

TECHNICAL BULLETIN

**Combustion Calculations,
Normalisations and Conversions**

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Combustion & Environmental Monitoring

Combustion Calculations, Normalisations and Conversions

Introduction

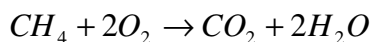
This document provides detailed information on use of calculations within analyser systems, to give derived values, normalisations, combustion efficiency data, along with other useful measurement conversions.

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1. Calculation of Carbon Dioxide (CO₂) values

1.1 Calculating the CO₂ max value

Most stack gases contain carbon dioxide as a result of the combustion of carbon and oxygen. For example, the chemical equation for combustion of methane in air is:



The maximum concentration of CO₂ will occur for stoichiometric combustion, i.e. where all the fuel reacts with the oxygen in the combustion air. The actual concentration depends on the relative amounts of carbon, hydrogen and other combustibles in the fuel. CO₂ max values for common fuel types are shown in Table 1.

Table 1 CO₂ max values for common fuel types, assuming the gases are dry.

FUEL	CO ₂ max (%)
Wood	19.7
Natural Gas	11.9
Light Fuel Oil	15.5
Heavy Fuel Oil	15.8
Propane	13.8
Anthracite	19.1
Lignite (Peat)	18.6
Bituminous Coal	18.4

For other hydrocarbon fuels, CO₂ max can readily be calculated.

$$CO_2 \text{ max} = \frac{\text{No. of } CO_2 \text{ molecules produced by complete combustion of fuel}}{\text{Total no. of molecules of combustion products}}$$

$$\text{For wet gases: } CO_2 \text{ max} = \frac{c}{c + \frac{h}{2} + \frac{79.1}{20.9} \times \left(c + \frac{h}{4}\right)} \%$$

$$\text{For dry gases: } CO_2 \text{ max} = \frac{c}{c + \frac{79.1}{20.9} \times \left(c + \frac{h}{4}\right)} \%$$

where c and h are the number of carbon and hydrogen atoms, respectively, in each hydrocarbon molecule. The two terms differ because the wet gas figure includes the water produced during combustion.

The measured concentration will never be as high as CO₂ max since the calculation ignores a number of real-world factors such as moisture in the fuel and dilution of flue gas by air leaks downstream of the combustion process.

These equations may be used even where the fuel is not a pure hydrocarbon, but the result will be somewhat less accurate.

1.2 Calculation of the CO₂ concentration

We can calculate the concentration of carbon dioxide [CO₂] in the stack gas if we know the oxygen concentration [O₂] and CO₂ max or fuel type.

$$[\text{CO}_2] = \frac{\text{CO}_2 \text{ max} \times (20.9 - [\text{O}_2])}{20.9}$$

If the [O₂] is a dry measurement, we must use a dry CO₂ max and [CO₂] is also dry basis. If the [O₂] is a wet measurement from an in-situ analyser, then we must use the wet CO₂ max to get a wet [CO₂].

2 Calculations of Efficiency using British Standard BS845

The efficiency calculation is based on British Standard BS845:Part 1:1987 *Assessing thermal performance of boilers for steam, hot water and high temperature heat transfer fluids*. It is similar to the methods DIN 1942 and ASME PTC 4.1.

The Standard identifies a number of loss mechanisms in combustion processes. Three of these mechanisms can be detected by flue gas analysis:

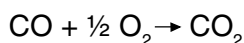
- 1 Loss due to sensible heat in dry gases, L₁
- 2 Loss due to enthalpy of water vapour, L₂
- 3 Loss due to unburned gases, L₃

The efficiency of the boiler is found by subtracting the sum of the losses from 100%. The calculation shows the efficiency as a fraction of the gross calorific value of the fuel.

$$\text{Efficiency} = 100\% - L_1 - L_2 - L_3$$

This calculation ignores a number of terms which are generally small but which may be significant in some circumstances. These include

- Losses due to unburned fuel in ash
- Radiative and convective losses in the boiler
- Water vapour concentration of the ambient air
- The enthalpy of combustion of hydrocarbons to CO + H₂O, since L₃ is based on the reaction



In spite of its limitations, the efficiency calculation will give a useful measure of the efficiency of combustion in most practical applications.

