



Designation: D3588 – 98 (Reapproved 2017)^{ε1}

Standard Practice for Calculating Heat Value, Compressibility Factor, and Relative Density of Gaseous Fuels¹

This standard is issued under the fixed designation D3588; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ϵ) indicates an editorial change since the last revision or reapproval.

^{ε1} NOTE—Note 2 was editorially corrected in April 2020.

1. Scope

1.1 This practice covers procedures for calculating heating value, relative density, and compressibility factor at base conditions (14.696 psia and 60°F (15.6°C)) for natural gas mixtures from compositional analysis.² It applies to all common types of utility gaseous fuels, for example, dry natural gas, reformed gas, oil gas (both high and low Btu), propane-air, carbureted water gas, coke oven gas, and retort coal gas, for which suitable methods of analysis as described in Section 6 are available. Calculation procedures for other base conditions are given.

1.2 The values stated in inch-pound units are to be regarded as the standard. The SI units given in parentheses are for information only.

1.3 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

1.4 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.*

¹ This practice is under the jurisdiction of ASTM Committee D03 on Gaseous Fuels and is the direct responsibility of Subcommittee D03.03 on Determination of Heating Value and Relative Density of Gaseous Fuels.

Current edition approved April 1, 2017. Published April 2017. Originally approved in 1998. Last previous edition approved in 2011 as D3588 – 98(2011). DOI: 10.1520/D3588-98R17E01.

² A more rigorous calculation of $Z(T,P)$ at both base conditions and higher pressures can be made using the calculation procedures in “Compressibility and Super Compressibility for Natural Gas and Other Hydrocarbon Gases,” American Gas Association Transmission Measurement Committee Report 8, AGA Cat. No. XQ1285, 1985, AGA, 1515 Wilson Blvd., Arlington, VA 22209.

2. Referenced Documents

2.1 ASTM Standards:³

D1717 Test Method for Test for Analysis of Commercial Butane-Butene Mixtures and Isobutylene by Gas Chromatography (Withdrawn 1984)⁴

D1945 Test Method for Analysis of Natural Gas by Gas Chromatography

D1946 Practice for Analysis of Reformed Gas by Gas Chromatography

D2163 Test Method for Determination of Hydrocarbons in Liquefied Petroleum (LP) Gases and Propane/Propene Mixtures by Gas Chromatography

D2650 Test Method for Chemical Composition of Gases by Mass Spectrometry

2.2 GPA Standards:

GPA 2145 Physical Constants for the Paraffin Hydrocarbons and Other Components in Natural Gas⁵

GPA Standard 2166 Methods of Obtaining Natural Gas Samples for Analysis by Gas Chromatography⁵

GPA 2172 Calculation of Gross Heating Value, Relative Density, and Compressibility Factor for Natural Gas Mixtures from Compositional Analysis^{5,6}

GPA Standard 2261 Method of Analysis for Natural Gas and Similar Gaseous Mixtures by Gas Chromatography⁵

³ For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

⁴ The last approved version of this historical standard is referenced on www.astm.org.

⁵ Available from Gas Processors Association (GPA), 6526 E. 60th St., Tulsa, OK 74145, <http://www.gasprocessors.com>.

⁶ The sole source of supply of the program in either BASIC or FORTRAN suitable for running on computers known to the committee at this time is the Gas Processors Association. If you are aware of alternative suppliers, please provide this information to ASTM International Headquarters. Your comments will receive careful consideration at a meeting of the responsible technical committee¹, which you may attend.

GPA Technical Publication TP-17 Table of Physical Properties of Hydrocarbons for Extended Analysis of Natural Gases⁵

GPSA Data Book, Fig. 23-2, Physical Constants⁵

2.3 TRC Document:

TRC Thermodynamic Tables—Hydrocarbons⁷

2.4 ANSI Standard:

ANSI Z 132.1-1969: Base Conditions of Pressure and Temperature for the Volumetric Measurement of Natural Gas^{8,9}

3. Terminology

3.1 Definitions:

3.1.1 *British thermal unit*—the defined International Tables British thermal unit (Btu).

