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Generation and analysis of toxic gases in fire — Calculation of species yields, equivalence ratios and combustion efficiency in experimental fires

Production et analyse des gaz toxiques dans le feu — Calcul des taux de production des espèces, des rapports d'équivalence et de l'efficacité de combustion dans les feux expérimentaux

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Foreword

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The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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For an explanation on the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT) see the following URL: www.iso.org/iso/foreword.html.

This document was prepared by Technical Committee ISO/TC 92, *Fire safety*, Subcommittee SC 3, *Fire threat to people and environment*.

This third edition cancels and replaces the second edition (ISO 19703:2010), which has been technically revised.

The main changes compared to the previous edition are as follows:

- redundant symbols have been deleted;
- missing symbols have been added;
- units of some symbols in formulae and tables have been corrected to conform with the ISO/IEC Directives, Part 2;
- unnecessary formulae have been deleted;
- mistakes in formulae have been corrected.

Introduction

It is the view of committees ISO TC 92/SC 3, ISO TC 92/SC 4, and IEC TC 89 that commercial products should not be regulated solely on the basis of the toxic potency of the effluent produced when the product is combusted in a bench-scale test apparatus (physical fire model). Rather, the information that characterizes the toxic potency of the effluent should be used in a fire risk or hazard assessment that includes the other factors that contribute to determining the magnitude and impact of the effluent. It is intended that the characterization of

a) the apparatus used to generate the effluent, and

b) the effluent itself

be in a form usable in such a fire safety assessment.

As described in ISO 13571, the time to incapacitation in a fire is determined by the integrated exposure of a person to the fire effluent components. The toxic species concentrations depend on both the yields originally generated and the successive dilution in air. The former are commonly obtained using a bench-scale apparatus (in which a specimen from a commercial product is burned) or a real-scale fire test of the commercial product. These yields, expressed as the mass of effluent component per mass of fuel consumed, are then inserted into a fluid mechanical model which estimates the rate of fuel consumption, transport and dilution of the effluent throughout the building as the fire evolves.

For the engineering analysis to produce accurate results, it is preferred that the yield data come from an apparatus that has been demonstrated to produce yields comparable to those produced when the full product is burned. In addition to depending on the chemical composition, conformation and physical properties of the test specimen, toxic-product yields are sensitive to the combustion conditions in the apparatus. Thus, one means of increasing the likelihood that the yields from a bench-scale apparatus are accurate is to operate it under combustion conditions similar to those expected when the real product burns. As described in ISO 19706, the important conditions include whether the fuel is flaming or non-flaming, the degree of flame extension, the fuel/air equivalence ratio and the thermal environment. Similarly, these parameters should be known for a real-scale fire test.

The yields of toxic gases, the combustion efficiency and the equivalence ratio are likely to be sensitive to the manner in which the test specimen is sampled from the whole commercial product. There can be difficulty or alternative ways of obtaining a proper test specimen. That is not the subject of this document, which presumes that a specimen has been selected for study and characterizes the combustion conditions and the yields of effluent species for that specimen.

For those experimental fires in which time-resolved data are available, the methods in this document should be used to produce either instantaneous or averaged values. The application can be influenced by changes in the chemistry of the test specimen during combustion. For those fire tests limited to producing time-averaged gas concentrations, the calculated values produced by the methods in this document are limited to being averages as well. In real fires, combustion conditions, the fuel chemistry and the composition of fire effluent from many common materials and products vary continuously during the course of the fire. Thus, how well the average yields obtained using these methods correspond to the yields in a given real fire has much to do with the stage of the fire, the pace of fire development and the chemical nature of the materials and products exposed.

This document provides definitions and equations for the calculation of toxic product yields and the fire conditions under which they have been derived in terms of equivalence ratio and combustion efficiency. Sample calculations for practical cases are provided.

Generation and analysis of toxic gases in fire — Calculation of species yields, equivalence ratios and combustion efficiency in experimental fires

1 Scope

This document provides definitions and equations for the calculation of toxic product yields and the fire conditions under which they have been derived in terms of equivalence ratio and combustion efficiency. Sample calculations for practical cases are provided. The methods are intended to be used to produce either instantaneous or averaged values for those experimental fires in which time-resolved data are available.

This document is intended to provide guidance to fire researchers for

- recording appropriate experimental fire data,
- calculating average yields of gases and smoke in fire effluents in fire tests and fire-like combustion in reduced scale apparatus,
- characterizing burning behaviour in experimental fires in terms of equivalence ratio and combustion efficiency using oxygen consumption and product generation data.

This document does not provide guidance on the operating procedure of any particular piece of apparatus or interpretation of data obtained therein (e.g. toxicological significance of results).

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 13943, *Fire safety — Vocabulary*

3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 13943 and the following apply.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

- IEC Electropedia: available at http://www.electropedia.org/
- ISO Online browsing platform: available at http://www.iso.org/obp

3.1
mass concentration of gas
mass of gas per unit volume

Note 1 to entry: The mass concentration of a gas shall be derived directly from the measured volume fraction and its molar mass or measured directly.

Note 2 to entry: Mass concentration is typically expressed in units of grams per cubic metre.

3.2

mass concentration of particles

mass of solid and liquid aerosol particles per unit volume

Note 1 to entry: Mass concentration of particles is typically expressed in units of grams per cubic metre.

3.3

molar mass

mass of 1 mole

Note 1 to entry: Molar mass is normally expressed in units of grams per mole.

3.4

recovery of element

⟨in a specified combustion product⟩ degree of conversion of an element in the test specimen to a corresponding gas

Note 1 to entry: It is the ratio of the actual yield to notional yield of the gas containing that element.

3.5

relative atomic mass

average mass of one atom of an element divided by one twelfth of the mass of one atom of carbon (isotope ^{12}C)

3.6

stoichiometric oxygen-to-fuel mass ratio

amount of oxygen needed by a material for complete combustion

Note 1 to entry: Stoichiometric oxygen-to-fuel mass ratio is typically expressed in units of grams of oxygen per gram or kilogram of burnt material.

3.7

uncertainty

uncertainty of measurement

parameter, associated with the result of a measurement, that characterizes the dispersion of the values that could reasonably be attributed to the measurement

Note 1 to entry: The description and propagation of uncertainty in measurements are described in ISO/IEC Guide 98-3[24].

[SOURCE: ISO/IEC Guide 98-3:2008, 2.2.3, modified—The term has been changed from “uncertainty (of measurement)” to “uncertainty”; “uncertainty of measurement” has been added as an admitted term; the original Notes 1, 2 and 3 to entry have been deleted and a new Note 1 to entry has been added.]

3.8

expanded uncertainty

quantity defining an interval about the result of a measurement that may be expected to encompass a large fraction of the distribution of values that could reasonably be attributed to the measurement

Note 1 to entry: Adapted from ISO/IEC Guide 98-3:2008, 2.3.5.

4 Symbols and units

Table 1 — Symbols

Symbol	Quantity	Typical unit
A	extinction area of smoke	square metre
$A_{\sigma f}$ or A_{SEA}	specific extinction area of smoke per unit mass of material burned	square metres per gram or square metres per kilogram
D_{MO}	mass optical density ($\log_{10}$ analogue of A_{SEA})	square metres per gram or square metres per kilogram
$F_{R,E}$	recovery fraction of element E in gas containing E	dimensionless
ΔH_{act}	measured heat release in a combustion	kilojoules per gram
ΔH_{c}	net heat of combustion or enthalpy generated in complete combustion	kilojoules per gram
I/I_{0}	fraction of light transmitted through smoke	dimensionless
L	is the length of the light path through the smoke	metre
$m_{A,E}$	relative atomic mass of the element E	dimensionless
m_{E}	mass fraction of element E in the material	dimensionless
m_{fuel}	mass of fuel	gram
m_{gas}	total mass of the gas of interest	gram
$m_{m,loss}$	total mass loss of material	gram
$\dot{m}_{m,loss}$	material mass loss rate	grams per minute
$m_{O,act}$	actual mass of oxygen available for combustion	gram
$\dot{m}_{O,act}$	actual mass flow of oxygen available for combustion	grams per minute
$m_{O,stoich}$	stoichiometric mass of oxygen required for complete combustion	gram
m_{part}	total mass of particles	gram
M_{gas}	molar mass of the gas of interest	grams per mole
M_{poly}	molar mass of the polymer unit	grams per mole
n_{E}	number of atoms of element E in one molecule of gas	dimensionless
$\mathrm{n}_{E,poly}$	number of atoms of element E in the polymer unit	dimensionless
P_{amb}	ambient pressure	kilopascal
P_{std}	standard pressure	101,3 kPa
T_{C}	thermodynamic temperature of the gas of interest at the point of measurement	kelvin
V	volume of chamber	cubic meter
V_{eff}	total volume of fire effluent	cubic metre
$\dot{V}_{air}$	volume air flow	cubic metres per minute
$w_{O,cons}$	measured mass fraction of oxygen consumed per unit mass of fuel	dimensionless
$w_{O,der}$	derived mass fraction of oxygen consumed per unit mass of fuel	dimensionless
$w_{Oex,poly}$	mass fraction of oxygen in polymer that contributes to the formation of oxygen-containing products	dimensionless
$w_{O,gases}$	mass fraction of oxygen consumed in the form of the major oxygen-containing products ($w_{O,CO2}$ + $w_{O,CO}$ + $w_{O,H2O}$)	dimensionless
$w_{O,poly}$	mass fraction of oxygen in the polymer	dimensionless
Y_{gas}	measured mass yield of gas of interest	dimensionless
Y_{part}	measured mass yield of smoke particles	dimensionless
α	linear decadic absorption coefficient (or optical density)	inverse metre

