Agilent

Agilent NGA RGA

Reference Guide

Notices

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Contents

1 Introduction

2 Calibration

3 Metric Calculations

4 FPS Calculations

5 ISO 6976:2016 Calculations

6 Constants

7 References

1 Introduction

The NGA RGA Add-on provides the ability to generate a custom calculation file, a constants file, and a report template for a set of conditions defined either in the GPA, ASTM, or ISO based standards for Natural Gas. These calculations are based FPS (Foot Pound Second) units or on the Metric (meter kilogram Second) units. The FPS based calculations (Btu) may also be called English or Engineering and are used by GPA, ASTM, and other organizations in the United States. The Metric based calculations are used by ISO and other European standards. ISO 6976:1998 used superior heat value and inferior heat value. The updated ISO 6976:2016 has changed the term to Gross Heat value and Net Heat value. ISO 6976:2016 has also added 15.55°C (60°F) as a combustion temperature and metering temperature to the physical constants tables.

The NGA RGA Add-on requires a calibrated method and the names in the calibrated method to match the names in the Constants file.

There are five main calculations that must be made to enable all of the calculations that are possible. The five calculations are the:

- Superior or Gross heat value (molar)
- Inferior or Net heat value (molar)
- Mean molecular weight
- Relative density
- Compression factor

Each of these calculations require compound specific physical constants be used in the calculations.

Since the Add-on uses the calibrated method, the custom calculator, and the constants file to calculate the various Energy Values, the reference guide is organized in the following manner:

Calibration

Calculation

- Metric (kJ/m^3, kJ/mole, kJ/kg, Wobbe Index)
- FPS (Btu/ft^3, Btu/mole, Btu/lbm and GPM)
- ISO 6976:2016 (kJ/m^3, kJ/mole, kJ/kg, Wobbe Index)

Constants

Gas constant

References

2 Calibration

While most of the gas mixtures used for calibration are reported as Mole %, there are gas standards also available as Weight % and Volume %. It is then necessary to convert from Weight % or Volume % to mole % for the heating value calculations.

The conversion from Weight % to Mole % is given by:

$$\text{Mole\%}_{\text{i non-norm}} = \text{Weight\%}_i / \text{MW}_i \quad (1)$$

Where:

MW_i = molecular weight of compound i (g/mole for Metric and lb/lbmole for FPS)

The conversion form Volume % to Mole % is given by:

$$\text{Mole\%}_{\text{i non-norm}} = \text{Vol\%}_i / Z_i \quad (2)$$

Where:

Z_i = compression factor of compound i at metering temperature t_2 for Metric and 60°F for FPS)

The calculations use the appropriate constants for the compound from the physical constants tables to convert to Mole %.

NOTE

Z_i and MW_i are read from constant file, if the data is not found for one of the compounds the whole computations are in error.

3 Metric Calculations

The Metric calculations are primarily based on ISO 6976: 1995 with Cor. 2: 1997(E) and Cor.3:1999(E) and follows the following notation:

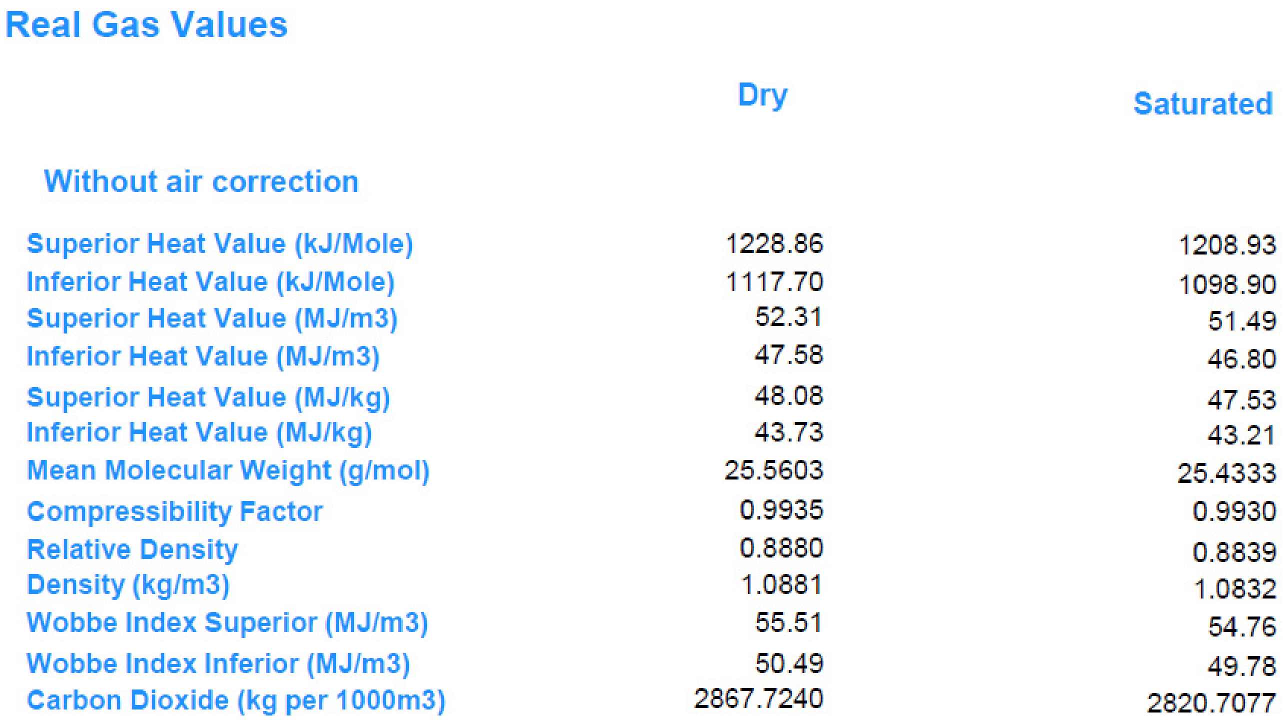
P_1, t_1: combustion pressure and temperature

P_2, t_2: metering pressure and temperature

A temperature in lowercase indicate a temperature in °C, if we use uppercase it indicates a temperature in °K.

$P_1 = P_2 = P_b = 101325$ Pa

The Metric calculation includes the provision for calculating the real, the saturated, and air corrected values for a Natural Gas mixture.