3.1.1.1 *Discussion*—The defining relationships are:

$$1 \text{ Btu} \cdot \text{lb}^{-1} = 2.326 \text{ J} \cdot \text{g}^{-1} \text{ (exact)}$$

$$1 \text{ lb} = 453.592 \text{ 37 g (exact)}$$

By these relationships, 1 Btu = 1 055.055 852 62 J (exact). For most purposes, the value (rounded) 1 Btu = 1055.056 J is adequate.

3.1.2 *compressibility factor* (z)—the ratio of the actual volume of a given mass of gas at a specified temperature and pressure to its volume calculated from the ideal gas law under the same conditions.

3.1.3 *gross heating value*—the amount of energy transferred as heat from the complete, ideal combustion of the gas with air, at standard temperature, in which all the water formed by the reaction condenses to liquid. The values for the pure gases appear in GPA Standard 2145, which is revised annually. If the gross heating value has a volumetric rather than a mass or molar basis, a base pressure must also be specified.

3.1.4 *net heating value*—the amount of energy transferred as heat from the total, ideal combustion of the gas at standard temperature in which all the water formed by the reaction remains in the vapor state. Condensation of any “spectator” water does not contribute to the net heating value. If the net heating value has a volumetric rather than a mass or molar basis, a base pressure must also be specified.

3.1.5 *relative density*—the ratio of the density of the gaseous fuel, under observed conditions of temperature and pressure, to the density of dry air (of normal carbon dioxide content) at the same temperature and pressure.

3.1.6 *standard cubic foot of gas*—the amount of gas that occupies 1 ft³ (0.028 m³) at a temperature of 60°F (15.6°C) under a given base pressure and either saturated with water vapor (wet) or free of water vapor (dry) as specified (see ANSI Z 132.1). In this practice, calculations have been made at 14.696 psia and 60°F (15.6°C), because the yearly update of GPA 2145 by the Thermodynamics Research Center, on which these calculations are based, are given for this base pressure.

⁷ Available from Thermodynamics Research Center, The Texas A&M University, College Station, TX 77843-3111.

⁸ Available from American National Standards Institute (ANSI), 25 W. 43rd St., 4th Floor, New York, NY 10036, <http://www.ansi.org>.

⁹ Supporting data have been filed at ASTM International Headquarters and may be obtained by requesting Research Report RR:D03-1007.

Conversions to other base conditions should be made at the end of the calculation to reduce roundoff errors.

3.1.7 *standard temperature (USA)*—60°F (15.6°C).

3.2 *Symbols:*

3.2.1 *Nomenclature:*

3.2.1.1 B —second virial coefficient for gas mixture

3.2.1.2 $\sqrt{\beta_{ij}}$ —summation factor for calculating real gas correction (alternate method)

3.2.1.3 (cor)—corrected for water content

3.2.1.4 (dry)—value on water-free basis

3.2.1.5 d —density for gas relative to the density of air.

3.2.1.6 d^{id} —ideal relative density or relative molar mass, that is, molar mass of gas relative to molar mass of air

3.2.1.7 G^{id} —molar mass ratio

3.2.1.8 H_m^{id} —gross heating value per unit mass

3.2.1.9 H_v^{id} —gross heating value per unit volume

3.2.1.10 H_n^{id} —gross heating value per unit mole

3.2.1.11 h_m^{id} —net heating value per unit mass

3.2.1.12 h_v^{id} —net heating value per unit volume

3.2.1.13 h_n^{id} —net heating value per unit mole

3.2.1.14 a, b, c—in Eq 1, integers required to balance the equation: C, carbon; H, hydrogen; S, sulfur; O, oxygen