Table 1 *(continued)*

Symbol	Quantity	Typical unit
α_k	light extinction coefficient	inverse metre
χ	combustion efficiency	dimensionless
χ_{cox}	combustion efficiency calculated from the generation efficiency of carbon in the fuel to oxides of carbon	dimensionless
χ_{O}	combustion efficiency calculated from oxygen depletion	dimensionless
χ_{prod}	combustion efficiency calculated from the oxygen in the major combustion products	dimensionless
ϕ	equivalence ratio	dimensionless
η	generation efficiency for oxides of carbon	dimensionless
φ_{gas}	volume fraction of the gas of interest	dimensionless
φ_{O}	volume fraction oxygen in the air supply (0,209 5 for dry air)	dimensionless
ρ_{gas}	mass concentration of the gas of interest	grams per cubic metre
$\rho_{m,loss}$	mass loss concentration of the material	grams per cubic metre
$\rho_{O,act}$	actual mass concentration of oxygen available for combustion	grams per cubic metre
ρ_{part}	mass concentration of the smoke particles	grams per cubic metre
$\sigma_{m,\alpha}$	mass specific extinction coefficient	square metres per gram or square metres per kilogram
Ψ_{gas}	notional yield (mass fraction) of gas of interest	dimensionless
Ψ_{O}	stoichiometric oxygen-to-fuel mass ratio	dimensionless

5 Appropriate input data required for calculations

5.1 Data handling

5.1.1 Uncertainty

In calculating the fire parameters described in this document, the uncertainty or error associated with each component shall be taken into account and they shall be combined in the correct manner[1]. Uncertainty is derived from accuracy (how close the measured value is to the true value) and precision (how well the values agree with each other). There are uncertainties relating to physically measured parameters (e.g. mass loss and gas concentrations).

Assuming all errors to be independent, the total error, δq, is obtained by summing the squares of the errors in accordance with the general Formula (1):

$$\delta q = \sqrt{\left(\frac{\delta q}{\delta a}\delta a\right)^2 + \ldots + \left(\frac{\delta q}{\delta z}\delta z\right)^2} \qquad (1)$$

In other words, evaluate the error caused by each of the individual measurements, then combine them by taking the root of the sum of the squares.

In empirically derived equations, uncertainties in “constant” values shall be treated similarly to measurement uncertainties. If a constant is truly constant, i.e. has negligible uncertainty, it can be neglected.

5.1.2 Significant figures and rounding off

When recording and reporting data, significant figures shall be handled properly. The general approach is to carry one digit beyond the last certain one. When rounding off, the typical rule is to round up when the figure to be dropped is 5 or more and round down when it is less than 5.

5.2 Test specimen information

5.2.1 Composition

Information shall be given where possible on the combustible fraction, organic and inorganic combustible components, inert components, elemental composition, empirical formula and molecular or formula weight.

Where the combustible in a fire experiment is a single, homogenous material, perhaps with dispersed additives, the molecular formula of the material shall be provided. Commercial products, however, are generally non-homogeneous combinations of materials, with each component containing one or more polymers and possibly multiple additives. For complex materials representative of commercial products, the yields, effective heats of combustion, etc. vary with time as the various components become involved. For some of the following (global) calculations, a simplification is the use of an empirical formula for the composite.

5.2.2 Net heat of combustion

The net heat of combustion for combustible components shall be required for some of the calculations (e.g. combustion efficiency).

5.3 Fire conditions

5.3.1 Apparatus

Give the name of the apparatus with a brief description of mode of operation (e.g. flow-through steady state, calorimeter and closed chamber system). Refer to the appropriate standard or other reference relating to the procedure.

5.3.2 Set-up procedure

The fire conditions are generally apparatus-dependent and largely dictated by the set-up procedure for the particular apparatus. The following information shall be required:

a) test specimen details, its mass, dimensions and orientation of the combustible;

b) thermal environment, in terms of the temperature (expressed in degrees Celsius) and irradiance (expressed in kilowatts per square metre) to which test specimen is subjected;

NOTE The temperature distribution and the radiation field in a test are frequently not uniform and, as a result, are rarely well documented. Sufficient information about the thermal and radiative conditions is intended to allow another person to reproduce the results using the same apparatus, compare the results with results for the same specimen tested in another apparatus, etc.

c) oxygen concentration in the air supply (volume percent or volume fraction);

d) volume of chamber or air flow. For a closed system, give the air volume (expressed in litres or cubic metres) and for an open system, give the air flow (expressed in litres per minute or in cubic metres per minute) and the dynamics of the flow. In both cases, give information on the atmospheric mixing conditions and the degree of homogeneity of the fire effluent.

5.4 Data collection

5.4.1 Data acquisition

Time-resolved data or time-integrated data may be acquired. The method of data acquisition shall be specified in the test protocol.

5.4.2 Measured data and observations

Most of the following data parameters shall be used to calculate yields, equivalence ratios and combustion efficiencies in experimental fires. Usually, the units applied to data should be dictated by the operational procedure associated with a particular piece of apparatus. The following are a number of suggested typical units:

a) mass loss of the test specimen, derived by measuring the test specimen mass before and after test to give overall mass loss (expressed in milligrams, grams or kilograms) or mass loss fraction (expressed in mass percent, grams per gram or kilograms per kilogram), or by measuring the specimen mass throughout a test to give mass loss rate (expressed in milligrams per second, grams per minute or kilograms per minute);

b) gas and vapour concentrations and oxygen depletion (expressed in volume percent, volume fraction, microlitres per litre, milligrams per litre or milligrams per cubic metre);

c) smoke particulate concentration (expressed in milligrams per litre or milligrams per cubic metre) and smoke obscuration (expressed in optical density per metre or square metres per kilogram);

d) heat release (expressed in kilojoules per gram), used to calculate combustion efficiency, forms part of the protocol for some apparatuses;

e) combustion mode, time to ignition (expressed in minutes or seconds) and whether the specimen flames or not throughout the test.

6 Calculation of yields of fire gases and smoke, stoichiometric oxygen-to-fuel mass ratio and recovery of key elements

6.1 Calculation of measured yields from fire gas concentration data

In experimental fires, the mass yield, Y_{gas}, of a gas shall be calculated from the measured mass concentration of the gas of interest and the mass loss concentration of the material in accordance with Formula (2) (see NOTES 1, 2 and 3):

$$Y_{\text{gas}} = \frac{\rho_{\text{gas}}}{\rho_{\text{m,loss}}} \tag{2}$$

where

ρ_{gas} is the mass concentration of the gas;

$\rho_{\text{m,loss}}$ is the mass loss concentration of the material.

Alternatively, Y_{gas} shall be calculated from the total mass of gas generated and the total mass loss of material in accordance with Formula (3):

$$Y_{\text{gas}} = \frac{m_{\text{gas}}}{m_{\text{m,loss}}} \tag{3}$$

where

m_{gas}	is the total mass of the gas;
$m_{\text{m,loss}}$	is the total mass loss of the material.

NOTE 1 These calculations can be derived from instantaneous data or from data which assumes that the gases are uniformly dispersed in a certain volume and that this volume is the same one in which the lost sample mass is (evenly) dispersed. If the dispersion is not uniform, the equations still work if the lost mass and the gas in question are dispersed equivalently. If a combustion gas is prone to surface losses within the apparatus, the apparent yield depends on where the concentration is being measured.

NOTE 2 In flow-through devices, the total effluent is generally well mixed at some distance downstream. For closed-box combustion systems, it is not necessarily so, especially if there are large molecular weight differences and large thermal gradients. If multiple fuels are involved, only some averaged combined yield can be calculated.

NOTE 3 In setting up these calculations, uncertainties relating to lost sample mass, fluctuations in the measured concentration, etc. occur.

The uncertainty shall be monitored. The calculated yield shall take account of and combine these uncertainties, enabling a sound basis for comparing yields under different combustion conditions, comparing yields from different materials and so on.

Whilst concentrations of the specific gas are most often measured in volume fractions, Formulae (4) and (5) show how to convert the volume fraction of a gas to its mass concentration:

$$\rho_{\text{gas}} = \varphi_{\text{gas}} \times \frac{M_{\text{gas}}}{22{,}414\,\text{dm}^3 \cdot \text{mol}^{-1}} \times \frac{273{,}15\,\text{K}}{T_{\text{C}}} \times \frac{P_{\text{amb}}}{101{,}325\,\text{kPa}} \tag{4}$$

where

ρ_{gas}	is the mass concentration of the gas;
φ_{gas}	is the volume fraction of the gas;
M_{gas}	is the molar mass of the gas;
T_{C}	is the thermodynamic temperature of the gas at the point of measurement;
P_{amb}	is the ambient pressure;
273,15 K	is the standard thermodynamic temperature;
101,325 kPa	is the standard pressure;
22,414 $\text{dm}^3 \cdot \text{mol}^{-1}$	is the molar volume of an ideal gas at standard temperature and pressure.

