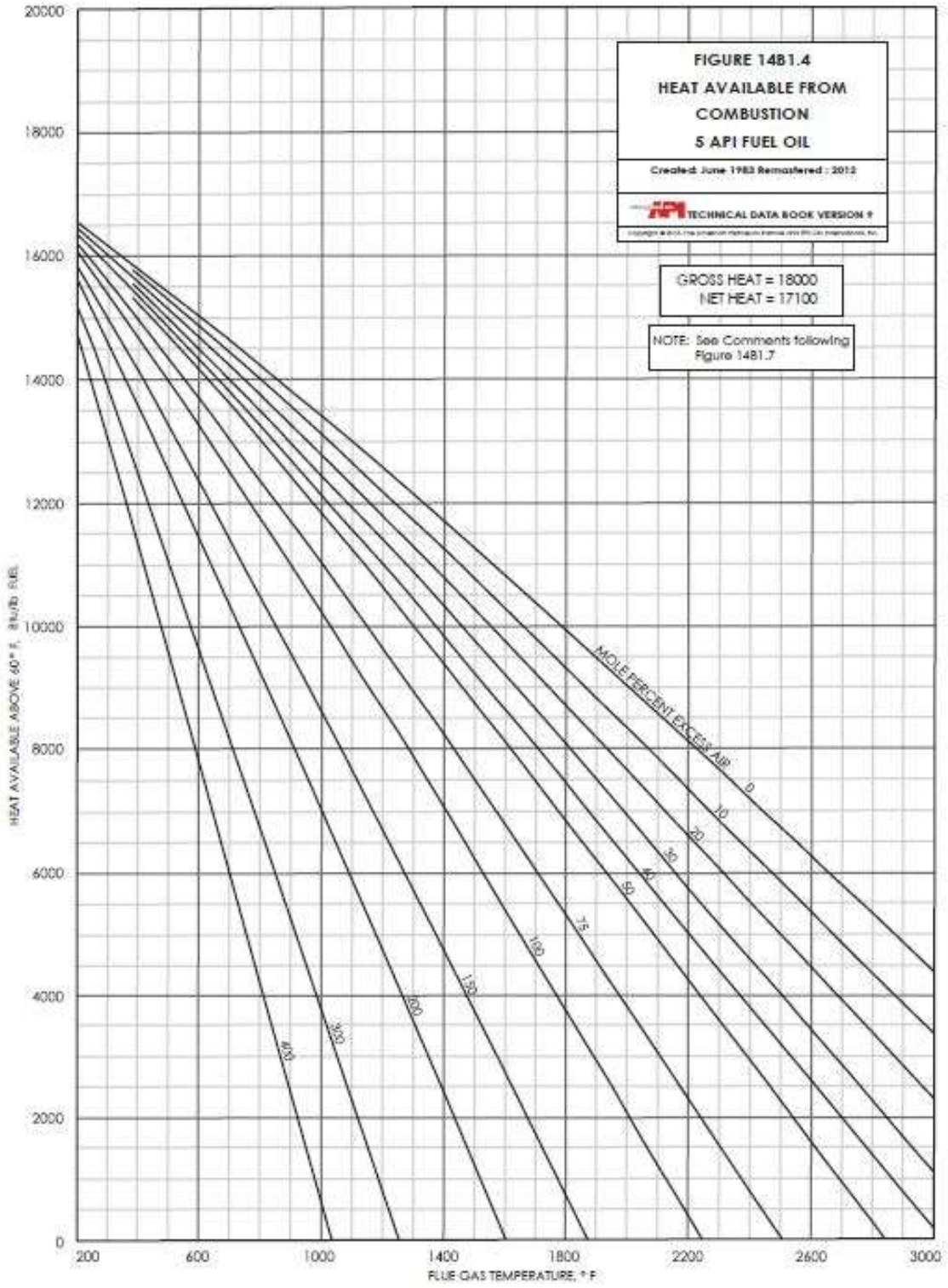


Figure 14B1.5 – Heat Available from Combustion: 10 API Fuel Oil