Real Gas Values

	Dry	Saturated
Without air correction		
Superior Heat Value (kJ/Mole)	1228.86	1208.93
Inferior Heat Value (kJ/Mole)	1117.70	1098.90
Superior Heat Value (MJ/m3)	52.31	51.49
Inferior Heat Value (MJ/m3)	47.58	46.80
Superior Heat Value (MJ/kg)	48.08	47.53
Inferior Heat Value (MJ/kg)	43.73	43.21
Mean Molecular Weight (g/mol)	25.5603	25.4333
Compressibility Factor	0.9935	0.9930
Relative Density	0.8880	0.8839
Density (kg/m3)	1.0881	1.0832
Wobbe Index Superior (MJ/m3)	55.51	54.76
Wobbe Index Inferior (MJ/m3)	50.49	49.78
Carbon Dioxide (kg per 1000m3)	2867.7240	2820.7077

Figure 1. The portion of the Metric_NGA_Report showing the calculated totals for gas mixture using the Metric based calculations

The following calculations are used. Section numbers are from ISO 6976: 1995 with Cor. 2: 1997(E) and Cor.3:1999(E) Natural gas - Calculation of calorific values, density, relative density and Wobbe Index from composition. The air correction has a separate reference.

Gas Mixture Heat Value (Mole)

Section 5 of ISO 6976: 1995 with Cor. 2: 1997(E) and Cor.3:1999(E).

$$H_{sup,\ mole} = \sum xi \times H_{sup,\ mole\ i} \quad (3)$$

Where:

$H_{sup,\ mole}$ = The gas mixture superior heat value (kJ/mol)

$H_{sup,\ mole\ i}$ = The compound i superior heat value (kJ/mol) at combustion T° t_1

NOTE

The same computation is applied for $H_{inf,\ mole}$ using the constant $H_{inf,mole\ i}$

Compressibility of the Gas Mixture

Section 4.2 of ISO 6976: 1995 with Cor. 2: 1997(E) and Cor.3:1999(E).

$$Z_{mix} = 1 - (\Sigma(x_i \times \sqrt{bi}))^2 \quad (4)$$

Where:

Z_{mix} = Compressibility of the gas mixture

$\sqrt{bi}$ = Summation factor of compound i at metering T° t_2

NOTE

In the constant file we have √bi called summation factor.

Mean Molecular Weight of the Gas Mixture

Section 6.1 of ISO 6976: 1995 with Cor. 2: 1997(E) and Cor.3:1999(E).

$$MW = \sum x_i \times MW_i \quad (5)$$

Where:

MW = Mean molecular weight of the gas mixture (g/mol)

MW_i = Molecular weight of the compound i (g/mol)

Relative Density of the Gas Mixture

Section 8.2 (real gas) of ISO 6976: 1995 with Cor. 2: 1997(E) and Cor.3:1999(E).

$$d = (MW/MW_{air}) \times (Z_{air}/Z_{mix}) \qquad \textbf{(6)}$$

Where:

d = relative density of the gas mixture

MW = Mean molecular weight of the gas mixture (g/mol)

MW_{air} = Molecular weight of air (28.9626 g/mol)

Z_{air} = Compressibility factor at metering T° t_2 (Z(Compress) in the constant file)

Z_{mix} = Compressibility of the gas mixture

Density of the Gas Mixture (Real Gas)

Section 8.2 (real gas) of ISO 6976: 1995 with Cor. 2: 1997(E) and Cor.3:1999(E).

$$\rho = (P_b/(R \times T_2)) \times (MW/1000)/Z_{mix} \qquad \textbf{(7)}$$

Where:

ρ = The density of the gas mixture (kg/m^3)

R = (Gas constant) = 8.3144621 J/(mol × K) = (Pa × m^3)/(mol × K)

T_2 = Metering T(°C) + 273.15 = Metering T(K)

P_b = 101325 Pa

Z_{mix} = Compressibility of the gas mixture

MW/1000 = Mean molecular weight or molar mass of the gas mixture (kg/mol)

Gas Mixture Heat Value (Mass)

Section 6.1 and 6.2 of ISO 6976: 1995 with Cor. 2: 1997(E) and Cor.3:1999(E).

$$H_{sup,\ mass} = H_{sup,\ mole}/MW \qquad \textbf{(8)}$$

Where:

$H_{sup,\ mass}$ = The gas mixture superior heat value (kJ/g);

$H_{sup,\ mole}$ = The gas mixture superior heat value (kJ/mol);

MW = Mean molecular weight or molar mass of the gas mixture (g/mol)

NOTE **The same computation is applied for H_{inf}, mass using $H_{inf,mole}$**

Gas Mixture Heat Value (Volume)

Section 7.2 of ISO 6976: 1995 with Cor. 2: 1997(E) and Cor.3:1999(E).

$$H_{\text{sup, volume}} = H_{\text{sup, mole}} \times (P_b/RT_2)/Z_{\text{mix}} \qquad (9)$$

Where:

$H_{\text{sup, volume}}$ = The gas mixture superior heat value (kJ/m^3);

$H_{\text{sup, mole}}$ = The gas mixture superior heat value (kJ/mol);

P_b = 101325 Pa;

R = (Gas constant) = 8.3144621 J/(mol × K) = (Pa × m^3)/(mol × K);

T_2= Metering temperature t_2(°C) + 273.15 = Metering T(K);

Z_{mix} = Compressibility of the gas mixture

NOTE

The same computation is applied for $H_{\text{inf, volume}}$ using $H_{\text{inf, mole}}$.

Wobbe Index

Section 8.2 of ISO 6976: 1995 with Cor. 2: 1997(E) and Cor.3:1999(E).

$$W_{sup} = H_{\text{sup, volume}}/(\sqrt{d}) \qquad (10)$$

Where:

W_{sup} = Wobbe index superior for the gas mixture (kJ/m^3);

$H_{\text{sup, volume}}$ = The gas mixture superior heat value (kJ/m^3);

d = Relative density of the gas mixture

NOTE

The same computation is applied for W_{inf} using $H_{\text{inf,volume}}$.

Amount of Carbon Dioxide

Volume for 1 mole of an ideal gas

$$V_{ideal} = n \times R \times T_2/P_b \tag{11}$$

Where:

V_{ideal} = Volume (m^3) of 1 mole of an ideal gas at the metering temperature and the base pressure

n = 1 mol

R = (Gas constant) = 8.3144621 J/(mol × K) = (Pa × m^3)/(mol × K)

T_2 = Metering T(°C) + 273.15 = Metering T(K)

P_b = 101325 Pa

Volume for 1 mole of the gas mixture

$$V_{real} = V_{ideal} \times Z_{mix} \tag{12}$$

Where:

V_{real} = Volume (m^3) of 1 mole of the gas mixture at the metering temperature and the base pressure

V_{ideal} = Volume (L) of 1 mole of an ideal gas calculated in **Equation 11**.