Thus, for fire effluent at 20 °C and standard pressure, Formula (4) simplifies to Formula (5):

$$\rho_{\text{gas}} = \varphi_{\text{gas}} \times \frac{M_{\text{gas}}}{24{,}055\,\text{dm}^3 \cdot \text{mol}^{-1}} \tag{5}$$

EXAMPLE The calculations for a well-ventilated fire atmosphere where mass loss concentration of the material is 25 $\text{g} \cdot \text{m}^{-3}$ and the volume fraction of carbon monoxide (CO) is 0,125% (or 0,001 25) at 20 °C are shown in Formulae (6) and (7):

$$\rho_{\text{CO}} = 0{,}001\,25 \times \frac{28{,}01\,\text{g} \cdot \text{mol}^{-1}}{24{,}055\,\text{dm}^3 \cdot \text{mol}^{-1}} = 0{,}001\,456\,\text{g} \cdot \text{dm}^{-3} = 1{,}456\,\text{g} \cdot \text{m}^{-3} \tag{6}$$

$$Y_{\text{co}} = 1{,}456\,\text{g} \cdot \text{m}^{-3} / 25\,\text{g} \cdot \text{m}^{-3} = 0{,}058\,2 \tag{7}$$

where

ρ_{CO} is the mass concentration of CO;

Y_{CO} is the mass yield of CO (mass of CO per unit mass of material);

28,01 $g{\cdot}mol^{-1}$ is the molar mass of CO.

The relative atomic mass, molar mass and gas concentration conversion factors for the major fire gases are listed in Tables 2 and 3.

Table 2 — Relative atomic mass of key fire gas elements[2]

Element	Symbol	Relative atomic mass[a]
Carbon	C	12,011
Hydrogen	H	1,0079
Oxygen	O	15,999
Nitrogen	N	14,007
Chlorine	Cl	35,453
Bromine	Br	79,904
Fluorine	F	18,998
Sulfur	S	32,065
Phosphorus	P	30,973
Antimony	Sb	121,76

[a] Relative atomic mass values rounded to five significant figures.

Table 3 — Molar masses of common fire gases and volume fraction/mass concentration conversion factors

Gas or vapour	Formula	Molar mass[a] $g{\cdot}mol^{-1}$	Gas concentration conversion factors (at 20 °C and 101,3 kPa)	
			To convert volume fraction to concentration, multiply by density of the gas:	To convert concentration to volume fraction, divide by density of the gas:
Carbon dioxide[b]	CO_2	44,01	1 830 $g.m^{-3}$	
Carbon monoxide[b]	CO	28,01	1 164 $g.m^{-3}$	
Hydrogen cyanide	HCN	27,02	1 124 $g.m^{-3}$	
Nitrogen dioxide	NO_2	46,01	1 913 $g.m^{-3}$	
Nitrous oxide	N_2O	44,01	1 831 $g.m^{-3}$	
Nitric oxide	NO	30,01	1 248 $g.m^{-3}$	
Ammonia	NH_3	17,03	708 $g.m^{-3}$	
Hydrogen chloride	HCl	36,46	1 516 $g.m^{-3}$	
Hydrogen bromide	HBr	80,91	3 364 $g.m^{-3}$	
Hydrogen fluoride	HF	20,01	832 $g.m^{-3}$	
Hydrogen sulfide	H_2S	34,08	1 417 $g.m^{-3}$	
Sulfur dioxide	SO_2	64,06	2 663 $g.m^{-3}$	

NOTE The concentration of a gas equals to volume fraction x density.

Example calculations:

If $\varphi_{CO} = 0{,}01$ (i.e. 1 % or 10^4 μl/l), $m_{CO} = 0{,}01 \times 1\,164\ g{\cdot}m^{-3} = 11{,}64\ g{\cdot}m^{-3}$.

If $m_{HCN} = 0{,}281\ g{\cdot}m^{-3}$, $\varphi_{HCN} = 0{,}281\ g{\cdot}m^{-3} / 1\,124\ g{\cdot}m^{-3} = 0{,}000\,25$ (i.e. 0,025 % or 250 μl/l).

[a] Molar mass values are rounded to two decimal places.

[b] CO_2/CO volume ratio equals the CO_2/CO mass ratio divided by 1,571.

Table 3 *(continued)*

Gas or vapour	Formula	Molar mass[a] g·mol^{-1}	Gas concentration conversion factors (at 20 °C and 101,3 kPa)	
			To convert volume fraction to concentration, multiply by density of the gas:	**To convert concentration to volume fraction, divide by density of the gas:**
Water	H_2O	18,01	749 g.m^{-3}	
Phosphoric acid	H_3PO_4	97,99	4 074 g.m^{-3}	
Acrolein	C_3H_4O	56,06	2 331 g.m^{-3}	
Formaldehyde	CH_2O	30,03	1 248 g.m^{-3}	
Oxygen	O_2	32,00	1 331 g.m^{-3}	

NOTE The concentration of a gas equals to volume fraction x density.

Example calculations:

If φ_{CO} = 0,01 (i.e. 1 % or 10^4 µl/l), m_{CO} = 0,01 × 1 164 g·m^{-3} =11,64 g·m^{-3}.

If m_{HCN} = 0,281 g·m^{-3}, φ_{HCN} =0,281 g·m^{-3} /1 124 g·m^{-3} =0,000 25 (i.e. 0,025 % or 250 µl/l).

[a] Molar mass values are rounded to two decimal places.

[b] CO_2/CO volume ratio equals the CO_2/CO mass ratio divided by 1,571.

6.2 Calculation of notional gas yields

6.2.1 General

The notional yields of gases and vapours are a measure of the maximum theoretical combustion product yields. They are based on the composition of the material and are entirely material-dependent. Two primary methods for calculating notional yields are described in 6.2.2 and 6.2.3.

6.2.2 From the elemental composition

Provided the elemental composition of the base material is known (e.g. by elemental analysis), the maximum possible (notional) yield, Ψ_{gas}, of fire gas corresponding to each specified element, E, is calculated in accordance with Formula (8):

$$\Psi_{gas} = m_E \times \frac{M_{gas}}{n_E \times m_{A,E}} \qquad (8)$$

where

m_E is the mass fraction of element E in the material;

M_{gas} is the molar mass of the gas which is under consideration;

n_E is the number of atoms of element E in one molecule of the gas;

$m_{A,E}$ is the relative atomic mass of the element E.

EXAMPLE The notional yield, Ψ_{CO}, of CO from cellulose, $(C_6H_{10}O_5)_n$, is calculated as given by Formula (9):

$$\Psi_{CO} = 0{,}445 \times \frac{28{,}01\ \text{g}\cdot\text{mol}^{-1}}{1 \times 12{,}011\ \text{g}\cdot\text{mol}^{-1}} = 1{,}038 \qquad (9)$$

where

0,445 is the mass fraction of carbon in the cellulose;

28,01 g·mol^{-1} is the molar mass of CO;

1 is the number of atoms of carbon in one molecule of CO;

12,011 g·mol^{-1} is the molar mass of carbon.

Factors for calculating notional gas yields from the elemental composition and derived from the term $\frac{M_{\text{gas}}}{n_{\text{E}} \times m_{\text{A,E}}}$ in Formula(8), are given in Table 4.

Table 4 — Factors for calculating notional gas yields from the elemental composition of material

Gas or vapour		Element *E* considered in base material	Factor[a]
Formula	**Molar mass** g·mol-1		
CO_2	44,01	carbon	3,664
CO	28,01	carbon	2,332
H_2O	18,02	hydrogen	8,939
HCN	27,02	nitrogen	1,929
NO_2	46,01	nitrogen	3,284
N_2O	44,01	nitrogen	1,571
NO	30,01	nitrogen	2,142
NH_3	17,03	nitrogen	1,216
HCl	36,46	chlorine	1,028
HBr	80,92	bromine	1,013
HF	20,01	fluorine	1,053
H_2S	34,08	sulfur	1,063
H_3PO_4	97,98	phosphorus	3,163
SO_2	64,06	sulfur	1,998
Acrolein (C_3H_4O)	56,06	carbon	1,556
Formaldehyde (CH_2O)	30,03	carbon	2,500

[a] Factor $\frac{M_{\text{gas}}}{n_{\text{E}} \times m_{\text{A,E}}}$ rounded to four significant figures.

6.2.3 From the empirical formula

If the empirical formula of the material is known, the notional yield, Ψ_{gas}, shall be calculated from Formula (10):

$$\Psi_{\text{gas}} = \frac{n_{\text{E,poly}}}{n_{\text{E}}} \times \frac{M_{\text{gas}}}{M_{\text{poly}}} \qquad (10)$$

where

$n_{\text{E,poly}}$ is the number of atoms of element *E* in the empirical formula;

M_{poly} is the molar mass of the empirical formula.

EXAMPLE The notional yield, Ψ_{CO_2}, of carbon dioxide (CO_2) from polypropylene with the empirical formula (C_3H_6) is calculated as shown in Formula (11):

$$\Psi_{CO_2} = \frac{3}{1} \times \frac{44{,}01\,g \cdot mol^{-1}}{42{,}03\,g \cdot mol^{-1}} = 3{,}142 \tag{11}$$

where

Ψ_{CO_2}	is expressed in grams of CO_2 per gram of polymer;
1	is the number of atoms of carbon in one molecule of CO_2;
3	is the number of atoms of carbon in the polymer unit;
$44{,}01\,g \cdot mol^{-1}$	is the molar mass of CO_2;
$42{,}03\,g \cdot mol^{-1}$	is the molar mass of the polymer unit.

NOTE The notional yield of a gas that contains more than one element from the fuel molecule is determined by the least prevalent element (other than oxygen). Thus, the notional yield of HCN can be most often determined by the nitrogen content of the fuel. However, for a product gas like formaldehyde, it can be either the carbon or hydrogen fraction that provides the criterion, depending on the fuel composition.