The loss terms are calculated as follows:

2.1 Loss due to sensible heat in dry flue gases

This is essentially a measurement of the amount of hot air passing out of the stack.

$$L_1 = k_1 \times \frac{T_f - T_a}{[CO_2]}$$

$[CO_2]$ = Concentration of CO_2 in stack gases, % by volume
 T_f = Flue gas temperature in °C
 T_a = Temperature of ambient air in °C

2.2 Calculation of k_1

$$k_1 = \frac{253 \times [C]}{Q_{gr}} \quad (\text{this is known as the Siegert constant})$$

$[C]$ = Carbon content of fuel, % by mass
 Q_{gr} = Gross calorific value of fuel in kJ/kg

2.3 Loss due to enthalpy of the water vapour in the flue gases

This includes both the latent heat of vaporization of the water in the stack gases and the heat required to raise the water vapour to stack temperature.

$$L_2 = k_2 \times (1185 + T_f - 2 \times T_a)$$

T_f = Flue gas temperature in °C
 T_a = Temperature of ambient air in °C

2.4 Calculation of k_2

$$k_2 = 2.1 \times \frac{[H_2O] + 9 \times [H]}{Q_{gr}}$$

$[H_2O]$ = Water content of fuel, % by mass
 $[H]$ = Hydrogen content of fuel, % by mass
 Q_{gr} = Gross calorific value of fuel in kJ/kg

2.5 Loss due to unburned fuel in the flue gases

This is the heat lost by incomplete combustion of the fuel, based on the fraction of the fuel which leaves the stack unburned.

$$L_3 = k_3 \times \frac{[CO] + [H_xC_y]}{[CO_2] + [CO] + [H_xC_y]}$$

$[CO]$ = Concentration of CO in stack gases, % by volume
 $[H_xC_y]$ = Concentration of hydrocarbons in stack gases, % by volume
 $[CO_2]$ = Concentration of CO_2 in stack gases, % by volume

2.6 Calculation of k_3

$$k_3 = 1.25 \times [C] - 55$$

[C] = Carbon content of fuel, % by mass

Table 2 Values of [H], [C], k_1 , k_2 and k_3 for common fuel types

Fuel	[H] %	*[C] %	$k_1^{\#}$	k_2 (dry)	$k_3^{\#}$	Q_{gr} kJ/kg
Wood	3.0	97.0	0.64	0.00140	6	19538
Coke	0.4	99.6	0.75	0.00021	70	33864
Heavy fuel oil	11.5	88.5	0.48	0.00512	53	46219
Light fuel oil	13.0	87.0	0.51	0.00473	54	44250
Natural gas	24.4	75.6	0.35	0.00806	40	55080
Propane	18.2	81.8	0.42	0.00667	48	49664
Coal	4.0	96.0	0.62	0.00184	63	39484
Butane	17.2	82.8	0.43	0.00638	48	49102
Anthracite	3.0	97.0	0.67	0.00148	65	36918

**These values assume the fuel is a pure hydrocarbon.*

#Refer to Section 12 References

2.7 Calculations of 'k' factors when burning Mixed Fuels

Where mixed fuels are being burned in the process, the constants (k_1 , k_2 and k_3) should be calculated as:

Constant of Mixed Fuels (Type A & Type B) = $a \times \text{Constant A} + b \times \text{Constant B}$

where a & b are the fractions of components Fuel Type A and Fuel Type B respectively.

Example: where the fuel mix is 70 % wood and 30 % coal

k_1 for Wood = 0.68; k_1 for Coal = 0.62

Combined Fuel $k_1 = 0.7 \times 0.68 + 0.3 \times 0.62 = 0.66$

3 Calculations of Efficiency using UNI standards

The UNI 9166:1987 standards² use the following calculations for efficiency:

$$Q_s = \left(\frac{A1}{21 - [O_2]} + B \right) \times (T_f - T_a) \quad \text{when } [O_2] \text{ is measured}$$

$$Q_s = \left(\frac{A2}{[CO_2]} + B \right) \times (T_f - T_a) \quad \text{when } [CO_2] \text{ is measured}$$

where

- Q_s = % loss
- T_f = flue gas temperature in °C
- T_a = ambient temperature in °C
- $[O_2]$ = oxygen concentration (dry), % Vol.
- $[CO_2]$ = carbon dioxide concentration (dry), % Vol.
- A1, A2, B are fuel factors:

Fuel	A1	A2	B
Natural gas	0.66	0.38	0.010
Propane	0.63	0.42	0.008
Light fuel oil	0.68	0.50	0.007
Heavy fuel oil	0.68	0.52	0.007