Z_{mix} = Compressibility of the gas mixture

Amount of CO_2 produced during the combustion of 1 m^3 of the gas mixture

$$\text{Total } CO_2\text{ (g)} = \Sigma x_i \times (CN)_i \times MWCO_2/\ V_{real} \tag{13}$$

Where:

$(CN)_i$ = Number of carbon in the compound i

$MWCO_2$ = 44.01 g/mol

V_{real} = Volume (m^3) of 1 mole of the gas mixture calculated in **Equation 12**.

The calculation of the saturated values require the renormalization of the mole fraction.

Normalization

$$x_{i,\ norm,\ dry} = (Mole\%_{i,\ non\text{-}norm}) / (\Sigma Mole\%_{i,\ non\text{-}norm}) \tag{14}$$

Where:

$x_{i,\ norm,\ dry}$ = The mole fraction for the compound i (without air correction and water correction)

$Mole\%_{i,\ non\text{-}norm}$ = Mole% calculated in **Chapter 2**, “Calibration.”.

Optional: Water Correction (Saturated Case)

We are using the preferred computation described in Annex F section F.2 of ISO norm.

Add water to the compound list

$$x_{H2O,\ non\text{-}norm} = P_w / P_b \tag{15}$$

Where:

P_w = Water partial pressure (in Pa) at t_2 (°C)

610.5 Pa	0°C
1705 Pa	15°C
2338 Pa	20°C
3167 Pa	25°C

P_b = 101325 Pa

Normalization

$$x_{i,\ saturated} = x_{i,\ norm,\ dry} \times (P_b - P_w) / P_b \tag{16}$$

Where:

$x_{i,\ saturated}$ = The mole fraction for compound i after water correction

$x_{i,\ norm,\ dry}$ = The mole fraction for the compound i (without air correction and water correction)

For the following computation, xi will be the mole fraction of the compound i dry or saturated depending on the case we want to compute.

Optional: Air Correction

Discussed in ISO 6974-3 Standard, [Natural gas - Determination of composition with defined uncertainty by gas chromatography Part 3: Determination of hydrogen, helium, oxygen, nitrogen, carbon dioxide and hydrocarbons up to C8 using two packed columns] defines a means to correct for air in the sample by adjusting the nitrogen concentration for the air. See section 7.1.2.

Computation of the new value for x_{N2} and x_{O2} if $x_{O2} > 0.02$

$$x_{N2,\ \text{air removed}} = x_{N2} - (78/21) \times x_{O2} \tag{17}$$

Where:

$x_{N2,\ \text{air removed}}$ = The mole fraction of N_2 without the part of N_2 from the air

x_{N2} = The mole fraction of N_2 calculated previously (dry or saturated depending on the correction the user chose)

x_{O2} = The mole fraction of O_2 calculated previously (dry or saturated depending on the correction the user chose)

$$x_{O2,\ \text{air removed}} = 0 \tag{18}$$

Computation of the new value for x_{N2} and x_{O2} if $x_{O2} < 0.02$

If the column used is a sieve 13x:

$$x_{N2,\ \text{air removed}} = x_{N2} - (78/21) \times x_{O2} \tag{19}$$

Where:

$x_{N2,\ \text{air removed}}$ = The mole fraction of N_2 without the part of N_2 from the air

x_{N2} = The mole fraction of N_2 calculated previously (dry or saturated depending on the correction the user chose)

x_{O2} = The mole fraction of O_2 calculated previously (dry or saturated depending on the correction the user chose)

$$x_{O2,\ \text{air removed}} = 0 \tag{20}$$

If the column used is a Porapak:

$$x_{N2}\text{, air removed} = x_{N2} - (100/21) \times x_{O2} \tag{21}$$

Where:

$x_{N2,\ \text{air removed}}$ = The mole fraction of N_2 without the part of N_2 from the air

x_{N2} = The mole fraction of N_2 calculated previously (dry or saturated depending on the correction the user chose)

x_{O2} = The mole fraction of O_2 calculated previously (dry or saturated depending on the correction the user chose)

$$x_{O2,\ air\ removed} = 0 \tag{22}$$

If the column used is neither a sieve 13x, nor a Porapak:

$$x_{N2,\ air\ removed} = x_{N2} - (78/21) \times x_{O2} \tag{23}$$

Where:

$x_{N2,\ air\ removed}$ = The mole fraction of N_2 without the part of N_2 from the air

x_{N2} = The mole fraction of N_2 calculated previously (dry or saturated depending on the correction the user chose)

x_{O2} = The mole fraction of O_2 calculated previously (dry or saturated depending on the correction the user chose)

$$x_{O2,\ air\ removed} = 0 \tag{24}$$

Correction for all the mole fractions

$$x_{i,\ air\ corrected} = 100 \times (x_i / \Sigma\, x_i + x_{N2,\ air\ removed} + x_{O2,\ air\ removed}) \tag{25}$$

Where:

$x_{i,\ air\ corrected}$ = The mole fraction of compound i (except N_2 and O_2) corrected for the air

x_i = The mole fraction of compound i (except N_2 and O_2) calculated previously (dry or saturated depending on the correction the user chose)

$x_{N2,\ air\ removed}$ = The mole fraction of N_2 calculated in **Equation 17**, **Equation 19**, or **Equation 21**.

$$x_{O2,\ air\ removed} = 0 \tag{26}$$

$$x_{N2,\ air\ corrected} = 100 \times (x_{N2,\ air\ removed} / \Sigma\, x_i + x_{N2,\ air\ removed} + x_{O2,\ air\ removed}) \tag{27}$$

Where:

$x_{N2,\ air\ corrected}$ = The mole fraction of N_2 corrected for the air

$$x_{O2,\ air\ corrected} = 0 \tag{28}$$

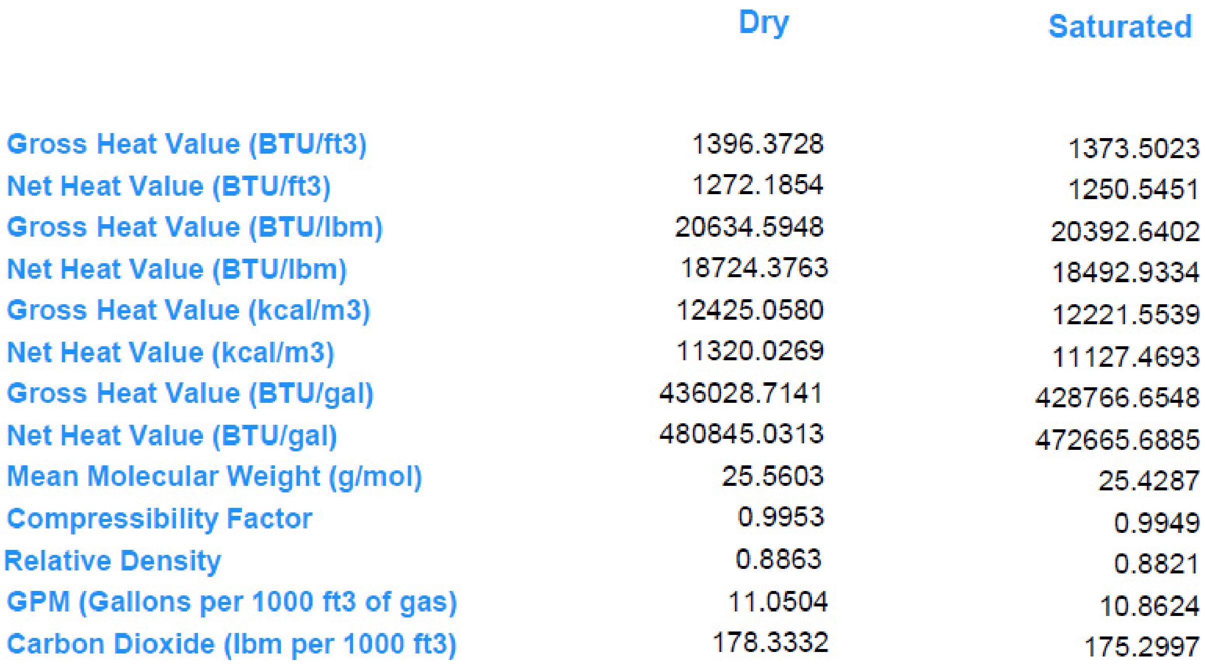
In the other formulas, x_i will refer to the mole fraction of the compound i (including O_2 and N_2) with or without air correction and with or without water correction depending on which corrections has been applied.

4 FPS Calculations

FPS (Foot Pound Second) provides the means to calculate using English based units. This provides the calculations also known as Engineering based calculations, which are used by the GPA and ASTM Natural Gas Standards.

The FPS calculation includes the provision for calculating the real and the saturated values for a Natural Gas mixture. The following calculations are used. If a section number is noted, it is from GPA Standard 2172.09 Calculation of Gross Heating Value, Relative Density, Compressibility and Theoretical Hydrocarbon Liquid Content for Natural Gas Mixtures for Custody Transfer. The standard uses the term Molar Mass. The calculations described use the term Molecular Weight.

Real Gas Values



	Dry	Saturated
Gross Heat Value (BTU/ft3)	1396.3728	1373.5023
Net Heat Value (BTU/ft3)	1272.1854	1250.5451
Gross Heat Value (BTU/lbm)	20634.5948	20392.6402
Net Heat Value (BTU/lbm)	18724.3763	18492.9334
Gross Heat Value (kcal/m3)	12425.0580	12221.5539
Net Heat Value (kcal/m3)	11320.0269	11127.4693
Gross Heat Value (BTU/gal)	436028.7141	428766.6548
Net Heat Value (BTU/gal)	480845.0313	472665.6885
Mean Molecular Weight (g/mol)	25.5603	25.4287
Compressibility Factor	0.9953	0.9949
Relative Density	0.8863	0.8821
GPM (Gallons per 1000 ft3 of gas)	11.0504	10.8624
Carbon Dioxide (lbm per 1000 ft3)	178.3332	175.2997

Figure 2. The portion of the FPS_NGA_Report showing the calculated totals for gas mixture using the FPS based calculations.

Normalization

$x_{i,\ norm} = (Mole\%_{i,\ non\text{-}norm}) / (\Sigma Mole\%_{i,\ non\text{-}norm})$ **(29)**

Where:

$x_{i,\ norm}$ = The mole fraction for the compound i (without air correction)

$Mole\%_{\ i,\ non\text{-}norm}$ = The calculation of Mole% from Volume% or Weight%. See **Chapter 2**, “Calibration” .

Optional: Water Correction (Saturated Case)

The mole fraction of water is calculated from the vapor pressure of water and the base pressure.

$x_{H2O,\ non\text{-}\ norm} = P_{H2O}/P_b$ **(30)**

Where:

P_{H2O} = Vapor pressure of water (psia) at 60 °F = 0.25640 psia.

P_b = metering pressure (psia)

Normalization

$x_{i,\ saturated} = x_{i,norm} \times (P_2\text{-}P_w)/P_2$ **(31)**

Where:

$x_{i,\ saturated}$ = The mole fraction for compound i after water correction

$x_{i,\ norm,\ dry}$ = The mole fraction for the compound i (without air correction and water correction)

Compressibility Factor of the Gas Mixture (Z_{sample}) at P_b (Near Atmospheric Pressure) and 60 °F

From GPA 2172 Section 7.3.

For the following computation, xi will be the mole fraction of the compound i dry or saturated depending on the case we want to compute.

$$Z_{sample} = 1 - P_b \times (\Sigma x_i \times b_i)^2 \qquad \textbf{(32)}$$

Where:

Z_{sample} = Compressibility factor of the gas at P_b

b_i = The summation factor of compound i at 60 °F ($psia^{-1}$)

P_b = Base pressure (psia)

Heat Value of a Real Gas (BTU/ft^3) (Volume)

From GPA 2172 Section 7.1 + Annex A2

$$H_{gross,v}(Pb) = \Sigma(x_i \times H_{gross,v,i}(60°F) \times (P_b/14.696))/Z_{sample} \qquad \textbf{(33)}$$

Where:

$H_{gross,v,i}(60°F)$ = Gross heat value (BTU/ft^3) of compound i at 60°F

P_b = Base pressure (psia)

Z_{sample} = Compressibility factor of the gas at P_b

NOTE

The same computation is applied for $H_{net, v}$ using $H_{net, v, i}$.