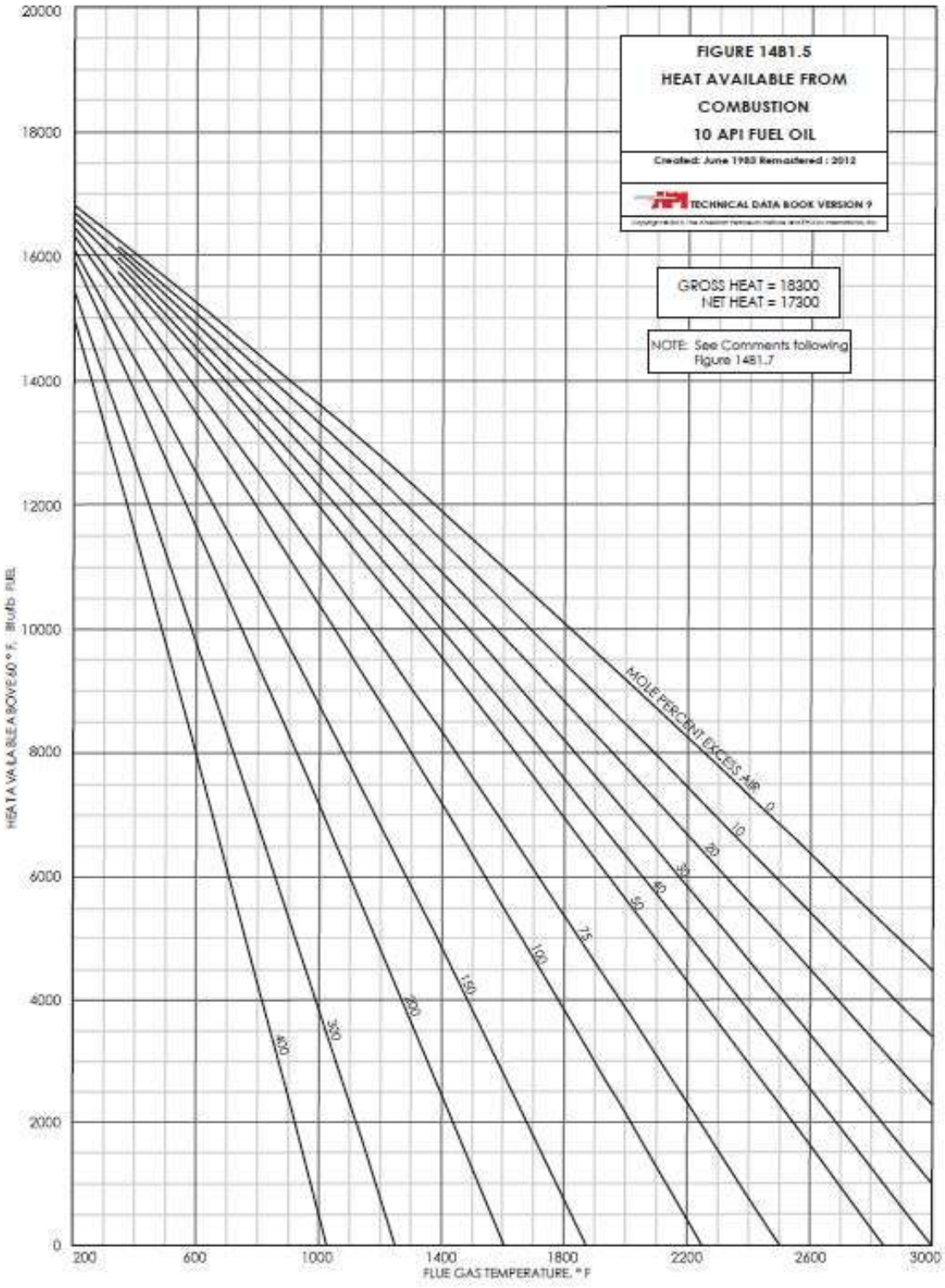


Figure 14B1.6 – Heat Available from Combustion: 