² Refer to Section 12 References

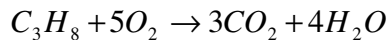
4.1 Calculating Excess Air

The Excess Air 'n' is calculated as:

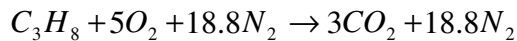
$$n = \frac{\text{Air not used}}{\text{Air required}}$$

$$n = \frac{[O_2]}{20.9 - [O_2]} \times \frac{V_o \text{ (dry)}}{A_o}$$

where V_o (dry) is the volume of the dry products of combustion and A_o is the volume of air at stoichiometry. The V_o / A_o factor is included to take account of the difference in the volume of combustion air and the volume of the products of combustion, since we define excess air in terms of the reactants but we actually measure the products. It can be calculated for any unknown fuel provided we can express the combustion process as a chemical equation, e.g. for combustion of propane.



If we include the nitrogen from the air, and remove the water, this equation becomes



Therefore

$$\frac{V_o \text{ (dry)}}{A_o} = \frac{3 + 18.8}{5 + 18.8} = 0.915$$

For hydrocarbon fuels, the V_o / A_o factor can be calculated from

$$\frac{V_o \text{ (dry)}}{A_o} = \frac{c + (3.73 \times (c + h/4))}{(1 + 3.73) \times (c + h/4)}$$

where c and h are the number of carbon and hydrogen atoms, respectively, per molecule of fuel. The factor 3.73 represents the contribution of N_2 to the total volume of the gases.

4.2 V_o (dry)/ A_o Values

For most commonly-used fuels, the V_o (dry)/ A_o factor³ will be between 0.89 and 0.98 (see table below); if no information is available on the fuel composition then a value of 0.95 is traditionally used.

FUEL	V_o (dry)/ A_o
Wood	0.98
Natural Gas	0.90
Light Fuel Oil	0.93
Heavy Fuel Oil	0.94
Propane	0.92
Anthracite	0.98
Lignite (Peat)	0.96
Bituminous Coal	0.98
Coke Oven Gas	0.90
Enriched Blast Furnace	1.95
Lean Blast Furnace	1.95
BOS Gas	1.25

³ Refer to Section 12 References

4.3 Lambda Factor

The Lambda factor is widely used as a measure of combustion air. It is calculated as:

$$\lambda = \frac{\text{Air input}}{\text{Air required}}$$

Excess air is calculated as:

$$n = \frac{\text{Air not used}}{\text{Air required}}$$

Therefore, $\lambda = 1 + n$

5 Calculation of Oxygen Normalisation

To comply with environmental legislation, readings of flue gases must be normalised to a specific oxygen content.

The formula for Oxygen normalisation is:

$$[G_N] = [G] \times \frac{(20.9 - O_{2,ref})}{(20.9 - [O_2])}$$

where

- $[G_N]$ = normalised gas concentration
- $[G]$ = measured gas concentration
- $O_{2,ref}$ = Reference oxygen content, % Vol
- $[O_2]$ = O_2 reading, % Vol

6 Calculation of Mass Emissions Rate

In order for the mass emissions rate to be calculated the following data must be available:

Barometric pressure - atmosphere, mb or inHg

Flue gas water concentration - % Vol

Cross-sectional area of the duct - m² or ft²

Density Correction - Default 1.00

6.1 Velocity

The flue gas velocity has to be measured first, prior to the mass emissions rate being calculated. This should be made using a suitable flow measuring device such as a pitot type flow probe, in which case velocity is calculated using the following equation

$$v = 1.291 \times \sqrt{\frac{1013}{B} \times \frac{T + 273}{293} \times \frac{P}{K}}$$

where v = Velocity in m/s

T = Temperature in °C

P = Pitot Pressure in Pa

K = Probe K Factor*

B = Barometric pressure in mb

* *K Factor is the calibration factor applied to the specific probe, and depends on its geometry.*

6.2 Calculate volumetric flow

Volumetric flow in m³/s

$$\text{actual flow} = \text{Velocity} \times \text{area}$$

where area is in m²

Dry equivalent flow in m³/s

$$\text{dry flow} = \text{actual flow} \times \frac{100 - [\text{H}_2\text{O}]}{100}$$

where $[\text{H}_2\text{O}]$ is the flue gas water concentration in %

Normal dry flow in m³/s

$$\text{dry flow}_{\text{NORM}} = \text{dry flow} \times \frac{(T_0 + 273)}{(T + 273)} \times \frac{B}{P_0}$$

where T = probe temperature in °C

T_0 = reference temperature in °C

NORM = normalised

B = atmospheric pressure in mbar

P_0 = reference pressure in mb

Flow is usually normalised to standard temperature and pressure (STP) which is defined as 0 °C and 1013 mb. Where flow is normalised to normal temperature and pressure (NTP), the reference values should be quoted.