3.2.1.15 (*id*)—ideal gas state

3.2.1.16 (*l*)—liquid phase

3.2.1.17 M —molar mass

3.2.1.18 m —mass flow rate

3.2.1.19 n —number of components

3.2.1.20 P —pressure in absolute units (psia)

3.2.1.21 Q^{id} —ideal energy per unit time released as heat upon combustion

3.2.1.22 R —gas constant, 10.7316 psia.ft³/(lb mol•R) in this practice (based upon $R = 8.314 \text{ 48 J}/(\text{mol} \cdot \text{K})$)

3.2.1.23 (sat)—denotes saturation value

3.2.1.24 T —absolute temperature, °R = °F + 459.67 or $K = °C + 273.15$

3.2.1.25 (T , P)—value dependent upon temperature and pressure

3.2.1.26 V —gas volumetric flow rate

3.2.1.27 x —mole fraction

3.2.1.28 Z —gas compressibility factor repeatability of property

3.2.1.29 δ —repeatability of property

3.2.1.30 ρ —density in mass per unit volume

3.2.1.31 $\sum_{j=1}^n$ —property summed for Components 1 through n , where n represents the total number of components in the mixture

3.2.2 *Superscripts:*

3.2.2.1 *id*—ideal gas value

3.2.2.2 *l*—liquid

3.2.2.3 σ —value at saturation (vapor pressure)

3.2.2.4 '—reproducibility

3.2.3 *Subscripts:*

3.2.3.1 *a*—value for air

3.2.3.2 *a*—relative number of atoms of carbon in Eq 1

- 3.2.3.3 *b*—relative number of atoms of hydrogen in Eq 1
- 3.2.3.4 *c*—relative number of atoms of sulfur in Eq 1
- 3.2.3.5 *j*—property for component *j*
- 3.2.3.6 *ii*—non-ideal gas property for component *i*
- 3.2.3.7 *ij*—non-ideal gas property for mixture of *i* and *j*
- 3.2.3.8 *jj*—non-ideal gas property for component *j*
- 3.2.3.9 *w*—value for water
- 3.2.3.10 1—property for Component 1
- 3.2.3.11 2—property for Component 2

4. Summary of Practice

4.1 The ideal gas heating value and ideal gas relative density at base conditions (14.696 psia and 60°F (5.6°C)) are calculated from the molar composition and the respective ideal gas values for the components; these values are then adjusted by means of a calculated compressibility factor.

5. Significance and Use

5.1 The heating value is a measure of the suitability of a pure gas or a gas mixture for use as a fuel; it indicates the amount of energy that can be obtained as heat by burning a unit of gas. For use as heating agents, the relative merits of gases from different sources and having different compositions can be compared readily on the basis of their heating values. Therefore, the heating value is used as a parameter for determining the price of gas in custody transfer. It is also an essential factor in calculating the efficiencies of energy conversion devices such as gas-fired turbines. The heating values of a gas depend not only upon the temperature and pressure, but also upon the degree of saturation with water vapor. However, some calorimetric methods for measuring heating values are based upon the gas being saturated with water at the specified conditions.

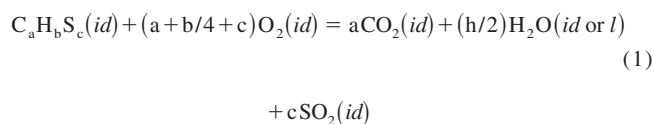
5.2 The relative density (specific gravity) of a gas quantifies the density of the gas as compared with that of air under the same conditions.

6. Methods of Analysis

6.1 Determine the molar composition of the gas in accordance with any ASTM or GPA method that yields the complete composition, exclusive of water, but including all other components present in amounts of 0.1 % or more, in terms of components or groups of components listed in Table 1. At least 98 % of the sample must be reported as individual components (that is, not more than a total of 2 % reported as groups of components such as butanes, pentanes, hexanes, butenes, and so forth). Any group used must be one of those listed in Table 1 for which average values appear. The following test methods are applicable to this practice when appropriate for the sample under test: Test Methods D1717, D1945, D2163, and D2650.