15 API Fuel Oil

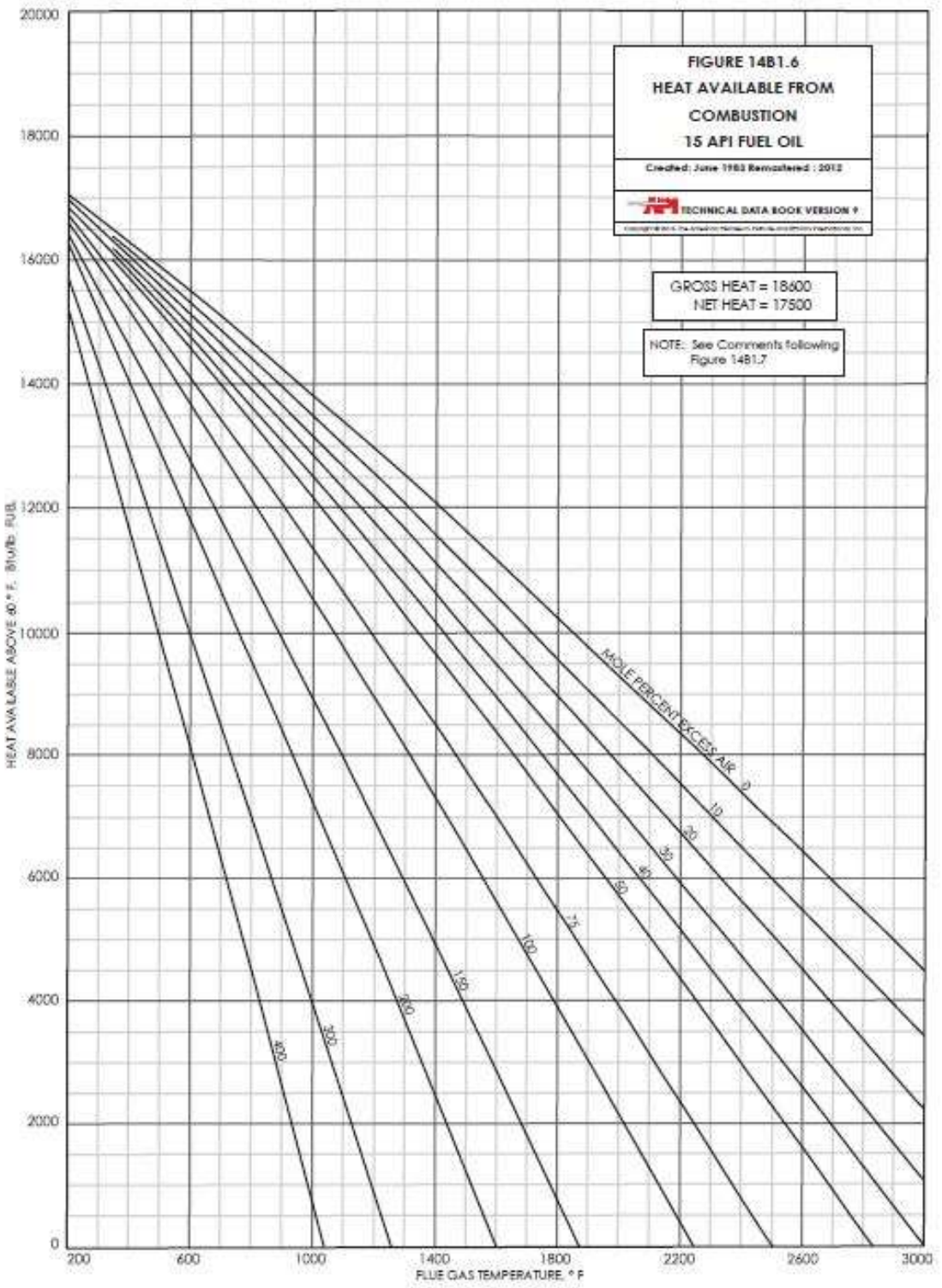
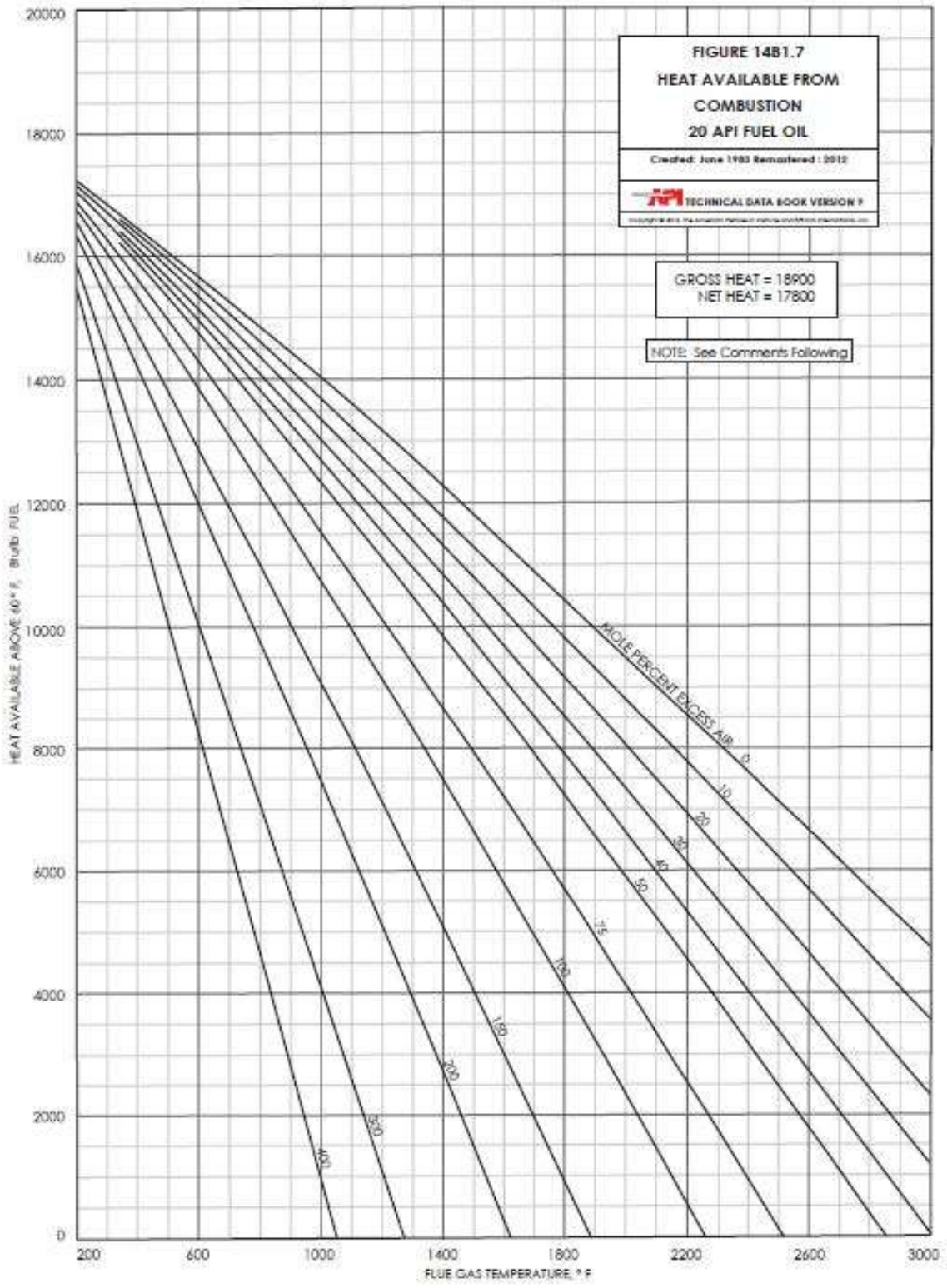