6.3 Calculation of recovery of elements in key products

The recovery fraction of an element in a key combustion product (alternatively, the conversion efficiency of an element in the test specimen to a corresponding gas) shall be calculated from the measured yield, Y_{gas}, of the gas of interest relative to its notional yield, Ψ_{gas}. For a material containing element E, this corresponds to Formula (12):

$$\eta_{E,\,gas} = Y_{gas}/\Psi_{gas} \tag{12}$$

where

Y_{gas}	is derived from Formulae (2) to (7);
Ψ_{gas}	is derived from Formulae (8) to (11);
$\eta_{E,\,gas}$	is the recovery fraction or conversion efficiency of element E in gas containing E.

6.4 Calculation of stoichiometric oxygen-to-fuel mass ratio

6.4.1 General

Stoichiometric oxygen-to-fuel mass ratio is the amount of oxygen needed by a material for complete combustion. Its derivation is somewhat more complex than notional gas yields and should be calculated by one of the three primary methods as described in 6.4.2 to 6.4.4.

6.4.2 From the chemical equation for complete combustion

6.4.2.1 For fuels containing C, H, O, for complete combustion to carbon dioxide and water

For the complete combustion of fuels containing C, H, O, the products only consist of CO_2 and gaseous H_2O. For organic fuels which contain oxygen, the requirement of oxygen from air for complete combustion is less than for those which do not contain oxygen. For a polymer with the general formula $C_aH_bO_c$, Formulae (13) to (15) apply:

$$C_aH_bO_c + zO_2 \rightarrow aCO_2 + b/2\ H_2O \tag{13}$$

and

$$z = \frac{2a + (b/2) - c}{2} \tag{14}$$

where

z is the (stoichiometric) number of moles of O_2 required for complete combustion of one mole of $C_aH_bO_c$;

a is the number of atoms of carbon in $C_aH_bO_c$;

b is the number of atoms of hydrogen in $C_aH_bO_c$;

c is the number of atoms of oxygen in $C_aH_bO_c$.

The stoichiometric oxygen-to-fuel mass ratio required for complete combustion is then calculated from Formula (15):

$$\Psi_0 = \frac{z \times 32{,}00}{M_{\text{poly}}} \tag{15}$$

where

Ψ_0 is the stoichiometric oxygen-to-fuel mass ratio, expressed in grams of oxygen per gram of polymer;

32,00 $g \cdot mol^{-1}$ is the molar mass of oxygen.

EXAMPLE The stoichiometric combustion equation for polymethyl methacrylate (PMMA) is given by Formulae (16) and (17):

$$C_{1,0}H_{1,6}O_{0,4} + 1{,}20\ O_2 \rightarrow CO_2 + 0{,}80\ H_2O \tag{16}$$

$$\Psi_0 = \frac{1{,}20 \times 32{,}00}{20{,}02} = 1{,}918 \tag{17}$$

where

1,0 is the number of atoms of carbon in $C_{1,0}H_{1,6}O_{0,4}$;

1,6 is the number of atoms of hydrogen in $C_{1,0}H_{1,6}O_{0,4}$;

0,4 is the number of atoms of oxygen in $C_{1,0}H_{1,6}O_{0,4}$;

1,20 is the (stoichiometric) number of moles of O_2 required for complete combustion of one mole of $C_{1,0}H_{1,6}O_{0,4}$;

1,918 is the calculated stoichiometric oxygen-to-fuel mass ratio of PMMA, expressed in grams of oxygen per gram of PMMA.

6.4.2.2 For fuels containing hetero-elements

For the complete combustion of fuels containing (organically-bound) elements in addition to C, H and O, it is assumed that nitrogen generates gaseous N_2, halogens generate gaseous acid gases (HCl, HBr, etc.) and sulfur generates gaseous SO_2.

Combustion equations for this type of test material are more complex because, for example, hydrogen from the material is used to form acid gases as well as water and sulfur consumes oxygen to form SO_2. For a halogenated material with the general formula of $C_aH_bO_cN_dCl_eBr_fF_gS_h$, the equation for stoichiometric oxygen-to-fuel mass ratio is given by Formula (18):

$$z=\frac{2a+2h-c+\left(b-e-f-g\right)/2}{2} \tag{18}$$

where

z is the (stoichiometric) number of moles of O_2 required for complete combustion of one mole of $C_aH_bO_cN_dCl_eBr_fF_gS_h$;

a is the number of atoms of carbon in $C_aH_bO_cN_dCl_eBr_fF_gS_h$;

b is the number of atoms of hydrogen in $C_aH_bO_cN_dCl_eBr_fF_gS_h$;

c is the number of atoms of oxygen in $C_aH_bO_cN_dCl_eBr_fF_gS_h$;

d is the number of atoms of nitrogen in $C_aH_bO_cN_dCl_eBr_fF_gS_h$;

e is the number of atoms of chlorine in $C_aH_bO_cN_dCl_eBr_fF_gS_h$;

f is the number of atoms of bromine in $C_aH_bO_cN_dCl_eBr_fF_gS_h$;

g is the number of atoms of fluorine in $C_aH_bO_cN_dCl_eBr_fF_gS_h$;

h is the number of atoms of sulphur in $C_aH_bO_cN_dCl_eBr_fF_gS_h$.

EXAMPLE The stoichiometric combustion equation for unplasticized polyvinyl chloride (C_2H_3Cl) is given by Formulae (19) to (20):

$$C_2H_3Cl + 2{,}5\ O_2 \rightarrow 2CO_2 + H_2O + HCl \tag{19}$$

and

$$\Psi_O=\frac{2{,}5\times 32{,}00}{62{,}5}=1{,}280 \tag{20}$$

where

2,5 is the (stoichiometric) number of moles of O_2 required for complete combustion of one mole of C_2H_3Cl;

$62{,}5\ g{\cdot}mol^{-1}$ is the molar mass of C_2H_3Cl;

1,280 is the calculated stoichiometric oxygen-to-fuel mass ratio for C_2H_3Cl, expressed in grams of oxygen per gram of C_2H_3Cl.

6.4.3 From the net heat of combustion, ΔH_c

It has been empirically determined that when a material burns, for every gram of oxygen consumed, the heat released is approximately 13,1 $kJ{\cdot}g^{-1}$ (accurate to ±5 %)[3]. Thus, if the net heat, ΔH_c, generated in complete combustion is known (e.g. as measured by bomb calorimetry), the stoichiometric oxygen-to-fuel mass ratio shall be calculated as given by Formula (21):

$$\Psi_0 = \Delta H_c / 13{,}1 \tag{21}$$

where

ΔH_c is the net heat or enthalpy per unit mass of fuel consumed, generated in complete combustion. It assumes that any water produced is in the gaseous state.

EXAMPLE The calculation for polystyrene is shown in Formula (22):

$$\Psi_0 = 39{,}2/13{,}1 = 2{,}99 \tag{22}$$

where

39,2 kJ·g^{-1}	is the net heat of complete combustion for polystyrene;
2,99	is the calculated stoichiometric oxygen-to-fuel mass ratio for polystyrene, expressed in grams of oxygen per gram of polystyrene.

NOTE From its chemical composition, Ψ_0 for polystyrene is 3,07 g·g^{-1}.

6.4.4 From the carbon content of the material

There is a less accurate correlation between the carbon content and stoichiometric oxygen-to-fuel mass ratio of polymeric materials empirically derived from the carbon content where the correlation coefficient, R^2, is 0,933, as shown in Formula (23):

$$\Psi_{0,\mathrm{poly}} = (m_C \times 3{,}87) - 0{,}339\ 9 \tag{23}$$

where

m_C	is the mass fraction of carbon in the material;
3,87 and 0,339 9	are empirically-derived mathematical coefficients.

EXAMPLE The calculation for polymethyl methacrylate is given by Formula (24):

$$\Psi_0 = (0{,}60 \times 3{,}87) - 0{,}339\ 9 = 1{,}98 \tag{24}$$

where

0,60	is the mass fraction of carbon in PMMA;
1,98	is the calculated stoichiometric oxygen-to-fuel mass ratio for PMMA, expressed in grams O_2 per gram of PMMA.

NOTE From its chemical composition, Ψ_0 for PMMA is 1,918 g·g^{-1}.

The step-wise procedures for calculating notional gas yields and stoichiometric oxygen-to-fuel mass ratio for a polymer containing C, O, H and X and for polyamide using chemical equation methods are summarized in Table 5.

Three methods for calculating stoichiometric oxygen-to-fuel mass ratio for selected polymers are compared in Table 6.

Notional gas yields and stoichiometric oxygen-to-fuel mass ratio derived for a number of common polymers are listed in Tables 7, 8 and 9.

Table 5 — Example calculations for notional gas yields and stoichiometric oxygen-to-fuel mass ratio for a polymer containing C, O, H, X and for polyamide using chemical equation methods

Polymer Empirical formula	Contains C, H, O, X $C_aH_bO_cX_d$	Polyamide $C_{12}H_{22}O_2N_2$ $(C_1H_{1,83}O_{0,17}N_{0,17})^b$
Molar mass of polymer M_{poly}, grams	$(12 \times a) + (1 \times b) + (16 \times c) + (m_{A,X} \times d)^a$	$(12 \times 12) + (1 \times 22) + (16 \times 2) + (14 \times 2) = 226$ (= 18,83 relative to each C atom)
Notional yield CO_2 Ψ_{CO_2}, grams per gram	$a/1 \times 44/M_{poly}$	$12 \times 44/226 = 2{,}336$ g·g^{-1}
Notional yield CO Ψ_{CO}, grams per gram	$a/1 \times 28/M_{poly}$	$12 \times 28/226 = 1{,}487$ g·g^{-1}
Notional yield H_2O Ψ_{H_2O}, grams per gram	$b/2 \times 18/M_{poly}$	$22/2 \times 18/226 = 0{,}876$ g·g^{-1}
Stoichiometric oxygen-to-fuel mass ratio, z moles O_2[c]	$(2a + b/2 - c)/2$	$(24 + 11 - 2)/2 = 16{,}5$ mol
Stoichiometric oxygen-to-fuel mass ratio of polymer $\Psi_{O,poly}$, grams per gram	z mol $\times 32/M_{poly}$	$16{,}5 \times 32/226 = 2{,}336$ g·g^{-1}

[a] $m_{A,X}$ is the relative atomic mass of the element X, expressed in grams per mole.