Heat Value of a Real Gas (kcal/m^3) (Volume)

To convert BTU/ft^3 into kcal/m^3:

$$H_{v, kcal/m^3} = (0.25/0.0283169) \times H_{v, BTU/ft^3} \qquad \textbf{(34)}$$

Where:

1 BTU = 0.25 kcal

1 ft^3 = 0.0283169 m^3

Heat Value of a Real Gas (BTU/Gallon) (Volume)

From GPA 2172 Section 7.4.

$$H_v^{id}(\text{BTU/gal}) = \Sigma LF_i \times H_l^{id}(\text{BTU/gal})/LF_{total} \quad (35)$$

$$\text{Liquid Fraction } LF_i = x_i \times MW_i/d_l \quad (36)$$

where

x_i = mole fraction of compound i

MW_i = Molecular weight of compound i

d_l = Absolute density lbm/gal

$$\text{total liquid fraction } LF_{total} = \Sigma LF_i \quad (37)$$

NOTE **The same computation is applied for $H_{net, vg}$ using $H_{net, vg, i}$.**

Mean Molecular Weight of the Gas Mixture

$$MW = \Sigma\, x_i \times MW_i \quad (38)$$

Where:

MW = Mean molecular weight of the gas mixture (g/mol)

MW_i = Molecular weight of the compound i (g/mol)

Heat Value of a Real Gas (BTU/lbm) (Mass)

From GPA 2172 Section A.2.

$$H_{gross,m}(P_b) = \Sigma(x_i \times H_{gross,\, m,\, i}(60°F) \times MW_i)/\ MW_m \quad (39)$$

Where:

$H_{gross,\, m,\, i}(60°F)$ = Gross heat value (BTU/ lbm) of compound i at 60°F

P_b = Base pressure (psia)

Z_{sample} = Compressibility factor of the gas at P_b

M_i = The molecular mass of compound i

MW_i = molecular weight of compound i

MW_m = Mean molecular weight of the gas mixture (g/mol)

NOTE **The same computation is applied for $H_{net,\, m}$ using $H_{net,\, m,\, i}$.**

Gallons per 1000 CF of Real Gas

This is the Liquid Volume Equivalent expressed as Gallons per 1000 cubic feet of gas:

$$GPM = (\Sigma((x_i \times 1000) \times P_b)/(V_i \times 14.696))/Z_{sample} \qquad \textbf{(40)}$$

Where:

V_i = Cubic feet per gallon of compound i

P_b = Pressure base (psia)

Z_{sample} = Compressibility factor of the gas at P_b

Relative Density of the Gas Mixture

$$G = (MW/MW_{air}) \times (Z_{air}/Z_{sample}) \qquad \textbf{(41)}$$

Where:

G = Relative density real

MW = Mean molecular weight of the gas mixture (g/mol)

MW_{air} = Mean molecular weight of air (g/mol) = 28.693 g/mol

Z_{air} = Compressibility factor of air at 60°F = 0.9996

Z_{sample} = Compressibility factor of the gas at P_b

Amount of Carbon Dioxide

Volume for 1 mole of an ideal gas:

$$V_{ideal} = n \times R \times T/(P_b/14.696) \qquad \textbf{(42)}$$

Where:

V_{ideal} = volume (L) of 1 mole of an ideal gas at the metering temperature and the base pressure

n = 1 mol

R = (Gas constant) = 0.082057 L × atm/K × mol

T = metering T(K) = 288.6 K (= 60°F)

P_b = metering pressure (psia)

Volume for 1 mole of the gas mixture

$$V_{real} = V_{ideal} \times Z_{sample} \qquad (43)$$

Where:

V_{real} = volume (L) of 1 mole of the gas mixture at 60°F and the base pressure

V_{ideal} = volume (L) of 1 mole of an ideal gas calculated in **Equation 41**

Z_{sample} = Compressibility of the gas mixture

Amount of CO_2 produced during the combustion of 1000 ft^3 of the gas mixture

$$\text{Total } CO_2 \text{ (g)} = \Sigma x_i \times (CN)_i \times (MW_{CO2}/453.5924) \times (28316.85/V_{real}) \qquad (44)$$

Where:

$(CN)_i$ = The number of carbon in the compound i

MW_{CO2} = 44.01 g/mol

V_{real} = The volume (L) of 1 mole of the gas mixture calculated in **Equation 42**.

5 ISO 6976:2016 Calculations

The ISO 6976:2016 calculations are primarily based on ISO 6976:2016 and follows the following notation.

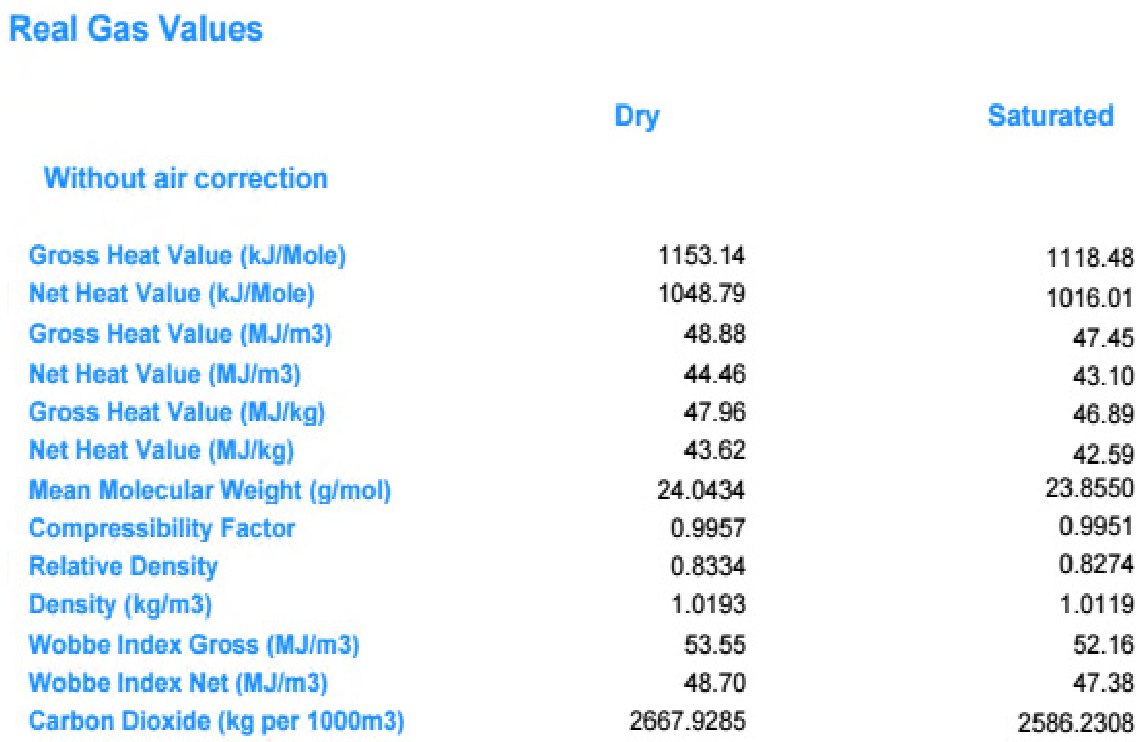
P_1, t_1: combustion pressure and temperature

P_2, t_2: metering pressure and temperature

A temperature in lowercase indicate a temperature in °C, if we use uppercase it indicate a temperature in °K.

$$P_1 = P_2 = P_b = 101325 \text{ Pa}$$

The ISO 6976:2016 calculation includes the provision for calculating the real, the saturated, and air corrected values for a Natural Gas mixture.