6.3 Calculate Mass Flow

To calculate the mass flow, use the following formula:

$$\text{mass flow in kg/min} = \text{dryflow}_{\text{STP}} \times m \times [G] \times 60 \times 10^{-6}$$

where $m = \text{mol.weight} / 22.414$, in kg/m^3

mol. weight = gram molecular weight

[G] = Concentration of measured gas in ppm

22.414 = molar volume in litres

Gas	mol.wt	m (kg/m ³)
CO	28	1.249
NO	30	1.338
NO ₂	46	2.052
SO ₂	64	2.858
NO _x	46	2.052
CO ₂	44	1.963

6.4 Example - Mass flow calculation

To calculate mass flow of NO_x in kg/hr where the given information is:

Velocity = 15 m/s (measured using flow probe)

Duct cross-sectional area = 20 m²

Flue gas water concentration = 15 %

Probe temperature = 55 °C

Atmospheric pressure = 1022 mb

Measured NO_x = 150 ppm

Step 1 actual flow = Velocity x area = 15 x 20 = 300 m³/s

Step 2 dry flow = actual flow x {(100 - [H₂O]) / 100} = 300 x {(100 - 15) / 100} = 255 m³/s

Step 3 dry flow_{STP} = dryflow x (273 / (T + 273)) x (B / 1013)
= 255 x {273 / (55 + 273)} x (1022 / 1013) = 214.1 m³/s

Step 4 mass flow in kg/min = dryflow_{STP} x m x [NO_x] x 60 x 10⁻⁶
= 214.1 x 2.052 x 150 x 60 x 10⁻⁶ = 3.95 kg/min

Step 5 mass flow in kg/hr = mass flow in kg/min x 60
= 3.95 x 60 = **237.0 kg/hr**

7 Calculation of NO_x

If the concentrations of NO and NO₂ are both measured, then for most practical purposes:

$$[NO_x] = [NO] + [NO_2]$$

However if the proportion of NO₂ is small (< 10 %), sufficient accuracy may be obtained by measuring only NO and multiplying by an estimated 'NO_x factor'. The additional proportion of NO₂ is sometimes referred to as the 'NO₂ factor', and expressed as a percentage (%).

They are related thus:

$$NO_x \text{ factor} = 1 + (NO_2 \text{ factor} / 100)$$

Example:

$$\begin{aligned} [NO] &= 100 \text{ ppm} \\ NO_x \text{ factor} &= 1.05 \text{ (NO}_2 \text{ factor} = 5 \%) \\ [NO_x] &= 100 \times 1.05 = 105 \text{ ppm} \end{aligned}$$

8 Conversion of Dry measurement readings to Wet readings

Extractive analysers usually report measurement data on a dry basis. In order to report data as 'Wet' analysis, we require information on the percentage water content of the flue gas.

For example, the typical water content for coal burning boilers is approximately 6 to 8%. Where the analysis is wet, the water content is displayed in percentage terms (%).

The formula for wet analysis is as follows:

$$[G_{wet}] = [G_{dry}] \times \left(\frac{100 - [H_2O]}{100} \right)$$

$$\begin{aligned} [H_2O] &= \% \text{ water content of stack gas by volume} \\ [G_{wet}] &= \text{gas concentration wet} \\ [G_{dry}] &= \text{gas concentration dry} \end{aligned}$$

9 Conversion of Wet measurement readings to Dry readings

In-situ analysers normally report measurement data on a wet basis. In order to report data as 'Dry' analysis, we require information on the percentage water content of the flue gas.

For example, the typical water content for coal burning boilers is approximately 6 to 8%. Where the analysis is wet, the water content is displayed in percentage terms (%).