[b] Empirical formula re-based to one carbon atom.

[c] This assumes that nitrogen in the material is converted to N_2. In practice, a small proportion is converted to nitrogen products containing hydrogen or oxygen. The error is considered to be small.

Table 6 — Examples of stoichiometric oxygen-to-fuel mass ratio derived by three methods

Generic polymer type	**Empirical formula**	ΔH_c[a,b,c] kJ·g^{-1}	**Mass fraction of carbon in polymer** m_C	**Stoichiometric oxygen -to-fuel mass ratio of polymer,** $\Psi_{O,poly}$ g·g^{-1}		
				From elemental composition	**From** ΔH_c[d]	**From carbon content**[e]
Polyethylene	C_2H_4	43,1 to 43,6	0,857	3,420	3,29 to 3,32	2,98
Polystyrene	C_8H_8	39,2 to 39,9	0,923	3,080	2,99 to 3,05	3,23
Polymethylmethacrylate	$C_5H_8O_2$	24,9 to 25,2	0,600	1,920	1,90 to 1,92	1,98
Polycarbonate	$C_{16}H_{14}O_3$	29,7 to 29,8	0,754	2,260	2,27	2,58
Polyethylene terephthalate	$C_{10}H_8O_4$	21,3 to 22,0	0,625	1,665	1,63 to 1,68	2,08
Polyester, unsaturated	$C_{5,77}H_{6,25}O_{1,63}$	20,3 to 28,5	0,682	2,051	1,55 to 2,18	2,30
Polyvinyl chloride	C_2H_3Cl	16,4 to 16,9	0,384	1,280	1,25 to 1,29	1,15

[a] Reference [4].

[b] Reference [5].

[c] Reference [6].

[d] Calculation uses 13,1 as a divisor[3].

[e] From empirical correlation derived from data given in References [4],[5] and [6]; see Formula (23) where $\Psi_{O,poly} = (m_C \times 3{,}87) - 0{,}339\,9$ and $R^2 = 0{,}933$.

Table 6 *(continued)*

Generic polymer type	Empirical formula	ΔH_c[a,b,c] kJ·g^{-1}	Mass fraction of carbon in polymer m_C	Stoichiometric oxygen -to-fuel mass ratio of polymer, $\Psi_{O,poly}$ g·g^{-1}		
				From elemental composition	From ΔH_c[d]	From carbon content[e]
Polytetrafluoroethylene	C_2F_4	6,2 to 5,00	0,240	0,640	0,473	0,59
Polyacrylonitrile	C_3H_3N	30,8 to 31,0	0,679	2,270	2,35 to 2,37	2,29
Polyamide	$C_6H_{11}NO$	29,5 to 30,8	0,637	2,330	2,25 to 2,35	2,13
Polyurethane foam, rigid	$C_{6,3}H_{7,1}NO_{2,1}$	~27 to 22,7	0,662	2,100	2,06 to 1,73	2,22
Polyurethane foam, flexible	—	23,2 to 31,6	—	—	1,77 to 2,41	—
Wool	—	20,7 to 26,6	—	—	1,58 to 2,03	—
Cellulosics (e.g. pine-wood)	$CH_{1,7}O_{0,83}$	16,0 to 20,4	0,445	1,197	1,22 to 1,56	1,38

[a] Reference [4].

[b] Reference [5].

[c] Reference [6].

[d] Calculation uses 13,1 as a divisor[3].

[e] From empirical correlation derived from data given in References [4],[5] and [6]; see Formula (23) where $\Psi_{O,poly} = (m_C \times 3{,}87) - 0{,}339\,9$ and $R^2 = 0{,}933$.

Table 7 — Notional gas yields and stoichiometric oxygen-to-fuel mass ratio for common polymers containing C, H, O, in the structure

Material	Empirical formula	Mass fraction of carbon in polymer m_C	Ψ_O[a] g·g^{-1}	Notional gas yields[b]	
				Ψ_{CO2} g·g^{-1}	Ψ_{CO} g·g^{-1}
Polyethylene	CH_2	0,857	3,421	3,140	2,000
Polypropylene	CH_2	0,857	3,421	3,140	2,000
Polystyrene	CH	0,923	3,070	3,380	2,150
Polymethylmethacrylate	$CH_{1,6}O_{0,40}$	0,600	1,920	2,200	1,400
Cellulose	$CH_{1,7}O_{0,83}$	0,445	1,197	1,630	1,040

[a] Stoichiometric oxygen-to-fuel mass ratio, Ψ_O, (used to calculate the equivalence ratio, ϕ) has been calculated from the chemical composition of the polymer and the equation for complete combustion.

EXAMPLE 1 Stoichiometric oxygen-to-fuel mass ratio for complete combustion of polyethylene:

$CH_2 + 1{,}5\ O_2 = CO_2 + H_2O$;

14,03 g + 48,00 g→48,00/14,03;

$\Psi_O = 3{,}421$ g·g^{-1}.

EXAMPLE 2 Stoichiometric oxygen-to-fuel mass ratio for complete combustion of polyester:

$CH_{1,4}O_{0,22} + 1{,}24O_2 = CO_2 + 0{,}7\ H_2O$;

16,92 g + 39,70 g→39,70/16,92;

$\Psi_O = 2{,}346$ g·g^{-1}.

[b] Notional gas yields, expressed in grams per gram: $\Psi_{CO_2} = m_C \times 3{,}67$;

$\Psi_{CO} = m_C \times 2{,}33$.

[c] The values given in this table are examples only and not necessarily characteristic of the whole family of polymers.

Table 7 *(continued)*

Material	Empirical formula	Mass fraction of carbon in polymer m_C	Ψ_O[a] g·g⁻¹	Notional gas yields[b]	
				Ψ_{CO2} g·g⁻¹	Ψ_{CO} g·g⁻¹
Viscose	$CH_{1,7}O_{0,83}$	0,44,5	1,197	1,630	1,040
Polyester[c]	$CH_{1,4}O_{0,22}$	0,709	2,340	2,600	1,650
Polyethylene terephthalate	$CH_{0,80}O_{0,40}$	0,625	1,667	2,292	1,458
Polycarbonate	$CH_{0,88}O_{0,19}$	0,754	2,260	2,760	1,760

[a] Stoichiometric oxygen-to-fuel mass ratio, Ψ_O, (used to calculate the equivalence ratio, ϕ) has been calculated from the chemical composition of the polymer and the equation for complete combustion.

EXAMPLE 1 Stoichiometric oxygen-to-fuel mass ratio for complete combustion of polyethylene:

$CH_2 + 1,5\ O_2 = CO_2 + H_2O$;

14,03 g + 48,00 g→48,00/14,03;

$\Psi_O = 3,421\ g{\cdot}g^{-1}$.

EXAMPLE 2 Stoichiometric oxygen-to-fuel mass ratio for complete combustion of polyester:

$CH_{1,4}O_{0,22} + 1,24O_2 = CO_2 + 0,7\ H_2O$;

16,92 g + 39,70 g→39,70/16,92;

$\Psi_O = 2,346\ g{\cdot}g^{-1}$.

[b] Notional gas yields, expressed in grams per gram: $\Psi_{CO_2} = m_C \times 3,67$;

$\Psi_{CO} = m_C \times 2,33$.

[c] The values given in this table are examples only and not necessarily characteristic of the whole family of polymers.

Table 8 — Notional gas yields and stoichiometric oxygen-to-fuel mass ratio for common polymers containing C, H, O, N in the structure

Material	Empirical formula[a]	m_C	m_N	Ψ_O[b] g·g⁻¹	Notional gas yields[d]			
					Ψ_{CO_2} g·g⁻¹	Ψ_{CO} g·g⁻¹	Ψ_{HCN} g·g⁻¹	Ψ_{NO_2} g·g⁻¹
Poly acrylonitrile PAN	$CHN_{0,33}$	0,681	0,264	2,270	2,500	1,590	0,510	0,870
Polyamide	$CH_{1,8}O_{0,17}N_{0,17}$	0,637	0,126	2,330	2,330	1,480	0,240	0,415
Polyurethane foam, flexible	$CH_{1,8}O_{0,35}N_{0,06}$	0,593	0,042	2,010	2,170	1,380	0,080	0,140
Polyurethane foam, rigid	$CH_{1,2}O_{0,22}N_{0,10}$	0,662	0,077	2,100	2,430	1,545	0,150	0,250

[a] The values given in this table are examples only and not necessarily characteristic of the whole family of polymers.

[b] Stoichiometric oxygen-to-fuel mass ratio, $\Psi_{O,}$ (used to calculate equivalence ratio, ϕ) has been calculated from the chemical composition of the polymer and the equation for complete combustion.

[c] Approximate values for wool.

[d] Notional gas yields: $\Psi_{CO_2} = m_C \times 3,67$;

$\Psi_{CO} = m_C \times 2,33$;

$\Psi_{HCN} = m_N \times 1,93$;

$\Psi_{NO_2} = m_N \times 3,29$.