7. Calculation—Ideal Gas Values; Ideal Heating Value

7.1 An ideal combustion reaction in general terms for fuel and air in the ideal gas state is:



where *id* denotes the ideal gas state and *l* denotes liquid phase. The ideal net heating value results when all the water remains in the ideal gas state. The ideal gross heating value results when all the water formed by the reaction condenses to liquid. For water, the reduction from $H_2O(id)$ to $H_2O(l)$ is $H_w^{id} - H_w^l$, the ideal enthalpy of vaporization, which is somewhat larger than the enthalpy of vaporization $H_w^v - H_w^l$.

7.1.1 Because the gross heating value results from an ideal combustion reaction, ideal gas relationships apply. The ideal gross heating value per unit mass for a mixture, H_m^{id} , is:

$$H_m^{id} = \sum_{j=1}^n x_j M_j H_{m,j}^{id} / \sum_{j=1}^n x_j M_j \quad (2)$$

where: x_j is the mole fraction of Component *j*, M_j is the molar mass of Component *j* from Table 1, and *n* is the total number of components.

7.1.2 $H_{m,j}^{id}$ is the pure component, ideal gross heating value per unit mass for Component *j* (at 60°F (15.6°C) in Table 1). Values of H_m^{id} are independent of pressure, but they vary with temperature.

7.2 Ideal Gas Density

7.2.1 The ideal gas density, ρ^{id} , is:

$$\rho^{id} = (P/RT) \sum_{j=1}^n x_j M_j = MP/RT \quad (3)$$

where: *M* is the molar mass of the mixture,

$$M = \sum_{j=1}^n x_j M_j \quad (4)$$

P is the base pressure in absolute units (psia), *R* is the gas constant, 10.7316 psia.ft³/(lb mol•°R) in this practice, based upon $R = 8.31448 \text{ J}/(\text{mol}\cdot\text{K})$, *T* is the base temperature in absolute units (°R = °F + 459.67). Values of the ideal gas density at 60°F (15.6°C) and 14.696 psia are in GPA Standard 2145.

7.3 Ideal Relative Density:

7.3.1 The ideal relative density d^{id} is:

$$d^{id} = \sum_{j=1}^n x_j d_j = \sum_{j=1}^n x_j M_j / M_a = M / M_a \quad (5)$$

where: M_a is the molar mass of air. The ideal relative density is the molar mass ratio.

7.4 Gross Heating Value per Unit Volume:

7.4.1 Multiplication of the gross heating value per unit mass by the ideal gas density provides the gross heating value per unit volume, H_v^{id} :

$$H_v^{id} = \rho^{id} H_m^{id} = \sum_{j=1}^n x_j H_{v,j}^{id} \quad (6)$$

$H_{v,j}^{id}$ is the pure component gross heating value per unit volume for Component *j* at specified temperature and pressure (60°F (15.6°C) and 14.696 psia in Table 1, ideal gas values).