Figure 14B1.7 – Heat Available from Combustion: 20 API Fuel Oil



Comments on Figures 14B1.1 through 14B1.7

Purpose

The heat available from the combustion of refinery gases and fuel oils to gaseous products is given in Figures 14B1.1 through 14B1.7 as a function of the flue gas temperature and percent excess air.

Limitations

An allowance was made for an average sulfur and inerts content in the fuel, but not for the presence of water.

Reliability

The estimated average deviation of these figures is 1 percent for the fuels defined in the Introduction.

Special Comments

Figures 14B1.1 and 14B1.2 were derived using only mixtures of paraffin gases. The figure more nearly corresponding to the gross heat of combustion of the fuel gas can be used without interpolation with very little error. In correcting for the variation in impurities, however, the available heat needs to be adjusted in proportion to the weight percentage of the hydrocarbon present in the fuel gas. When hydrogen sulfide is present, consider half of the reported quantity is hydrocarbon (i.e., a source of heat) and the other half as an inert gas (see Example).

Figures 14B1.3 through 14B1.7 represent the heat available from fuel oils having API gravities of 0, 5, 10, 15, and 20 °API. If the impurities are known to be appreciably different from the average values, then the available heat may be corrected in direct proportion to the weight percentage of the hydrocarbon present in the fuel, with sulfur considered an inert material. The average impurities used to develop the figures are tabulated in the Introduction.

Interpolation between the figures is not necessary. The available heat at any flue gas temperature and percent of excess air can be read from the chart, which most nearly corresponds to the API gravity of the fuel oil.

Literature Source

These charts were patterned after those of Maxwell (4). The figures were updated to be consistent with the more recent enthalpy data in Chapter 7.

Example

Estimate the heat available from the combustion of a refinery gas having a gross heat of combustion of 1200 Btu/ft^3 (60 °F) with 100 percent excess air. The fuel contains the following impurities: 8.0 percent by weight hydrogen sulfide and 12.0 percent by weight inert gases. The flue gases exit at 2000 °F.

1200 Btu/ft^3 (60 °F) is closer to 1000 than 1600, therefore, Figure 14B1.1 is recommended. Because the amount of impurities is significantly larger than the average values, it is recommended that the heat available be corrected. From Figure 14B1.1, the uncorrected heat available is 1950 Btu/lb-fuel for the average fuel containing 8.3 percent total hydrogen sulfide and inert gases (or 91.7% hydrocarbons) from Table 14-0.1. For the example refinery gas, half the hydrogen sulfide, or 4 percent by weight, needs to be considered inert gases. Therefore, the total amount of impurities is 4 + 12 = 16 percent by weight.

Total heat available = (1950) (100 – 16) / (100 – 8.3) = 1786 Btu/lb-fuel.