Table 8 *(continued)*

Material	Empirical formula[a]	m_C	m_N	Ψ_O[b] $g \cdot g^{-1}$	Notional gas yields[d]			
					Ψ_{CO_2} $g \cdot g^{-1}$	Ψ_{CO} $g \cdot g^{-1}$	Ψ_{HCN} $g \cdot g^{-1}$	Ψ_{NO_2} $g \cdot g^{-1}$
Polyisocyanurate foam, rigid	$CH_{1,0}O_{0,19}N_{0,11}$	0,682	0,088	2,100	2,430	1,545	0,171	0,286
Aramid fibres	$CH_{0,71}O_{0,14}N_{0,14}$	0,710	0,118	2,094	2,600	1,650	0,230	0,390
Wool[c]	$CH_{1,62}O_{0,38}N_{0,27}S_{0,03}$	0,491	N = 0,155 S = 0,039 O = 0,249	1,590	1,800	1,145	0,290	0,490

[a] The values given in this table are examples only and not necessarily characteristic of the whole family of polymers.

[b] Stoichiometric oxygen-to-fuel mass ratio, Ψ_O, (used to calculate equivalence ratio, ϕ) has been calculated from the chemical composition of the polymer and the equation for complete combustion.

[c] Approximate values for wool.

[d] Notional gas yields:

$$\Psi_{CO_2} = m_C \times 3{,}67;$$

$$\Psi_{CO} = m_C \times 2{,}33;$$

$$\Psi_{HCN} = m_N \times 1{,}93;$$

$$\Psi_{NO_2} = m_N \times 3{,}29.$$

Table 9 — Notional gas yields and stoichiometric oxygen-to-fuel mass ratio for common polymers containing C, H, O, X in the structure[a]

Material	Empirical formula	m_C	m_{Cl}	m_F	Ψ_O[b] $g \cdot g^{-1}$	Notional yields[f]			
						Ψ_{CO_2}	Ψ_{CO} $g \cdot g^{-1}$	Ψ_{HCl} $g \cdot g^{-1}$	Ψ_{HF} $g \cdot g^{-1}$
Polyvinyl chloride (PVC)	$CH_{1,5}Cl_{0,50}$	0,384	0,567	—	1,280	1,410	0,895	0,585	—
Polyvinyl chloride plasticized	$CH_{1,5}Cl_{0,50}$ + 50 % DOP[c]	0,56	0,28	—	1,917[c]	2,060	1,300	0,290	—
Poly tetra fluoroethylene (PTFE)	CF_2	0,240	—	0,75	0,64[d] 0,32[e]	0,880	0,560	—	0,790

[a] The stoichiometric number of moles of oxygen required for complete combustion of halogenated polymers is as follows [see Formula (18)]:

$$z = \frac{2a - c + (b - e - f - g)/2}{2}$$

The general formula for the polymer is $C_aH_bO_cN_dCl_eBr_fF_g$.

[b] Stoichiometric oxygen-to-fuel mass ratio, Ψ_O, (used to calculate equivalence ratio, ϕ) has been calculated from the chemical composition of the polymer and the equation for complete combustion.

[c] The formula for dioctylphthalate (DOP) is $C_{24}H_{36}O_4$; $\Psi_{DOP} = 2{,}553\ g \cdot g^{-1}$.

[d] Oxygen-to-fuel mass ratio assumes no H_2O in the reaction, i.e. $CF_2 + O_2 \rightarrow CO_2 + F_2$.

[e] Oxygen-to-fuel mass ratio assumes H_2O in the reaction, i.e. $CF_2 + ½O_2 + (H_2O) \rightarrow CO_2 + 2HF$.

[f] Notional gas yields:

$$\Psi_{CO_2} = m_C \times 3{,}67;$$

$$\Psi_{CO} = m_C \times 2{,}33;$$

$$\Psi_{HCl} = m_{Cl} \times 1{,}03;$$

$\Psi_{HF} = m_F \times 1{,}05$ (assumes H_2O in the reaction as in table footnote e).

6.5 Calculation of smoke yields

6.5.1 General

Smoke is an aerosol consisting of liquid droplets, solid particles and two-phase combinations of the two. It can be measured as a function of its gravimetric properties (the mass of smoke particles), of its light-obscuring properties or by combination of gravimetric and optical measurements [7][8].

6.5.2 Smoke yields based on mass of smoke particulates

Gravimetric methods give mass of particles for each gram of mass loss of material. Most systems use simple filter-based sampling devices, whilst other methods are more sophisticated and can characterize the smoke by fractionating the particles into different sizes.

The yield of smoke as particles shall be calculated from its mass concentration (grams per cubic metre) and the mass loss concentration of the material (grams per cubic metre) as given by Formula (25):

$$Y_{\mathrm{part}} = \frac{\rho_{\mathrm{part}}}{\rho_{\mathrm{m,loss}}} \tag{25}$$

where

Y_{part} is the measured mass yield of smoke particles;

ρ_{part} is the mass concentration of the smoke particles;

$\rho_{\mathrm{m,loss}}$ is the mass loss concentration of the material.

Alternatively, Y_{part} shall be calculated from the total mass of particles generated and the total mass loss of material as given by Formula (26):

$$Y_{\mathrm{part}} = \frac{m_{\mathrm{part}}}{m_{\mathrm{m,loss}}} \tag{26}$$

where

m_{part} is the total mass of particles;

$m_{\mathrm{m,loss}}$ is the total material mass loss.

6.5.3 Smoke yields based on light obscuring properties

Smoke can also be quantified in terms of its extinction coefficient, α_{k}, derived from Bouguer's law [Formulae (27) and (28)], which describes the attenuation of monochromatic light by smoke:

$$I/I_{\mathrm{o}} = \mathrm{e}^{-(\alpha_{\mathrm{k}} L)} \tag{27}$$

$$\alpha_{\mathrm{k}} = \frac{1}{L} \times \ln\left(I_{\mathrm{o}}/I\right) \tag{28}$$

where

α_k is the light extinction coefficient, expressed as inverse metres;

I_0 is the intensity of incident light;

I is the intensity of transmitted light (at the detector);

L is the length of the light path through the smoke.

Correlations have been established between visibility in smoke and its extinction coefficient, such that their product is a constant, but the value of the constant depends on the contrast and illumination of the target being viewed.

In some studies, base-10 logarithms are used to calculate the optical density per unit light path length, α, formally designated the linear decadic absorption coefficient, as given by Formulae (29) and (30):

$$\alpha = \frac{1}{L} \times \log_{10}\left(I_0 / I\right) \tag{29}$$

$$\alpha \times 2{,}303 = \alpha_k \tag{30}$$

where

α is the linear decadic absorption coefficient (optical density), expressed as inverse metres;

2,303 is the base-10 logarithm conversion factor that gives the extinction coefficient, α_k, in Formula (28).

The extinction area, A, of the smoke is the total effective cross-sectional area of all the smoke particles and this is related to the volume, V, of the chamber in which it is contained as given by Formulae (31) and (32):

$$A = \alpha_k \times V \tag{31}$$

or

$$A = 2{,}303 \times \alpha \times V \tag{32}$$

where

A is the extinction area of the smoke;

V is the volume of the chamber in which the smoke is contained.

The specific extinction area ($A_{\sigma f}$ or A_{SEA}) is a normalized parameter relating the extinction area of smoke to the mass of material burned by Formula (33):

$$A_{\sigma f} = A / m_{m,loss} \text{ or } A_{SEA} = A / m_{m,loss} \tag{33}$$

where $A_{\sigma f}$ or A_{SEA} is the extinction area of smoke per kilogram of material burned.

The relationships in Formula (33) can also be expressed as Formula (34):

$$A_{\sigma f} = \alpha_k \times V_{eff} / m_{m,loss} \text{ or } A_{SEA} = \alpha_k \times V_{eff} / m_{m,loss} \tag{34}$$

where V_{eff} is the total volume of effluent.

NOTE V_{eff} and V are equal under static condition but different under flowing condition.

The relationships in Formula (34) can also be expressed as Formula (35):

$$A_{\sigma f} = \alpha_k / \rho_{m,loss} \text{ or } A_{SEA} = \alpha_k / \rho_{m,loss} \tag{35}$$

A parameter known as the mass optical density, $D_{MO,}$ is the $\log_{10}$ analogue and usually refers to mass in grams rather than kilograms. The specific extinction areas ($A_{\sigma f}$ or A_{SEA}) can be converted to values based on $\log_e$ and kilograms as given by Formula (36):

$$A_{\sigma f} = D_{MO} \times 2{,}303 \times 1\,000 \text{ or } A_{SEA} = D_{MO} \times 2{,}303 \times 1\,000 \tag{36}$$

Various other derivations are used in the literature. They are given in more detail in References [7],[8] and [9].

6.5.4 Relationship between mass measurement and light obscuration

Both large- and bench-scale test procedures tend to monitor the optical/obscurational properties of smoke. However, the mass concentration of smoke is sometimes useful (e.g. for input to field and zone computational models). A relationship between optical properties and mass concentration has been developed for post-flame generated smoke for a wide range of fuels under well-ventilated conditions[8]. Again, Bouguer's law is the basis, relating the ratio of the transmitted and incident intensities to the mass concentration, ρ_{part} , of the smoke, the path length, L, through the smoke and the specific mass extinction coefficient, $\sigma_{m,\alpha}$, using Formula (37):

$$I/I_0 = \exp(-\sigma_{m,\alpha} \times \rho_{part} \times L) \tag{37}$$

The estimated mean value for $\sigma_{m,\alpha}$ is 8,7 $m^2 \cdot g^{-1}$ with an expanded uncertainty[24] (at the 95 % confidence interval) of 1,1 $m^2 \cdot g^{-1}$.