Real Gas Values

	Dry	Saturated
Without air correction		
Gross Heat Value (kJ/Mole)	1153.14	1118.48
Net Heat Value (kJ/Mole)	1048.79	1016.01
Gross Heat Value (MJ/m3)	48.88	47.45
Net Heat Value (MJ/m3)	44.46	43.10
Gross Heat Value (MJ/kg)	47.96	46.89
Net Heat Value (MJ/kg)	43.62	42.59
Mean Molecular Weight (g/mol)	24.0434	23.8550
Compressibility Factor	0.9957	0.9951
Relative Density	0.8334	0.8274
Density (kg/m3)	1.0193	1.0119
Wobbe Index Gross (MJ/m3)	53.55	52.16
Wobbe Index Net (MJ/m3)	48.70	47.38
Carbon Dioxide (kg per 1000m3)	2667.9285	2586.2308

Figure 3. The portion of the ISO 6975:2016_NGA_Report showing the calculated totals for gas mixture using the ISO 6975:2016 based calculations.

The following calculations are used. Section numbers are from ISO 6976: 2016 Natural gas - Calculation of calorific values, density, relative density and Wobbe Index from composition. The air correction has a separate reference.

Gas Mixture Heat Value (Mole)

Section 7.1 and 7.2 of ISO 6976:2016.

$$H_{G,\,mole} = \Sigma\, x_i \times H_{G\ mole\ I} \tag{45}$$

Where:

$H_{G,\,mole}$ = The gas mixture gross heat value (kJ/mol) at combustion T° t_1

$H_{G,\,mole\ I}$ = The compound I gross heat value (kJ/mol) at combustion T° t_1

NOTE **The same computation is applied for $H_{N,\,mole}$ using the constant $H_{N,mole\ i}$**

Compressibility of the Gas Mixture

Section 6.2 of ISO 6976:2016.

$$Z_{mix} = 1 - (\Sigma(x_i \times \sqrt{bi}))^2 \tag{46}$$

Where:

Z_{mix} = Compressibility of the gas mixture

$\sqrt{bi}$ = Summation factor of compound i at metering T° t_2

NOTE **In the constant file we have √bi called summation factor.**

Mean Molecular Weight of the Gas Mixture

Equation 5 in Section 8.1 of ISO 6976:2018.

$$MW = \Sigma\, x_i \times MW_i \tag{47}$$

Where:

MW = Mean molecular weight of the gas mixture (g/mol)

MW_i = Molecular weight of the compound i (g/mol)

Relative Density of the Gas Mixture

Section 10.5 (real gas) of ISO 6976:2016.

$$G = (MW/MW_{air}) \times (Z_{air}/Z_{mix}) \tag{48}$$

Where:

G = relative density of the gas mixture

MW = Mean molecular weight of the gas mixture (g/mol)

MW_{air} = Molecular weight of air (28.9626 g/mol)

Z_{air} = Compressibility factor at metering T° t_2 (Z(Compress) in the constant file)

Z_{mix} = Compressibility of the gas mixture

Density of the Gas Mixture (Real Gas)

Section 10.6 (real gas) of ISO 6976:2016.

$$G\ (t_2,p_2) = (P_b/(R \times T_2)) \times (MW/1000)/Z_{mix} \tag{49}$$

Where:

G = The density of the gas mixture (kg/m^3)

R = (Gas constant) = 8.3144621 J/(mol × K) = ($Pa \times m^3$)/(mol × K)

T_2 = Metering T(°C) + 273.15 = Metering T(K)

P_b = 101325 Pa

Z_{mix} = Compressibility of the gas mixture

MW/1000 = Mean molecular weight or molar mass of the gas mixture (kg/mol)

Gas Mixture Heat Value (Mass)

Section 6.1 and 6.2 of ISO 6976:2016.

$$H_{G,\ mass} = H_{G,\ mole}/MW \tag{50}$$

Where:

$H_{G,\ mass}$ = The gas mixture superior heat value (kJ/g);

$H_{G,\ mole}$ = The gas mixture superior heat value (kJ/mol);

MW = Mean molecular weight or molar mass of the gas mixture (g/mol)

NOTE

The same computation is applied for $H_{N,\ mass}$, mass using $H_{N,mole}$

Gas Mixture Heat Value (Volume)

Section 7.2 of ISO 6976:2016.

$$H_{G,\ \mathrm{volume}} = H_{G,\ \mathrm{mole}} \times (P_b/RT_2)/Z_{mix} \quad (51)$$

Where:

$H_{G,\ \mathrm{volume}}$ = The gas mixture superior heat value (kJ/m^3);

$H_{G,\ \mathrm{mole}}$ = The gas mixture superior heat value (kJ/mol);

P_b = 101325 Pa;

R = (Gas constant) = 8.3144621 J/(mol × K) = (Pa × m^3)/(mol × K);

T_2= Metering temperature t_2(°C) + 273.15 = Metering T(K);

Z_{mix} = Compressibility of the gas mixture

NOTE

The same computation is applied for $H_{N,\ \mathrm{volume}}$ using $H_{N,\ \mathrm{mole}}$.

Wobbe Index

Sections 10.7 and 10.8 of ISO 6976:2016.

$$W_G = H_{G,\ \mathrm{volume}}/(\sqrt{d}) \quad (52)$$

Where:

W_G = Wobbe index superior for the gas mixture (kJ/m^3);

$H_{G,\ \mathrm{volume}}$ = The gas mixture superior heat value (kJ/m^3);

d = Relative density of the gas mixture

NOTE

The same computation is applied for W_N using $H_{N,\mathrm{volume}}$.