7.4.2 Conversion of values in Table 1 to different pressure bases results from multiplying by the pressure ratio:

$$H_v^{id}(P) = H_v^{id}(P = 14.696) \times P/14.696 \quad (7)$$

7.5 Real Gas Values—Compressibility Factor:

TABLE 1 Properties of Natural Gas Components at 60°F and 14.696 psia^A

Compound	Formula	Molar Mass, lb·lbmol ^{-1B}	Molar Mass, Ratio, G ^{idC}	Ideal Gross Heating Value ^D			Ideal Net Heating Value			Summation Factor, b _H , psia ⁻¹
				H _v ^{id} , kJ·mol ⁻¹	H _m ^{id} , Btu·lbm ⁻¹	H _v ^{id} , Btu·ft ⁻³	h _v ^{id} , kJ·mol ⁻¹	h _m ^{id} , Btu·lbm ⁻¹	h _v ^{id} , Btu·ft ⁻³	
Hydrogen	H ₂	2.0159	0.069 60	286.20	6 1022	324.2	241.79	51 566	273.93	0
Helium	He	4.0026	0.138 20	0	0	0	0	0	0	0
Water	H ₂ O	18.0153	0.622 02	44.409	1059.8	50.312	0	0	0	0.0623
Carbon monoxide	CO	28.010	0.967 11	282.9	4342	320.5	282.9	4 342	320.5	0.0053
Nitrogen	N ₂	28.0134	0.967 23	0	0	0	0	0	0	0.0044
Oxygen	O ₂	31.9988	1.104 8	0	0	0	0	0	0	0.0073
Hydrogen sulfide	H ₂ S	34.08	1.176 7	562.4	7 094.2	637.1	517.99	6 534	586.8	0.0253
Argon	Ar	39.948	1.379 3	0	0	0	0	0	0	0.0071
Carbon dioxide	CO ₂	44.010	1.519 6	0	0	0	0	0	0	0.0197
Air	^E	28.9625	1.000 0	0	0	0	0	0	0	0.0050
Methane	CH ₄	16.043	0.553 92	891.63	23 891	1010.0	802.71	21 511	909.4	0.0116
Ethane	C ₂ H ₆	30.070	1.038 2	1562.06	22 333	1769.7	1428.83	20 429	1618.7	0.0239
Propane	C ₃ H ₈	44.097	1.522 6	2220.99	21 653	2516.1	2043.3	19 922	2314.9	0.0344
<i>i</i> -Butane	C ₄ H ₁₀	58.123	2.006 8	2870.45	21 232	3251.9	2648.4	19 590	3000.4	0.0458
<i>n</i> -Butane	C ₄ H ₁₀	58.123	2.006 8	2879.63	21 300	3262.3	2657.6	19 658	3010.8	0.0478
<i>i</i> -Pentane	C ₅ H ₁₂	72.150	2.491 2	3531.5	21 043	4000.9	3265.0	19 456	3699.0	0.0581
<i>n</i> -Pentane	C ₅ H ₁₂	72.150	2.491 2	3535.8	21 085	4008.9	3269.3	19 481	3703.9	0.0631
<i>n</i> -Hexane	C ₆ H ₁₄	86.177	2.975 5	4198.1	20 943	4755.9	3887.2	19 393	4403.9	0.0802
<i>n</i> -Heptane	C ₇ H ₁₆	100.204	3.459 8	4857.2	20 839	5502.5	4501.9	19 315	5100.3	0.0944
<i>n</i> -Octane	C ₈ H ₁₈	114.231	3.944 1	5515.9	20 759	6248.9	5116.2	19 256	5796.2	0.1137
<i>n</i> -Nonane	C ₉ H ₂₀	128.258	4.428 4	6175.9	20 701	6996.5	5731.8	19 213	6493.6	0.1331
<i>n</i> -Decane	C ₁₀ H ₂₂	142.285	4.912 7	6834.9	20 651	7742.9	6346.4	19 176	7189.9	0.1538
Neopentane	C ₅ H ₁₂	72.015	2.491 2	3517.27	20 958	3985	3250.8	19 371	3683	...
2-Methylpentane	C ₆ H ₁₄	86.177	2.975 5	4190.43	20 905	4747	3879.6	19 355	4395	0.080
3-Methylpentane	C ₆ H ₁₄	86.177	2.975 5	4193.03	20 918	4750	3882.2	19 367	4398	0.080
2,2-Dimethylbutane	C ₆ H ₁₄	86.177	2.975 5	4180.63	20 856	4736	3869.8	19 306	4384	0.080
2,3-Dimethylbutane	C ₆ H ₁₄	86.177	2.975 5	4188.41	20 895	4745	3877.5	19 344	4393	0.080
Cyclopropane	C ₃ H ₆	42.081	1.452 9	2092.78	21 381	2371	1959.6	20 020	2220	...
Cyclobutane	C ₄ H ₈	56.108	1.937 3	2747.08	21 049	2747	2569.4	19 688	2911	...
Cyclopentane	C ₅ H ₁₀	70.134	2.421 5	3322.04	20 364	3764	3100.0	19 003	3512	...
Cyclohexane	C ₆ H ₁₂	84.161	2.905 9	3955.84	20 208	4482	3689.4	18 847	4180	...
Ethyne (acetylene)	C ₂ H ₂	26.038	0.899 0	1301.32	21 487	1474	1256.9	20 753	1424	0.021
Ethene (ethylene)	C ₂ H ₄	28.054	0.968 6	1412.06	21 640	1600	1323.2	20 278	1499	0.020
Propene (propylene)	C ₃ H ₆	42.081	1.452 9	2059.35	21 039	2333	1926.1	19 678	2182	0.033
Benzene	C ₆ H ₆	78.114	2.697 1	3202.74	18 177	3742	3169.5	17 444	3591	0.069
Butanes (ave)	C ₄ H ₁₀	58.123	2.006 8	2875	21 266	3257	2653	19 623	3006	0.046
Pentanes (ave)	C ₅ H ₁₂	72.150	2.491 2	3534	21 056	4003	3267	19 469	3702	0.062
Hexanes (ave)	C ₆ H ₁₄	86.177	2.975 5	4190	20 904	4747	3879	19 353	4395	0.080
Butenes (ave)	C ₄ H ₈	56.108	1.937 2	2716	20 811	3077	2538	19 450	2876	0.046
Pentenes (ave)	C ₅ H ₁₀	70.134	2.421 5	3375	20 691	3824	3153	19 328	3572	0.060