14C Enthalpy of Flue Gas Components

Figure 14C1.1 – Enthalpy of Flue Gas Components at Low Pressures: H2O CO CO2 SO3

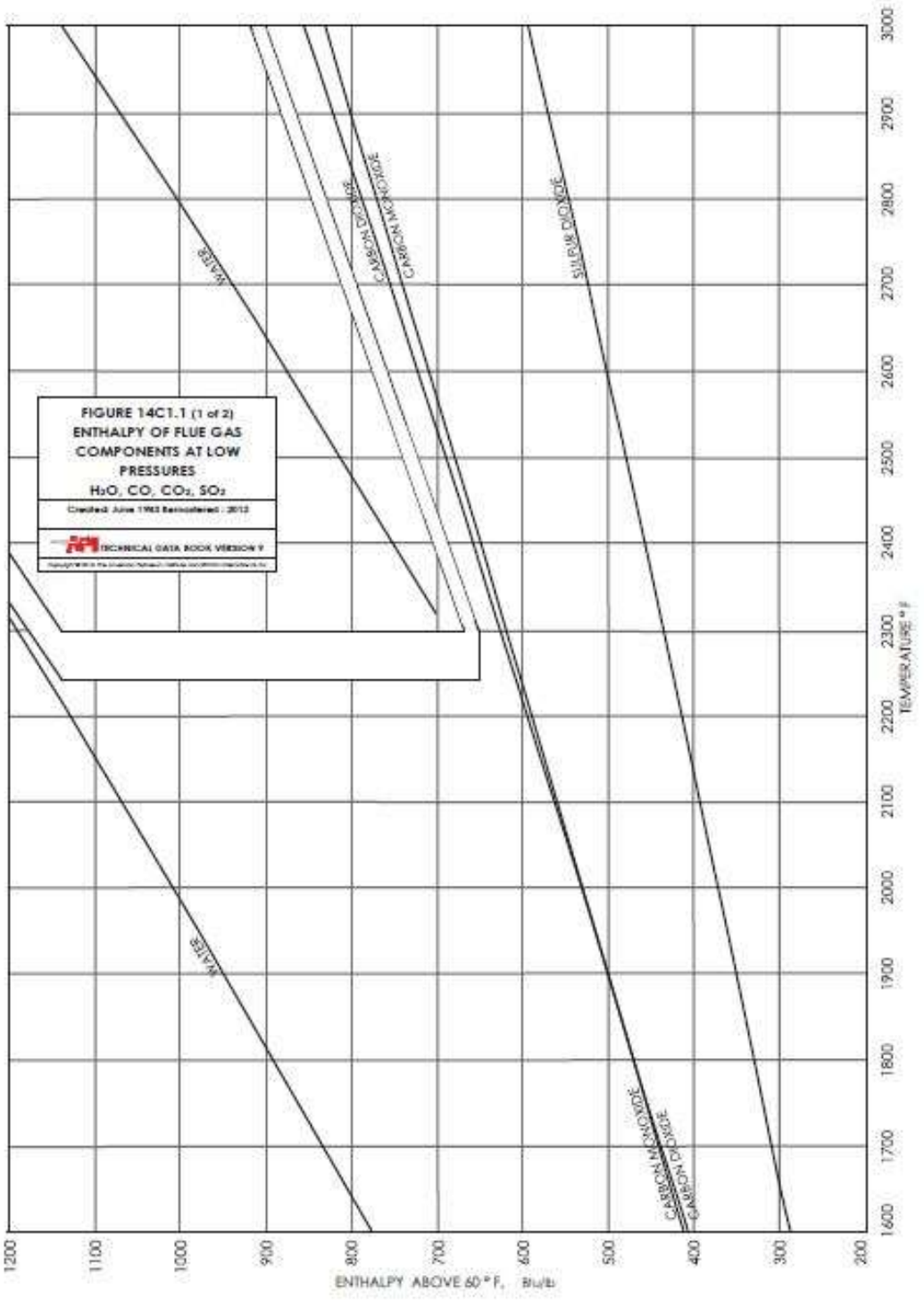


Figure 14C1.1 (Continued)