Amount of Carbon Dioxide

Volume for 1 mole of an ideal gas

$$V_{ideal} = n \times R \times T_2/P_b \quad \textbf{(53)}$$

Where:

V_{ideal} = Volume (m^3) of 1 mole of an ideal gas at the metering temperature and the base pressure

n = 1 mol

R = (Gas constant) = 8.3144621 J/(mol × K) = (Pa × m^3)/(mol × K)

T_2 = Metering T(°C) + 273.15 = Metering T(K)

P_b = 101325 Pa

Volume for 1 mole of the gas mixture

$$V_{real} = V_{ideal} \times Z_{mix} \quad \textbf{(54)}$$

Where:

V_{real} = Volume (m^3) of 1 mole of the gas mixture at the metering temperature and the base pressure

V_{ideal} = Volume (L) of 1 mole of an ideal gas calculated in **Equation 53**.

Z_{mix} = Compressibility of the gas mixture

Amount of CO_2 produced during the combustion of 1 m^3 of the gas mixture

$$\text{Total } CO_2 \text{ (g)} = \Sigma x_i \times (CN)_i \times MWCO_2/\ V_{real} \quad \textbf{(55)}$$

Where:

$(CN)_i$ = Number of carbon in the compound i

$MWCO_2$ = 44.01 g/mol

V_{real} = Volume (m^3) of 1 mole of the gas mixture calculated in **Equation 54**.

The calculation of the saturated values require the renormalization of the mole fraction.

Normalization

$$x_{i,\ norm,\ dry} = (Mole\%_{i,\ non\text{-}norm}) / (\Sigma Mole\%_{i,\ non\text{-}norm}) \quad \textbf{(56)}$$

Where:

$x_{i,\ norm,\ dry}$ = The mole fraction for the compound i (without air correction and water correction)

$Mole\%_{i,\ non\text{-}norm}$ = Mole% calculated in **Chapter 2**, “Calibration.”.

Optional: Water Correction (Saturated Case)

We are using the preferred computation described in Annex F section F.2 of ISO norm.

Add water to the compound list

$$x_{H2O,\ non\text{-}norm} = P_w/P_b \qquad \mathbf{(57)}$$

Where:

P_w = Water partial pressure (in Pa) at t_2 (°C)

610.5 Pa	0°C
1705 Pa	15°C
1767 Pa	15.55°C
2338 Pa	20°C
3167 Pa	25°C

P_b = 101325 Pa

Normalization

$$x_{i,\ saturated} = x_{i,\ norm,\ dry} \times (P_b\text{-}P_w)/P_b \qquad \mathbf{(58)}$$

Where:

$x_{i,\ saturated}$ = The mole fraction for compound i after water correction

$x_{i,\ norm,\ dry}$ = The mole fraction for the compound i (without air correction and water correction)

For the following computation, x_i will be the mole fraction of the compound i dry or saturated depending on the case we want to compute.

Optional: Air Correction

Discussed in ISO 6974-3 Standard, [Natural gas - Determination of composition with defined uncertainty by gas chromatography Part 3: Determination of hydrogen, helium, oxygen, nitrogen, carbon dioxide and hydrocarbons up to C8 using two packed columns] defines a means to correct for air in the sample by adjusting the nitrogen concentration for the air. See section 7.1.2.

Computation of the new value for x_{N2} and x_{O2} if $x_{O2} > 0.02$

$$x_{N2,\text{ air removed}} = x_{N2} - (78/21) \times x_{O2} \tag{59}$$

Where:

$x_{N2,\text{ air removed}}$ = The mole fraction of N_2 without the part of N_2 from the air

x_{N2} = The mole fraction of N_2 calculated previously (dry or saturated depending on the correction the user chose)

x_{O2} = The mole fraction of O_2 calculated previously (dry or saturated depending on the correction the user chose)

$$x_{O2,\text{ air removed}} = 0 \tag{60}$$

Computation of the new value for x_{N2} and x_{O2} if $x_{O2} < 0.02$

If the column used is a sieve 13x:

$$x_{N2,\text{ air removed}} = x_{N2} - (78/21) \times x_{O2} \tag{61}$$

Where:

$x_{N2,\text{ air removed}}$ = The mole fraction of N_2 without the part of N_2 from the air

x_{N2} = The mole fraction of N_2 calculated previously (dry or saturated depending on the correction the user chose)

x_{O2} = The mole fraction of O_2 calculated previously (dry or saturated depending on the correction the user chose)

$$x_{O2,\text{ air removed}} = 0 \tag{62}$$

If the column used is a Porapak:

$$x_{N2}\text{, air removed} = x_{N2} - (100/21) \times x_{O2} \tag{63}$$

Where:

$x_{N2,\text{ air removed}}$ = The mole fraction of N_2 without the part of N_2 from the air

x_{N2} = The mole fraction of N_2 calculated previously (dry or saturated depending on the correction the user chose)

x_{O2} = The mole fraction of O_2 calculated previously (dry or saturated depending on the correction the user chose)

$$x_{O2,\ \text{air removed}} = 0 \quad (64)$$

If the column used is neither a sieve 13x, nor a Porapak:

$$x_{N2,\ \text{air removed}} = x_{N2} - (78/21) \times x_{O2} \quad (65)$$

Where:

$x_{N2,\ \text{air removed}}$ = The mole fraction of N_2 without the part of N_2 from the air

x_{N2} = The mole fraction of N_2 calculated previously (dry or saturated depending on the correction the user chose)

x_{O2} = The mole fraction of O_2 calculated previously (dry or saturated depending on the correction the user chose)

$$x_{O2,\ \text{air removed}} = 0 \quad (66)$$

Correction for all the mole fractions

$$x_{i,\ \text{air corrected}} = 100 \times (x_i / \Sigma\, x_i + x_{N2,\ \text{air removed}} + x_{O2,\ \text{air removed}}) \quad (67)$$

Where:

$x_{i,\ \text{air corrected}}$ = The mole fraction of compound i (except N_2 and O_2) corrected for the air

x_i = The mole fraction of compound i (except N_2 and O_2) calculated previously (dry or saturated depending on the correction the user chose)

$x_{N2,\ \text{air removed}}$ = The mole fraction of N_2 calculated in **Equation 59**, **Equation 61**, or **Equation 63**.

$$x_{O2,\ \text{air removed}} = 0 \quad (68)$$

$$x_{N2,\ \text{air corrected}} = 100 \times (x_{N2,\ \text{air removed}} / \Sigma\, x_i + x_{N2,\ \text{air removed}} + x_{O2,\ \text{air removed}}) \quad (69)$$

Where:

$x_{N2,\ \text{air corrected}}$ = The mole fraction of N_2 corrected for the air

$x_{O2,\ \text{air corrected}} = 0$

In the other formulas, x_i will refer to the mole fraction of the compound i (including O_2 and N_2) with or without air correction and with or without water correction depending on which corrections has been applied.