The formula for dry analysis is as follows:

$$[G_{dry}] = [G_{wet}] \times \left(\frac{100}{100 - [H_2O]} \right)$$
$$\begin{aligned} [H_2O] &= \% \text{ water content of stack gas by volume} \\ [G_{wet}] &= \text{gas concentration wet} \\ [G_{dry}] &= \text{gas concentration dry} \end{aligned}$$

10 Emissions concentrations

10.1 Conversion of mg/m³ to lb/ft³

$$1 \text{ mg/m}^3 = 6.243 \times 10^{-8} \text{ lb/ft}^3.$$

10.2 Conversion of lb/MMBtu to ng/J

$$1 \text{ ng/J} = 2.326 \times 10^{-3} \text{ lb / MMBtu}$$

10.3 Conversion Table - ppm to mg/m³

To convert from ppm to mg/m³ at STP

$$[G] \text{ mg/m}^3 = [G] \text{ ppm} \times \frac{\text{mol. wt.}}{\text{molar vol.}}$$

mol. wt. = gram molecular weight

Molar volume at STP (0 °C and 1013 mb) = 22.414 l

Conversion factors are given in table below.

0°C	101.3 kPa
1 ppm = x mg/m ³	
C	0.54
CO	1.25
CO ₂	1.96
NO	1.34
NO ₂	2.05
NO _x	2.05
HCl	1.63
HF	0.89
H ₂ S	1.52
NH ₃	0.76
SO ₂	2.86
SO ₃	3.57
CH ₄	0.72

10.4 F Factor

As an alternative to quoting emissions as a concentration value, some legislation requires mass emissions to be quoted as nanograms per joule (ng/J) or pounds per million Btu (usually shown as lb/MMBtu). The conversion requires a fuel-dependent F factor.

$$E = C \times F \times \frac{20.9}{20.9 - [O_2]}$$

where

- E = emission in lb/MMBtu or ng/J
- C = concentration in lb/ft³ or mg/m³
- F = F factor for the fuel in question
- [O₂] = oxygen concentration in %.

F factors for a number of common fuel types are shown in the table below:

Fuel	F	F	F
	ft ³ /MMBtu	m ³ /GJ	m ³ /MJ
Coke	9848	264.4	0.2644
Anthracite	9411	252.5	0.2525
Bituminous coal	9112	245.0	0.2450
Heavy fuel oil	8563	230.1	0.2301
Light fuel oil	8563	230.1	0.2301
Butane	8115	218.0	0.2180
Propane	8115	218.0	0.2180
Natural gas	8115	218.0	0.2180
Wood	8609	231.1	0.2311

for other fuels, F may be calculated as:

$$F = \frac{10^6 \times (3.64 \times [H] + 1.53 \times [C] + 0.57 \times [S] + 0.14 \times [N] - 0.46 \times [O])}{Q_{gr}} \text{ ft}^3/\text{MMBtu}$$

$$F = \frac{26854 \times (3.64 \times [H] + 1.53 \times [C] + 0.57 \times [S] + 0.14 \times [N] - 0.46 \times [O])}{Q_{gr}} \text{ m}^3/\text{GJ}$$

where [X] is the elemental content of component X in the fuel, expressed as % by mass and Q_{gr} is the gross heating value in Btu/lb.

NOTE: These figures have been determined at 0 °C (32 °F). To convert to a different temperature, multiply by

$$\frac{T + 273}{273}$$

T = Temperature in °C

11 Table of Flue Gas Water Content at Various Dewpoint Temperatures

The table shows the approximate water content of flue gas for a range of dewpoint temperatures.

DP °C	% v/v	g/m ³
-40	0.01	0.12
-30	0.04	0.34
-20	0.10	0.89
-10	0.26	2.14
0	0.61	4.87
10	1.22	9.44
20	2.32	17.4
30	4.21	30.5
40	7.33	51.4
50	12.26	83.3
60	19.81	131
70	30.99	198
80	47.07	293
90	69.56	421

⁵ Refer to Section 12 References

All calculations and formulae are British Standard BS 845: Part1 : 1987 unless otherwise indicated.

1. British Standard BS 845: Part 1: 1987 Assessing thermal performance of boilers for steam, hot water and high temperature heat transfer fluids.

Technical Data on Fuel (7th ed), JW Rose & JR Cooper, Scottish Academic Press, London 1977

2. UNI 9166:1987 standards are those used by the Italian environment agency for the calculation of efficiency

3. Spiers, H.M. 'Technical Data of Fuel' (1962) pp. 99, British National Committee, World Energy Conference

4. 40CFR 60.45 - Standards of Performance for Fossil-fuel-fired Steam Generators for which construction is commenced after August 17th, 1971; Code of Federal Regulations, Washington DC, U.S.A.

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