^A This table is consistent with GPA 2145-89, but it is necessary to use the values from the most recent edition of GPA 2145 for custody transfer calculations.

^B 1984 Atomic Weights: C = 12.011, H = 1.00794, O = 15.9994, N = 14.0067, S = 32.06.

^C Molar mass ratio is the ratio of the molar mass of the gas to that of air.

^D Based upon ideal reaction; the entry for water represents the total enthalpy of vaporization.

^E Composition from: F. E. Jones, *J. Res. Nat. Bur. Stand.*, Vol. 83, 419, 1978.

7.5.1 The compressibility factor is:

$$Z(T,P) = \rho^{id} / \rho = (MP/RT) / \rho \quad (8)$$

where ρ is the real gas density in mass per unit volume. At conditions near ambient, the truncated virial equation of state satisfactorily represents the volumetric behavior of natural gas:

$$Z(T,P) = 1 + BP/RT \quad (9)$$

where B is the second virial coefficient for the gas mixture. The second virial coefficient for a mixture is:

$$B = x_1^2 B_{11} + x_2^2 B_{22} + \dots + x_n^2 B_{nn} + 2x_1x_2B_{12} + \dots + 2x_{n-1}x_nB_{n-1,n} \quad (10)$$

$$= \sum_{i=1}^n \sum_{j=1}^n x_i x_j B_{ij}$$

where B_{jj} is the second virial coefficient for Component j and B_{ij} is the second cross virial coefficient for Components i and j . The second virial coefficients are functions of temperature. Eq 9 can be used with Eq 10 for calculation of the compressibility factor for the various pressure bases, but it is not accurate at pressures greater than two atmospheres. Special treatment is not required for H₂ and He at mole fractions up to 0.01. Calculations can be made with $B_{ij} = 0$ for hydrogen and helium.

7.5.2 Eq 9 and Eq 10 for calculation of $Z(T,P)$ for a gas mixture are rigorous but require considerable calculations and information that is not always available. An alternative, approximate expression for $Z(T,P)$ that is more convenient for hand calculations is: