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# Coal and coke — Calculation of analyses to different bases

*Charbon et coke — Calculs pour les analyses par rapport à différentes bases*



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# Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

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. www.iso.org/directives

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The committee responsible for this document is ISO/TC 27, *Solid mineral fuels*, Subcommittee SC 5, *Methods of analysis*.

This fourth edition cancels and replaces the third edition (ISO 1170:2013), of which it constitutes a minor revision. This edition includes the following changes compared to the previous edition:

— updating of referenced documents;

— adding Terms and Definitions to form Clause 3 “Terms, Definitions and Symbols”

— use of “mass fraction” instead of “content”;

— converting Annex A from normative to informative.

# Coal and coke — Calculation of analyses to different bases

## 1 Scope

This document gives equations that allow analytical data relating to coal and coke to be expressed on the various different bases in common use. Consideration is given to corrections that can be applied to certain determined values for coal prior to their calculation to other bases.

## 2 Normatives 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 602, *Coal — Determination of mineral matter*

## 3 Terms, definitions and symbols

### 3.1 Terms and definitions

No terms and definitions are listed in this document.

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

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at http://www.electropedia.org/



### 3.2 Symbols

The symbols used in the subsequent clauses are as follows, with suffixes (separated by a comma) “ad” (air-dried), “ar” (as-received), “d” (dry), “daf” (dry, ash-free) or “dmmf” (dry, mineral-matter-free) where appropriate.

$w_A$ ash, expressed as percent mass fraction

$w_C$ carbon mass fraction, expressed as percent

$w_{Cl}$ chlorine mass fraction, expressed as percent

$w_{Cl,inorg}$ inorganic chlorine mass fraction, expressed as percent

$w_{CO_2}$ carbon dioxide mass fraction, expressed as percent

$w_H$ hydrogen mass fraction, excluding hydrogen in the moisture, but including the hydrogen from water of hydration in minerals, expressed as percent

$w_{H_2O}$ moisture mass fraction, expressed as percent

$w_h$ water of hydration in the mineral matter, expressed as percent mass fraction

$w_{MM}$ mineral matter mass fraction, expressed as percent (see Annex A)

$w_N$ nitrogen mass fraction, expressed as percent

$w_{O}$ oxygen mass fraction, excluding oxygen in the moisture but including the oxygen from water of hydration in minerals, expressed as percent

$w_{S,o}$ organic sulfur mass fraction, expressed as percent

$w_{S,p}$ pyritic sulfur mass fraction, expressed as percent

$w_{S,s}$ sulfate sulfur mass fraction, expressed as percent

$w_{S,T}$ total sulfur mass fraction, expressed as percent

$w_{V}$ volatile matter mass fraction, expressed as percent

$F_{Cl}$ national correction factor for the estimation of the inorganic chlorine mass fraction

$F_{h}$ national correction factor for the estimation of water of hydration

$F_{MM}$ national correction factor for the estimation of the mineral matter (see Annex A)

## 4 Principle

In order to convert an analytical result expressed on one basis to another basis, it is multiplied by a factor calculated from the appropriate formulae (see Table 1) after insertion of the requisite numerical values.

## 5 Calculations for coal analyses

### 5.1 General

In International Standards covering the analysis of coal, it is generally specified that the determination shall be carried out on an air-dried test sample. However, in making use of these analyses, it is sometimes necessary to express or report the results on some other basis. The bases in common use are “air-dried”, “as-received”, “dry”, “dry, ash-free”, and “dry, mineral-matter-free”.



### 5.2 Procedure

Any analytical value (except net calorific value) on a particular basis may be converted to any other basis by multiplying it by the appropriate factor calculated from the formulae given in Table 1, after insertion of the requisite numerical values for the symbols (for determination of moisture, see ISO 589, ISO 5068-1, ISO 5068-2 or ISO 11722 (as appropriate); for ash, see ISO 1171).

However, in some determinations, there is a direct involvement of the mineral matter and, in these cases, it is essential to apply a correction to the air-dried result prior to its calculation to the dry, mineral-matter-free basis. This correction is dependent on the nature, as well as the quantity, of the mineral matter present. The mineral matter is determined using ISO 602. If it is not possible or not desired to determine the mineral matter for any given sample, the formula recommended by the national standards organization of the country of origin of the sample should be used and should be quoted in full, together with the analysis. An example for a formula and further explanations are given in Annex A. All the determinations that may be expressed on the dry, mineral-matter-free basis are considered individually below.

If it is necessary to calculate an analytical result expressed on the dry, mineral-matter-free basis back to any other basis, then it is essential that any correction deducted during the application of any Formulae (1) to (10) inclusive be added back to the dry, mineral-matter-free value before applying the appropriate formula from Table 1.

 

## 5.3 Carbon

Total carbon, as determined in coal, comprises both organic carbon and carbonate carbon in the mineral matter. It is reported on the air-dried basis (see ISO 609, ISO 625, or ISO 29541). In order to convert the total carbon mass fraction as analysed to a dry, mineral-matter-free basis, subtract the carbonate carbon before the conversion as given in Formula (1):

$$w_{\text{C,dmmf}} = (w_{\text{C,ad}} - 0{,}273\ w_{\text{CO}_2\text{,ad}}) \times \frac{100}{100 - (w_{\text{H}_2\text{O,ad}} + w_{\text{MM,ad}})} \tag{1}$$

## 5.4 Hydrogen

The hydrogen mass fraction reported on the air-dried basis includes the hydrogen of the coal substance and the hydrogen present (as water) in the mineral matter (see ISO 609, ISO 625 or ISO 29541). The hydrogen present as moisture in the air-dried sample shall be deducted before reporting $w_{\text{H.ad}}$. Before calculating the hydrogen of the coal substance to a dry, mineral-matter-free basis, it is also necessary to deduct the hydrogen of the mineral matter as given in Formula (2):

$$w_{\text{H,dmmf}} = \left(w_{\text{H,ad}} - \frac{w_{\text{h,ad}}}{9}\right) \times \frac{100}{100 - (w_{\text{H}_2\text{O,ad}} + w_{\text{MM,ad}})} \tag{2}$$

Since the water of hydration in the mineral matter cannot readily be determined, it is generally estimated from a knowledge of the minerals likely to be present and the total mineral matter as given in Formula (3):

$$w_{\text{h,ad}} = F_{\text{h}} \times w_{\text{A,ad}} \tag{3}$$

where $F_{\text{h}}$ is a national factor, depending of the actual type of coal. If no national factor is available, a value of $F_{\text{h}}$ equal to 0,1 may be used to achieve an approximate result.



## 5.5 Nitrogen

The nitrogen mass fraction is reported on the air-dried basis (see ISO 29541). There is no nitrogen in the mineral state normally associated with coal, and the calculation to a dry, mineral-matter-free-basis is as given in Formula (4):

$$w_{\text{N,dmmf}} = w_{\text{N,ad}} \times \frac{100}{100 - (w_{\text{H}_2\text{O,ad}} + w_{\text{MM,ad}})} \tag{4}$$

## 5.6 Sulfur

The total sulfur mass fraction, $w_{\text{S,T}}$, as reported on the air-dried basis (see ISO 334, ISO 351, ISO 19579 or ISO 20336), includes organic sulfur, $w_{\text{S,o}}$, pyritic sulfur, $w_{\text{S,p}}$, and sulfate sulfur, $w_{\text{S,s}}$. The pyritic sulfur and the sulfate sulfur are determined and the organic sulfur is obtained by difference (see ISO 157). In order to convert the total sulfur mass fraction to a dry, mineral-matter-free basis, subtract the mass fractionof pyritic and sulfate sulfur as given in Formula (5):

$$w_{\text{S,o,dmmf}} = (w_{\text{S,T,ad}} - w_{\text{S,p,ad}} - w_{\text{S,s,ad}}) \times \frac{100}{100 - (w_{\text{H}_2\text{O,ad}} + w_{\text{MM,ad}})} \tag{5}$$

## 5.7 Oxygen

Although oxygen is a significant component of coal and coke, there has been insufficient demand for its direct determination to justify continuation of an ISO standard.

The oxygen mass fraction is calculated by difference on an air-dried basis as given in Formula (6), which is taken from ISO 17247:

$$w_{O,ad} = 100 - (w_{C,ad} + w_{H,ad} + w_{N,ad} + w_{S,T,ad} + w_{A,ad} + w_{H_2O,ad}) \quad (6)$$

The calculated "oxygen by difference" includes the oxygen in the coal substance, in the carbonate minerals (as carbon dioxide) and in the water of hydration of the mineral matter.

The oxygen mass fraction on a dry, mineral-matter-free basis can be calculated as given in Formula (7):

$$w_{O,dmmf} = 100 - (w_{C,dmmf} + w_{H,dmmf} + w_{N,dmmf} + w_{S,T,dmmf}) \quad (7)$$

It is necessary to exercise caution with the estimated result derived for "oxygen by difference" as it incorporates the summation of errors in the results of the other elements.

## 5.8 Chlorine

The chlorine mass fraction is reported on the air-dried basis (see ISO 587 or ISO 18806) and includes chlorine from the mineral matter and chlorine combined with the coal substance. It is, therefore, necessary to subtract the inorganic chlorine before calculating to the dry, mineral-matter-free basis as given in Formula (8):

$$w_{Cl,o,dmmf} = (w_{Cl,ad} - w_{Cl,inorg,ad}) \times \frac{100}{100 - (w_{H_2O,ad} + w_{MM,ad})} \quad (8)$$

The mass fraction of inorganic chlorine may be calculated using a national factor, $F_{Cl}$, as given in Formula (9):

$$w_{Cl,inorg,ad} = F_{Cl} \times w_{Cl,ad} \quad (9)$$

For higher rank coal, no chlorine combined with the coal matter has been found[20]. Therefore, a value $F_{Cl} = 1$ may be used for these coals.

## 5.9 Volatile matter

The mineral matter associated with a sample also loses mass under the conditions of the volatile matter determination (see ISO 562), the magnitude of the loss being dependent on both the nature and the quantity of the minerals present.

Correction is, therefore, necessary prior to the calculation of the volatile matter to a dry, mineral-matter-free basis to take account of losses of sulfur, water of hydration, carbon dioxide and chlorine as given in Formula (10):

$$w_{V,dmmf} = (w_{V,ad} - w_{CO_2,ad} - 0{,}5 \times w_{S,p,ad} - w_{h,ad} - w_{Cl,ad}) \times \frac{100}{100 - (w_{H_2O,ad} + w_{MM,ad})} \quad (10)$$

The loss of mass from pyritic sulfur during devolatilization is approximately half of the sulfur bound in pyrite.

## 5.10 Net calorific value

The calculation of the net calorific value is dealt with in detail in ISO 1928, which, however, does not include calculation to a dry, mineral-matter-free basis as this basis is not of importance for net calorific values.

NOTE Net calorific values cannot be converted to any other basis by direct multiplying with the appropriate formulas in Table 1 as net calorific values includes a correction for the heat of vaporization related to the actual moisture.



 

## 6 Calculations for coke analyses

Coke analyses may be expressed on the “air-dried”, “as-received”, “dry” and “dry, ash-free” bases, and these values (except for net calorific value) are calculated by the use of the appropriate formulae given in Table 1, after insertion of requisite numerical values for the symbols (for determination of moisture, see ISO 579 and ISO 687; for ash, see ISO 1171).

It is not proposed at present to recommend the calculation for the conversion of analytical results for coke to a dry, mineral-matter-free basis.

## 7 Table for calculation to different bases

**Table 1 — Formulae for calculation of results to different bases**

| Basis of value given | Basis of value wanted | | | | |
|---|---|---|---|---|---|
| | **As analysed** (air-dried) (ad) | **As received**[a] (ar) | **Dry** (d) | **Dry, ash free** (daf) | **Dry, mineral matter free** (dmmf) |
| As analysed (air-dried) (ad) | — | $\frac{100-w_{H_2O,ar}}{100-w_{H_2O,ad}}$ | $\frac{100}{100-w_{H_2O,ad}}$ | $\frac{100}{100-(w_{H_2O,ad}+w_{A,ad})}$ | $\frac{100}{100-(w_{H_2O,ad}+w_{MM,ad})}$ |
| As received (ar) | $\frac{100-w_{H_2O,ad}}{100-w_{H_2O,ar}}$ | — | $\frac{100}{100-w_{H_2O,ar}}$ | $\frac{100}{100-(w_{H_2O,ar}+w_{A,ar})}$ | $\frac{100}{100-(w_{H_2O,ar}+w_{MM,ar})}$ |
| Dry (d) | $\frac{100-w_{H_2O,ad}}{100}$ | $\frac{100-w_{H_2O,ar}}{100}$ | — | $\frac{100}{100-w_{A,d}}$ | $\frac{100}{100-w_{MM,d}}$ |
| Dry, ash-free (daf) | $\frac{100-(w_{H_2O,ad}+w_{A,ad})}{100}$ | $\frac{100-(w_{H_2O,ar}+w_{A,ar})}{100}$ | $\frac{100-w_{A,d}}{100}$ | — | $\frac{100-w_{A,d}}{100-w_{MM,d}}$ |
| Dry, mineral-matter-free (dmmf) | $\frac{100-(w_{H_2O,ad}+w_{MM,ad})}{100}$ | $\frac{100-(w_{H_2O,ar}+w_{MM,ar})}{100}$ | $\frac{100-w_{MM,d}}{100}$ | $\frac{100-w_{MM,d}}{100-w_{A,d}}$ | — |

[a] Note that the formulae given for calculating results for the “as received” basis may be used to calculate them for any other moisture basis, for example moisture-holding capacity or bed moisture.