NOTE The value of 8,7 $m^2 \cdot g^{-1}$ becomes 10 $m^2 \cdot g^{-1}$ when corrected from He-Ne laser light to visible light[8] and it depends on the smoke produced being primarily carbonaceous soot. The value is stated to be smaller and more variable for smoke generated under smouldering or pyrolytic conditions as a result of the low light absorption of this type of smoke and variability in smoke droplet size.

Soot yields obtained during under-ventilated burning of polymeric fuels in a small-scale apparatus have been shown to be higher than those under well-ventilated conditions by a factor of approximately 2 ± 0,5[8].

7 Calculation of equivalence ratio

7.1 General

The equivalence ratio, ϕ, is defined as the actual fuel-to-air mass ratio divided by the stoichiometric fuel-to-air mass ratio, in accordance with Formula (38). In this document, fuel-to-oxygen ratios are used rather than fuel-to-air ratios:

$$\phi = \frac{\left(m_{fuel} / m_{O,act}\right)}{\left(m_{fuel} / m_{O,stoich}\right)} \tag{38}$$

where

m_{fuel} is the mass of fuel;

$m_{O,act}$ is the actual mass of oxygen available for combustion;

$m_{O,stoich}$ is the stoichiometric mass of oxygen required for complete combustion.

Formula (38) rearranges to Formulae (39) and (40):

$$\phi = \left(m_{\text{fuel}} / m_{\text{O,act}}\right) \times \left(m_{\text{O,stoich}} / m_{\text{fuel}}\right) \tag{39}$$

$$\phi = \left(m_{\text{fuel}} / m_{\text{O,act}}\right) \times \Psi_{\text{O}} \tag{40}$$

where Ψ_{O} is the oxygen-to-fuel mass ratio for stoichiometric combustion ($m_{\text{O,stoich}}/m_{\text{fuel}}$), also referred to as the stoichiometric oxygen-to-fuel mass ratio.

Formula (41) applies for systems which measure mass loss rate:

$$\phi = \left(\dot{m}_{\text{m,loss}} / \dot{m}_{\text{O,act}}\right) \times \Psi_{\text{O}} \tag{41}$$

where

$\dot{m}_{\text{m,loss}}$	is the material mass loss rate;
$\dot{m}_{\text{O,act}}$	is the actual mass flow of oxygen available for combustion.

and where the mass flow of oxygen is calculated from Formula (42):

$$\dot{m}_{\text{O,act}} = \dot{V}_{\text{air}} \times \varphi_{\text{o}} \times 1\,331\ \text{g} \cdot \text{m}^{-3} \tag{42}$$

where

$\dot{V}_{\text{air}}$	is the volume air flow;
φ_{o}	is the volume fraction of oxygen in the air supply (0,209 5 for dry air);
1 331 g·m^{-3}	is the density of oxygen at 20 °C and 1 atm.

Alternatively, for systems that measure mass loss concentration, Formula (43) applies:

$$\phi = \left(\rho_{m,loss} / \rho_{\text{O,act}}\right) \times \Psi_{\text{O}} \tag{43}$$

where

$\rho_{\text{m,loss}}$	is the material mass loss concentration;
$\rho_{\text{O,act}}$	is the actual mass concentration of oxygen available for combustion, calculated from φ_{O_2} × 1 331 g·m^{-3}.

For fuel lean mixtures (small or well-ventilated fires)	$\phi < 1$.
For stoichiometric mixtures	$\phi = 1$.
For fuel rich mixtures (ventilation-controlled fires)	$\phi > 1$.

NOTE In all fires, ranging from real-scale test fires to the burning of test specimens in bench-scale apparatus, both spatial and temporal variations in equivalence ratio occur. Any measurement of equivalence ratio (or any other fire parameter), therefore, represents the results of some degree of averaging. This has been expressed in terms of a "global" equivalence ratio[10]. The relationships between local transient equivalence ratios and global equivalence ratio estimates depend upon the extent of averaging within the system. The concept was originally developed to represent equivalence ratio measurements in the upper layer of enclosure fires over limited time periods, but has been extended to encompass the total fuel mass loss over the whole fire duration and the total air mass passing into the combustion zone. While combustion products yields are determined by the local availability of oxygen and fuel, the necessary detailed measurements are rarely performed and there is no general algorithm for combining the local yields of a gas into an overall yield for the full test specimen.

7.2 Derivation of ϕ for flow-through, steady-state experimental systems

For experimental fires where rates of air supply (oxygen) and mass loss rate (fuel) are controlled (e.g. flow-through and steady-state systems, such as a moving-tube furnace), determining a global equivalence ratio is relatively straightforward, provided the specimen combusts steadily and leaves no residue or leaves a residue of similar chemical composition to the initial specimen. Examples of tube furnace devices are described in DIN 53436-1[11], DIN 53436-2[12], DIN 53436-3[13], BS 7990[14] and ISO/TS 19700[25]. Examples of the calculation in this type of apparatus are given in Table 10.

Table 10 — Example calculations of equivalence ratio for a tube furnace for a hydrocarbon polymer and a cellulosic polymer

Characteristic	**Desired ventilation condition**	
	Well-ventilated flaming	**Ventilation-controlled flaming**
Apparatus setting		
Fuel mass loss rate (nominal grams per minute)	1,000	1,000
Primary air flow, (cubic metres per minute)	0,018 0	0,004 0
Primary air flow, (litres per minute)	18,0	4,0
Oxygen supply (cubic metres per minute)[a]	(0,209 5 × 0,018 0 × 1 331) = 5,019	(0,209 5 × 0,004 0 × 1 331) = 1,112
Fuel-to-oxygen mass ratio: ($m_{\text{fuel}}/m_{\text{O,act}}$)	1,000/5,019 = 0,199	1,000/1,112 = 0,899
Stoichiometric oxygen-to-fuel mass ratio, Ψ_0		
Hydrocarbon polymer[b]	3,422	3,422
Cellulosic polymer[c]	1,198	1,198
Equivalence ratio, $\phi = (m_{\text{fuel}}/m_{\text{O,act}}) \times \Psi_0$		

NOTE 1 This table highlights the strong influence of polymer type on the value of ϕ (and consequent ventilation condition) for a fixed air flow and mass loss rate.

NOTE 2 In tube furnaces, the mass loss of specimen is not monitored continuously (although it can be estimated from the concentrations of combustion products). Thus, in these systems one generally obtains an average global equivalence ratio for the test. Furthermore, since the oxygen is depleted at the downstream portion of the specimen, the systems do not measure a local equivalence ratio. For a uniform specimen that burns or pyrolyzes evenly, this can equate to the instantaneous value of ϕ. For a non-uniform specimen or one that burns in stages or one that leaves a residue that is different from the initial specimen, this might not be the case. The example above is for determining the average value.

NOTE 3 For some bench-scale non-steady state flow-through systems, where the fuel-to-air ratio varies rapidly during the test, the fire type and/or model cannot usually be described in terms of equivalence ratio. However, in a room fire test, it can be possible to characterize a portion of the test by a time-averaged global equivalence ratio, as is described in Note 2 of this table.

[a] The oxygen fraction is lower than 0,209 5 if room air is used.

[b] Hydrocarbon polymer (empirical formula, CH_2; $\Psi_0 = 3{,}422$).

[c] Cellulosic polymer (empirical formula, $C_6H_{10}O_5$; $\Psi_0 = 1{,}198$).

Table 10 *(continued)*

Characteristic	Desired ventilation condition	
	Well-ventilated flaming	**Ventilation-controlled flaming**
Hydrocarbon polymer[b]	0,199 × 3,422 = 0,68	0,899 × 3,422 = 3,08
Cellulosic polymer[c]	0,199 × 1,198 = 0,24	0,899 × 1,198 = 1,08
Actual ventilation condition		
Hydrocarbon polymer[b]	well-ventilated	ventilation-controlled
Cellulosic polymer[c]	well-ventilated	stoichiometric

NOTE 1 This table highlights the strong influence of polymer type on the value of ϕ (and consequent ventilation condition) for a fixed air flow and mass loss rate.

NOTE 2 In tube furnaces, the mass loss of specimen is not monitored continuously (although it can be estimated from the concentrations of combustion products). Thus, in these systems one generally obtains an average global equivalence ratio for the test. Furthermore, since the oxygen is depleted at the downstream portion of the specimen, the systems do not measure a local equivalence ratio. For a uniform specimen that burns or pyrolyzes evenly, this can equate to the instantaneous value of ϕ. For a non-uniform specimen or one that burns in stages or one that leaves a residue that is different from the initial specimen, this might not be the case. The example above is for determining the average value.

NOTE 3 For some bench-scale non-steady state flow-through systems, where the fuel-to-air ratio varies rapidly during the test, the fire type and/or model cannot usually be described in terms of equivalence ratio. However, in a room fire test, it can be possible to characterize a portion of the test by a time-averaged global equivalence ratio, as is described in Note 2 of this table.

[a] The oxygen fraction is lower than 0,209 5 if room air is used.

[b] Hydrocarbon polymer (empirical formula, CH_2; $\Psi_{\mathrm{O}} = 3{,}422$).

[c] Cellulosic polymer (empirical formula, $C_6H_{10}O_5$; $\Psi_{\mathrm{O}} = 1{,}198$).

7.3 Derivation of ϕ for flow-through, calorimeter experimental systems

There is a family of devices in which the air flow is metered and constant and the specimen mass is monitored continuously. When the sample mass loss rate is steady, as can be experienced with a thermoplastic material or liquid fuel, the equivalence ratio is also steady and the analysis in 7.1 applies. When the mass loss varies during a test (as is the case of most furnishing or internal finish products), a time-dependent form of Formula (40) is used, where the mass loss during a time interval determines the global equivalence ratio for that interval. The implementation and accuracy of oxygen control can thus be fairly easy or difficult according to the type of fire test devices used.

Examples of this type of device are the fire propagation apparatus (FPA)[15][16] used in two American standards (ASTM E 2058[17] and NFPA 287[18]) and the ventilation-controlled cone calorimeter[19].

NOTE 1 Calculation of the global equivalence ratio in the conventional ISO 5660-1[20] device is more complex. Some of the exhaust air flow passes the test specimen and is entrained in the fire plume; some of the exhaust air flow can be entrained downstream of the combustion zone. Thus, the use of the total exhaust flow in Formula (40) results in an artificially low value of ϕ. However, since the standard air flow always results in highly over-ventilated combustion, it is not intended that this device be used for determining toxic product yields except possibly for the smallest of real-scale fires.

NOTE 2 For some bench-scale non-steady state flow through systems, where the fuel-to-air ratio varies rapidly during the test, the fire type and/or model cannot usually be described in terms of equivalence ratio. However, in a room fire test, it can be possible to characterize a portion of the test by a time-averaged global equivalence ratio, as is described in the Note in 7.1.

7.4 Derivation of ϕ for closed chamber systems

For a closed cabinet apparatus, an instantaneous global equivalence ratio can only be calculated from the sample mass loss rate (or the cumulative concentrations of carbonaceous by-products, mainly CO_2 and CO) and the oxygen concentration in the chamber, provided the oxygen depletion is small and the air is well mixed. Generally, with these types of apparatus, however, the sample mass is not monitored, there is a significant decrease in oxygen concentration and it is possible for the mixing of the chamber gases to not be sufficient to create a homogeneous atmosphere during the test. Thus, determination of the instantaneous equivalence ratio is not possible and one shall determine an average global equivalence ratio based on the overall mass loss and oxygen depletion.

The operator should be aware that the yields of toxic products are likely to change when significant vitiation occurs in the vicinity of the flames above the test specimen, with large increases in several important toxic products. Thus, it is possible for the average global equivalence ratio to not be indicative of the toxicologically most important fraction of the specimen combustion.

7.5 Derivation of ϕ in room fire tests

When the air inflow and the mass of the test specimen(s) are monitored continuously, Formula (41) is used to determine a time-varying global equivalence ratio. However, all of the incoming air does not necessarily approach the combustion zone. Thus, as with ISO 5660-1[20], it is possible for the determined equivalence ratio values to not relate directly to those in a more closely controlled bench-scale device.

One approach is to calculate ϕ from Formula (43) using measurements of the total fuel and air derived from the composition of fire effluent samples (in terms of the oxides of carbon, soot, hydrocarbons and oxygen content).

8 Calculation of combustion efficiency

8.1 General

Combustion efficiency, χ, is defined as the ratio of the heat released in a combustion reaction to the theoretical heat of complete combustion.

In a perfectly efficient combustor, the atoms in the fuel would be converted to the thermodynamically most stable by-products (carbon to carbon dioxide, hydrogen to water, nitrogen to nitrogen gas, etc.) and the heat released would equal the enthalpy of reaction. However, this rarely happens in accidental fires and the processes are less than 100 % efficient.

This is partially due to considerable variations in local fuel and oxidizer concentrations in the immediate vicinity of diffusion flames, such that combustion efficiency tends to be less than predicted by stoichiometry, even under well-ventilated (low-ϕ) conditions. Under vitiated (high-ϕ) conditions, where the rate of oxygen supply is less than the rate of fuel supply, then combustion efficiency is further reduced. Furthermore, a material can burn inefficiently because of its chemical structure or because it is flame-retarded in some way.

Combustion efficiency is generally reported as a global value, averaged over the full burning time. (This can be misleading when considering toxicological implications, since most of the impact results from periods when the combustion efficiency is low).

There are different (but interrelated) ways of defining combustion efficiency. It can be based on

a) the fraction of possible heat that is released,

b) the fraction of the maximum oxygen consumption that occurs, or

c) the fraction of the maximum oxides of carbon that are formed.

The first of these is most important in calculating thermal hazard, the latter two in characterizing the toxicity of the fire atmosphere. The three methods of calculation are described in 8.2 to 8.4 and methods for b) and c) summarized in Table 11. Worked examples are given in Table 12.

NOTE When experimental data are used to calculate combustion efficiency values, they are subject to experimental variations and can, therefore generate values greater than 1.

8.2 Heat release efficiency

The formula for heat release efficiency is given by Formula (44):

$$\chi = \Delta H_{\mathrm{act}} / \Delta H_{\mathrm{c}} \tag{44}$$

where

χ is the combustion efficiency, expressed as a ratio or as a percent;

ΔH_{c} is the net heat of combustion and defined as the enthalpy, per unit mass of fuel consumed, generated in complete combustion with the water produced being in the gaseous state;

ΔH_{act} is the actual measured heat release of the combustion.

NOTE Enthalpy and heat release can be used interchangeably since the burning process is usually at constant pressure and does not perform any mechanical work.

The enthalpy (net heat) of complete combustion of a sample can be determined in an oxygen bomb calorimeter. The measurement of the actual heat release in a test apparatus is more complex. The heat released warms the ambient gases, heats some or all of the apparatus itself and can radiate a significant fraction to the external world. Thus, a true calorimetric measurement is extremely difficult and unlikely to be accurate.

Research leading to the development of the cone calorimeter showed that the heat release during burning is approximately 13,1 kilojoules per gram of oxygen consumed (±5 %) for most organic materials. Thus, for systems where the total amount of oxygen is known, ΔH_{c} can be determined from oxygen concentration measurements. (In a flow-through apparatus, both the flow of air/oxygen and the change in oxygen concentration shall be measured. In a closed system, only the latter is needed, but it is important to take care that the final value is taken after the chamber atmosphere has equilibrated).

8.3 Oxygen consumption efficiency

8.3.1 General

This ratio, χ_{O2}, shall be determined either directly from the change in oxygen concentration or indirectly from the appearance of oxygen in combustion products. Each requires knowing the empirical formula of the test sample, which might not be available, such that the measured gas data can be compared with the stoichiometric data. χ_{O2} can differ from χ because

a) as noted above, the heat release per mole of oxygen consumed during burning is a function of fuel composition, and

b) different combustion conditions can produce the same global thermal efficiency, but produce different oxygenated product yield distributions.

In carrying out calculations based on the empirical formula of the sample, a typical assumption is that the empirical formula of the mass lost during burning is the same as that of the original product. This is not the case for layered products or those composed of a mixture of components. The calculation also tends to be inaccurate to the extent that there is a solid residue, particularly a carbonaceous residue.

8.3.2 Oxygen depletion method

This method calculates combustion efficiency by direct measurement of oxygen depletion in the fire atmosphere and calculating the mass fraction of oxygen consumed as given by Formula (45):

$$\chi_{\mathrm{O}} = w_{\mathrm{O,cons}} / \Psi_{\mathrm{O}} \tag{45}$$

where

χ_O is the combustion efficiency ratio calculated from oxygen depletion;

$w_{O,cons}$ is the measured mass fraction of oxygen consumed per unit mass of fuel;

Ψ_O is the stoichiometric oxygen-to-fuel mass ratio.

8.3.3 Oxygen-in-products method

8.3.3.1 General

This is an indirect method where the total amount of combined oxygen in the major oxygen-containing combustion products (CO_2, CO and H_2O) is calculated and the amount of oxygen contributed from the base polymer or fuel is subtracted to give a derived mass fraction of oxygen consumed:

$$\chi_{prod} = w_{O,der}/\Psi_O \tag{46}$$

where

χ_{prod} is the combustion efficiency calculated from the oxygen contained in the major combustion products;

$w_{O,der}$ is a derived mass fraction of oxygen consumed per unit mass of fuel:

$$w_{O,der} = w_{O,gases} - w_{Oex,poly} \tag{47}$$

where

$w_{O,gases}$ is the measured mass fraction of oxygen consumed per unit mass of polymer in the form of the major oxygen-containing products ($w_{O,CO_2} + w_{O,CO} + w_{O,H_2O}$);

$w_{Oex,poly}$ is the mass fraction of oxygen in the burned polymer (fuel) that contributes to the oxygen-containing products.

8.3.3.2 Oxygen in CO_2, CO and H_2O ($w_{O,gases}$)

This procedure calculates and then sums the oxygen content in the major products.

Step 1 is to calculate the yields of CO_2, CO and H_2O, in accordance with Formulae (48) to (50), from the measured gas volume fraction, the corresponding density as listed in Table 3 for each gas and fuel mass loss concentration ($\rho_{m,loss}$):

$$Y_{CO_2} = (\varphi_{CO_2} \times 1\,830\ \text{g·m}^{-3})/\rho_{m,loss} \tag{48}$$

$$Y_{CO} = (\varphi_{CO} \times 1\,164\ \text{g·m}^{-3})/\rho_{m,loss} \tag{49}$$

$$Y_{H_2O} = (\varphi_{H_2O} \times 749\ \text{g·m}^{-3})/\rho_{m,loss} \tag{50}$$

where

Y is the yield, expressed as a mass fraction, for each product gas;

φ is the volume fraction of each product gas.

1 830 g·m^{-3}, 1 164 g·m^{-3} and 749 g·m^{-3} are the densities of CO_2, CO and H_2O gases, respectively (see Table 3).