6 Constants

Physical Constants

The physical constants table for the Metric calculations has entries for the following physical constants:

- Superior heating value for 0, 15, 20, and 25
- Inferior heating value for 0, 15, 20, and 25
- $\sqrt{bi}$ for 0, 15, and 20
- Molecular weight
- Compression factor for 0, 15, and 20
- Carbon number

The compound list includes compounds from ISO 6976, GPA 2145-09, and GPA 17T. The compounds from GPA 17T are listed at 15°C. The Heating values and Compressibility Factors are converted to the other temperatures using Annex J (Approximate conversion factors between reference states) in ISO 6976.

The physical constants table for the FPS calculations has entries for the following physical constants:

- Gross heating value (BTU/ft^3, BTU/lb, BTU/gal)
- Net heating value (BTU/ft^3, BTU/lb, BTU/gal)
- Summation factor
- Molecular weight
- Compression factor
- Carbon number °C
- Hydrogen number
- Boiling point
- ft^3gas/lb
- ft^3/gal liq
- Density liquid
- Lbs/1000 ft^3
- Critical temperature, critical pressure, critical volume, and acentric factor

Annex L (ISO 6976: 1995 with Cor. 2: 1997(E) and Cor.3: 1999(E)) lists the Superior (Gross) and Inferior (Net) heating values for the components of natural gas at 60°F. These values were used as the basis for calculation of the different gross heating values with the appropriate conversion factors for the unsaturated compounds listed in the ISO standard.

The values for ethylene and propylene are from GPA 2145-09. BTU/gal was not calculated for Ethylene since 60°F is above the critical temperature and an estimate is not provided by GPA2145-09. The Compressibility Factor was obtained from the NIST REFPROP (NIST Standard Reference Database 23 Version 9.1) if possible. If not the compressibility was calculated using the procedure outlined in Annex E.2 (ISO 6976: 1995 with Cor. 2: 1997(E) and Cor.3:1999(E)) using the Pitzer-Curl correlation. The ideal gas density is calculated. The density of the component at 60°F was determined using either NIST REFPROP or the NIST/TRC Web Thermo Tables (WTT) Professional Edition (Version 2-2012-1-Pro). From the Idea gas density and the liquid density the other factors can be calculated with the appropriate conversion factors.

The physical constants for cis-2-pentene, trans-2-pentene, and 2-methyl-2-butene were obtained from ASTM DS 4A Physical Constants of Hydrocarbons and Non-Hydrocarbon Compounds and the 2nd Edition. The Compressibility Factor for these compounds were calculated using the Pitzer-Curl correlation.

- Gross heating value for 0, 15, 15.55, 20, and 25
- Net heating value for 0, 15, 15.55, 20, and 25
- √bi for 0, 15, 15.55, and 20
- Molecular weight
- Compression factor for 0, 15, 15.55, and 20
- Carbon number

The compound list only includes compounds from ISO 6976:2016.

Gas Constant

The Committee on Data for Science and Technology (CODATA) periodically updates the values for the Gas Constant.

The value used in ISO 6976 -1995 gives the value of the Molar gas constant in Annex B, section B.1 as 8.314510 ± 0.000070 J mol^{-1} K^{-1}.

This is from CODATA Bulletin No. 63 (Nov 1986)
http://physics.nist.gov/cuu/pdf/codata86.pdf

GPA 2145 -09 gives the value of the Molar gas constant as 8.314 472 ± 0.000015 J mol^{-1} K^{-1}. This is the value is given in the:

- 1998 update **http://physics.nist.gov/cuu/pdf/all_1998.pdf**
- 2002 update **http://physics.nist.gov/cuu/pdf/all_2002.pdf**
- 2006 update **http://physics.nist.gov/cuu/pdf/all_2006.pdf**

The molar gas constant was update in 2010 to a value of 8.3144621 ± 0.0000075 J mol^{-1} K^{-1}.

Year	Value	Link
1986	8.314510 ± 0.000070 J mol^{-1} K^{-1}	**http://physics.nist.gov/cuu/pdf/codata86.pdf**
1998		**http://physics.nist.gov/cuu/pdf/all_1998.pdf**
2002		**http://physics.nist.gov/cuu/pdf/all_2002.pdf**
2006	8.314 472 ± 0.000015 J mol^{-1} K^{-1}	**http://physics.nist.gov/cuu/pdf/all_2006.pdf**
2010	8.3144621 ± 0.0000075 J mol^{-1} K^{-1}	

The following Gas Constant Values are used in the calculations:

For the Metric based calculations the value is 8.3144621. For the FPS calculation the gas constant was converted to L atm mol^{-1} K^{-1} for a value of 0.082057361 L atm mol^{-1} K^{-1}. If the gas constant value needs to be changed, it can be edited by opening the ccf file in the custom calculator and modifying the value.

If the most recent value is needed, it can be accessed from the NIST Reference on Constants, Units, and Uncertainty web page at:

http://physics.nist.gov/cgi-bin/cuu/Value?r|search_for=abbr_in!

7 References

GPA Standard 2145-09 Table of Physical Properties for Hydrocarbons and Other Compounds of Interest to the Natural Gas Industry.

GPA Standard 2172-09 Calculation of Gross Heating Value, Relative Density, Compressibility and Theoretical Hydrocarbon Liquid Content for Natural Gas Mixtures for Custody Transfer.

GPA TP17 (1998 Revision) Table of Physical Properties of Hydrocarbons for Extended Analysis of Natural Gases.

ISO 6976: 1995 with Cor. 2: 1997(E) and Cor.3:1999(E) Natural gas - Calculation of calorific values, density, relative density and Wobbe Index from composition.

ISO 6976: 2016(E) Natural gas - Calculation of calorific values, density, relative density and Wobbe Index from composition.

ASTM D3588-98 (Reapproved 2011) Standard Practice for Calculating Heat Value, Compressibility Factor, and Relative Density of Gaseous Fuels.

ASTM DS 4A Physical Constants of Hydrocarbons and Non-Hydrocarbon Compounds, 1971

ASTM DS 4B Physical Constants of Hydrocarbons and Non-Hydrocarbon Compounds, 2nd Edition, 1987

NIST Standard Reference Database 23 Version 9.1

NIST/TRC Web Thermo Tables (WTT) Professional Edition (Version 2-2012-1-Pro)

Updates and other reference Material are available at:

- **https://www.gpaglobal.org/publications/**
- **http://www.iso.org/iso/home/standards.htm**
- **http://www.astm.org/**

www.agilent.com

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