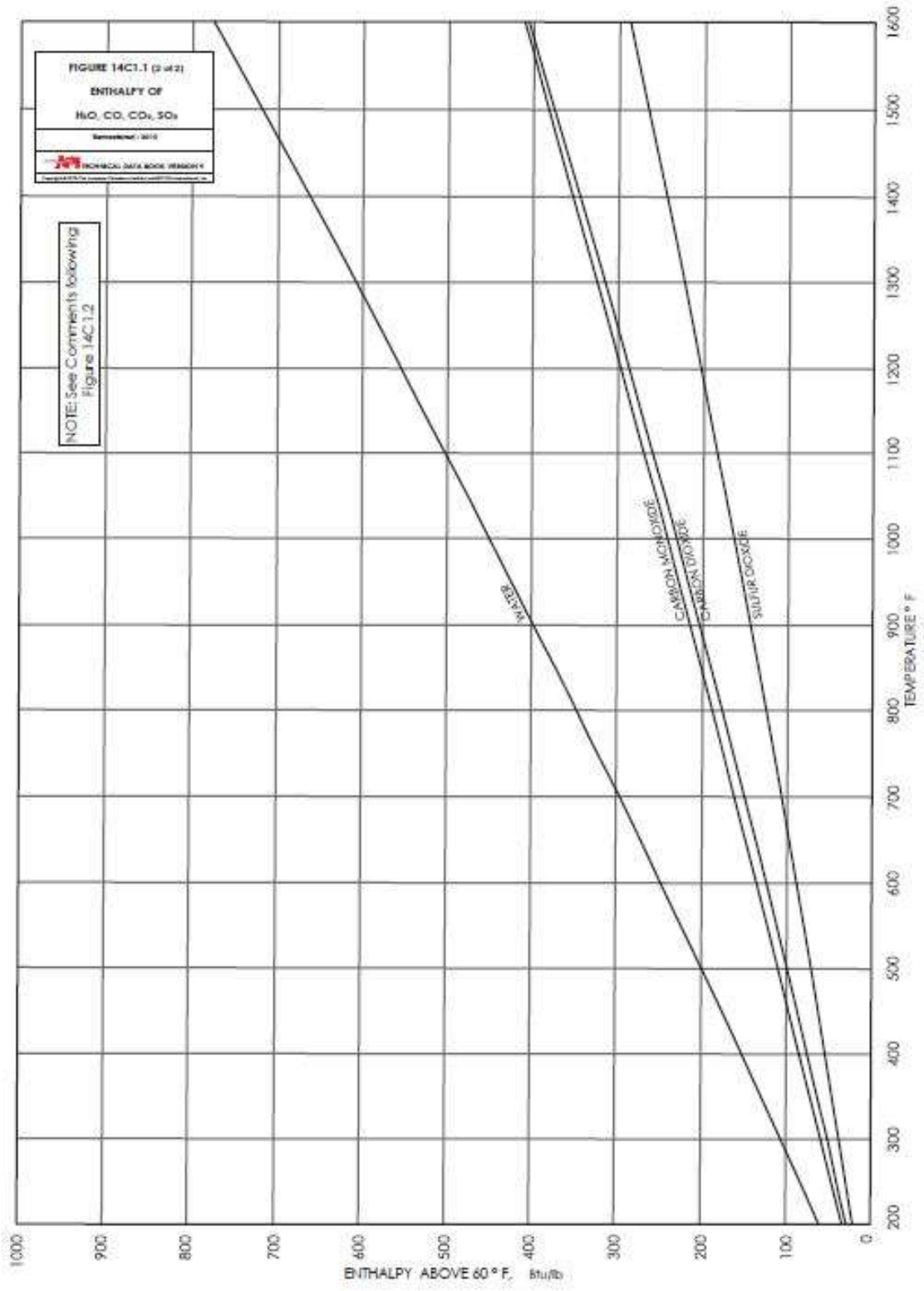


Figure 14C1.2 – Enthalpy of Flue Gas Components at Low Pressures: Air O2 N2

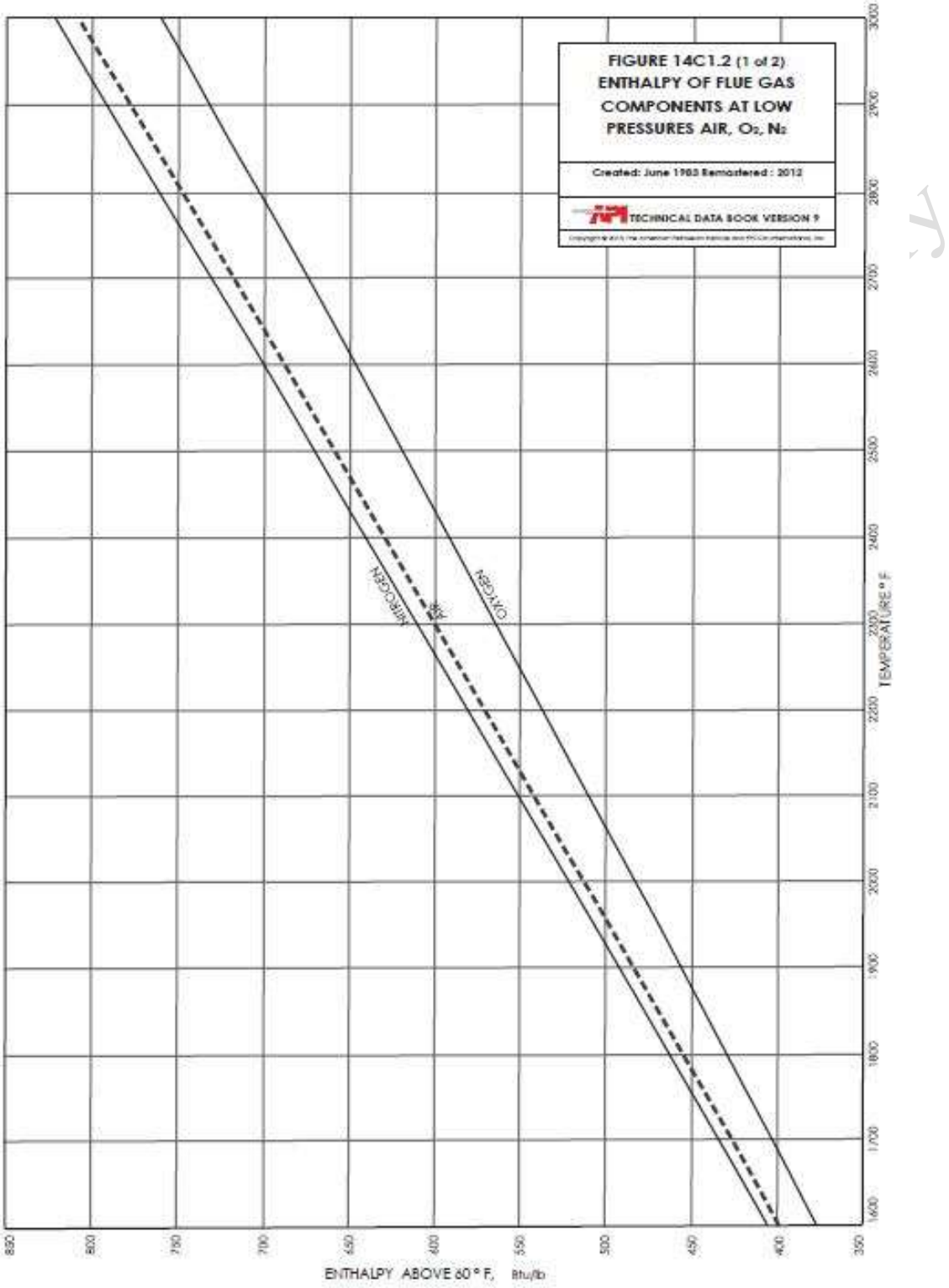
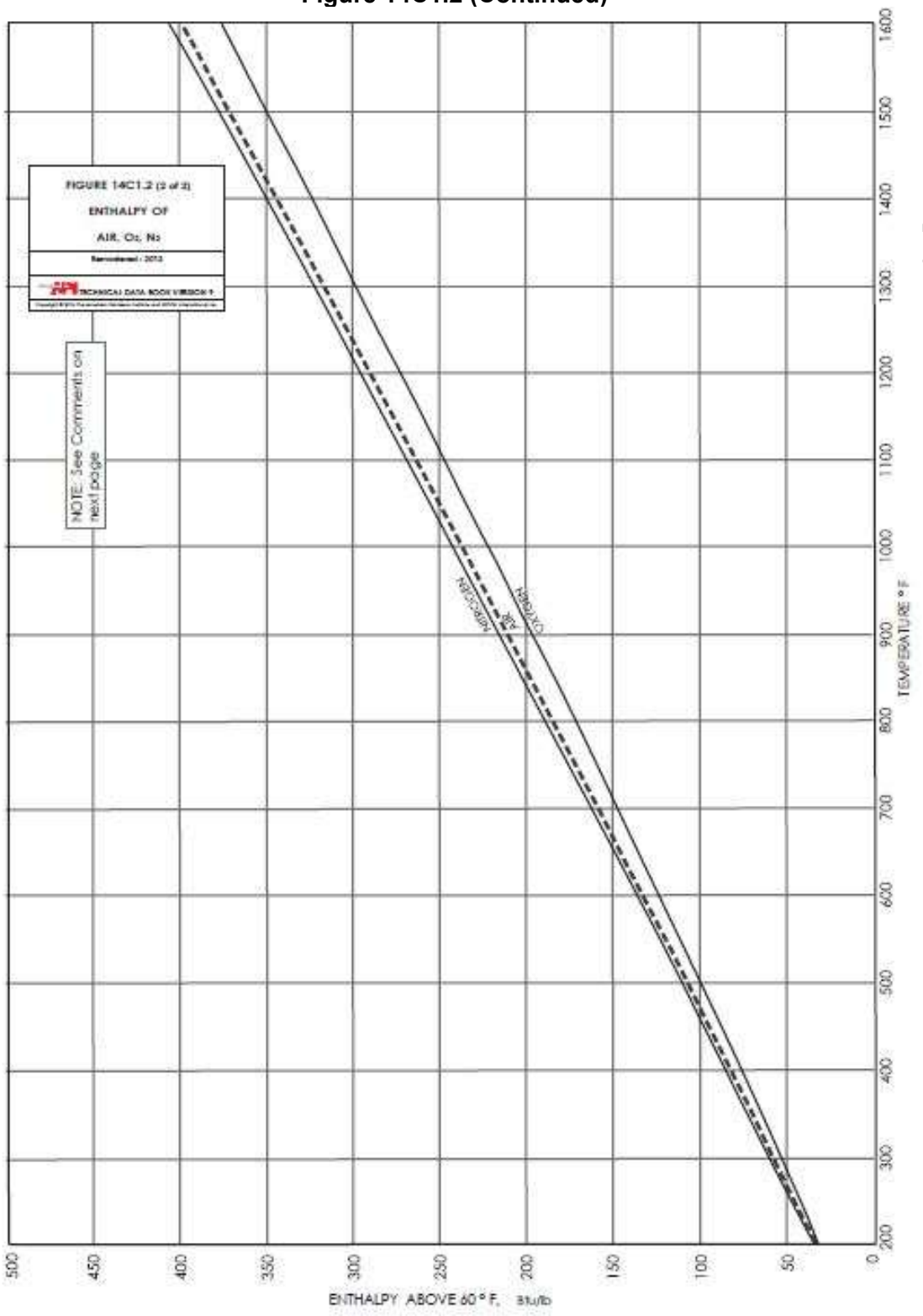


Figure 14C1.2 (Continued)



Comments of Figures 14C1.1 and 14C1.2

Purpose

The enthalpy above 60 °F for various flue gas components is plotted as a function of temperature. The enthalpy values are for low-pressure gases only (less than 50 psia).

Reliability

The estimated average deviation of these figures is 1 percent.

Special Comments

To prepare the figures, the ideal gas enthalpies given in Chapter 7 were converted to a basis of zero for the ideal gas at 60 °F. This basis is preferable for combustion calculations because standard heats of combustion are normally given at these conditions. The curve for air was obtained by assuming a composition of 21 percent by volume oxygen and 79 percent by volume nitrogen. No correction has been made for dissociation of the molecules at high temperatures.

Literature Source

The figures were plotted using the ideal gas enthalpy data given in Chapter 7.

14D Gross/Net Calorific Value of Solid Fuels

Procedure 14D1.1 – Gross/Net Calorific Value of Coals

Discussion

This procedure was last updated in 1983. The following equation is used to estimate the gross calorific value of coal:

$$Q_v = 146.58C + 568.78H + 29.4S - 6.58A - 51.53(O + N) \quad \textit{(14D1.1-1)}$$

where:

Q_v	=	*gross calorific value at constant volume, Btu/lb on a dry basis*
C	=	*weight percent of carbon*
H	=	*weight percent of hydrogen*
S	=	*weight percent of total sulfur*
A	=	*weight percent of ash*
(O + N)	=	*weight percent of oxygen plus nitrogen by difference*

The weight percents are on a dry basis.

The gross calorific value at constant pressure is obtained from the equation (14D1.1-2).

$$Q_p = Q_v + 2.6H - 0.33(O) \quad \textit{(14D1.1-2)}$$

where:

Q_p	=	*gross calorific value at constant pressure*

Equation (14D1.1-3) is used to calculate the net or low calorific value at constant pressure.

$$Q_p(net) = Q_v - 92.2H - 0.33(O) - 10.50M \quad \textit{(14D1.1-3)}$$

where:

Q_p *(net)*	=	*net calorific value at constant pressure*
M	=	*percent moisture in the coal*

Q_v, H, O are on a moist basis.

Procedure

Step 1: *Obtain the ultimate analysis and percent moisture of the coal.*

Step 2: *Use equation (14D1.1-1) or (14D1.1-2) to calculate the gross calorific value.*

Step 3: *Calculate the net calorific value from equations (14D1.1-1) and (14D1.1-3).*

Comments on Procedure 14D1.1

Purpose

This procedure may be used to predict the gross and net calorific value of a coal given the ultimate analysis and percent moisture of the coal.

Reliability

Gross caloric values estimated by this procedure have an average error of 115 Btu/lb.

Literature Source

Equations (14D1.1-1) through (14D1.1-3) were given in reference (3).

Example

Calculate the gross calorific value of an Illinois No. 6 coal with the following composition given on a dry basis:

carbon	=	*68.92%*
hydrogen	=	*5.01%*
nitrogen	=	*1.01%*
sulfur	=	*6.66%*
ash	=	*10.84%*
oxygen	=	*7.56% (by difference)*

From equation (14D1.1-1)

$$Q_v = 146.58(68.92) + 568.78(5.01) + 29.4(6.66) - 6.58(10.84) - 51.53(7.56 + 1.01)$$

= 12,635 Btu/lb

$$Q_p = 12{,}635 + 2.6(5.01) - 0.33(7.56)$$

= 12,646 Btu/lb

The experimental value is 12,773 Btu/lb.

Bibliography

1. ASTM D 388, “Standard Classification of Coals by Rank,” 1983 Annual Book of ASTM Standards, Volume 05.05.
2. Foster Wheeler Corporation, Standard Design Data (1960).
3. Institute of Gas Technology, Coal Conversion Systems Technical Data Book, U.S. Department of Energy (extant 1978).
4. Maxwell, J. B., Data Book on Hydrocarbons, D. Van Nostrand Co., Inc., Princeton, N.J. (1950).