Designation: D3180 – 15

Standard Practice for Calculating Coal and Coke Analyses from As-Determined to Different Bases[1]

This standard is issued under the fixed designation D3180; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This practice lists formulas that allow analytical data to be expressed in various bases in common use. Such bases are: as received, dry, equilibrium moisture, dry ash free, and others.

1.2 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

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

2. Referenced Documents

2.1 *ASTM Standards:*[2]

D388 Classification of Coals by Rank
D1412 Test Method for Equilibrium Moisture of Coal at 96 to 97 Percent Relative Humidity and 30°C
D2013 Practice for Preparing Coal Samples for Analysis
D3173 Test Method for Moisture in the Analysis Sample of Coal and Coke
D3174 Test Method for Ash in the Analysis Sample of Coal and Coke from Coal
D3302 Test Method for Total Moisture in Coal
D7582 Test Methods for Proximate Analysis of Coal and Coke by Macro Thermogravimetric Analysis
E29 Practice for Using Significant Digits in Test Data to Determine Conformance with Specifications

3. Terminology

3.1 *Definitions:*

3.1.1 *as-determined basis*—analytical data obtained from the analysis sample of coal or coke after conditioning and preparation to No. 60 (250-μm) sieve in accordance with Practice D2013 and Test Method D3302. As-determined data represents the numerical values obtained at the particular moisture level in the sample at the time of analysis. These values are normally converted, according to formulae contained herein, to conventional reporting bases.

3.1.2 *as-received basis*—analytical data calculated to the moisture condition of the sample as it arrived at the laboratory and before any processing or conditioning. If the sample has been maintained in a sealed state so that there has been no gain or loss, the as-received basis is equivalent to the moisture basis as sampled.

3.1.3 *dry basis*—data calculated to a theoretical base of no moisture associated with the sample. The numerical value as established by Test Methods D3173 or D7582 is used for converting the as-determined data to a dry basis.

3.1.4 *dry, ash-free basis*—data calculated to a theoretical base of no moisture or ash associated with the sample. Numerical values as established by Test Methods D3173, D3174, or, D7582 are used for converting the as-determined data to a moisture- and ash-free basis.

3.1.5 *equilibrium moisture base*—data calculated to the moisture level established as the equilibrium moisture. Numerical values as established by Test Method D1412 are used for the calculation.

4. Significance and Use

4.1 The calculations of analytical data for the coal and coke test parameters listed in Section 6, assume the analysis sample has been prepared according to Practice D2013 and Test Method D3302.

4.2 This practice provides formulas, to enable calculations of data from the as-determined analysis sample to various moisture bases, in common use by the coal and coke industry.

4.3 This practice provides guidance to enable calculations of weight-average data from various lots or sublots, which, initially, are provided at different moisture bases.

4.4 The principles given in this practice are applicable to the calculation of cumulative data (e.g., for trade purposes or for sieve analyses or washability analyses).

[1] This practice is under the jurisdiction of ASTM Committee D05 on Coal and Coke and is the direct responsibility of D05.21 on Methods of Analysis.

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

5. Applicable Parameters and Symbols Used

5.1 The calculation procedures defined in 6.3.3 and 6.4.2 are applicable to the following analysis parameters when expressed as weight percent, µg/g (trace elements) or Btu/lb (gross calorific value):

Ash
Carbon
Carbon dioxide
Chlorine
Calorific value (gross)
Fixed carbon
Major, minor and trace elements
Nitrogen
Sulfur
Sulfur forms (namely, pyritic, sulfate, organic)
Volatile matter

5.2 The symbols used in this practice:

A = ash; weight %
M = moisture, weight %
P = any analysis parameter listed in 5.1, weight % (except gross calorific value is Btu/lb)
ADL = air-dry loss, weight % of as-received sample. See Test Method D3302
H = hydrogen, weight %
Ox = oxygen, weight %

5.3 Subscripts used in this practice:

ad = as-determined
ar = as-received
d = dry
daf = dry, ash-free (equivalent to moisture and ash free, maf)

6. Methods for Calculating Data

6.1 Whenever calculating a test result from observed values, avoid rounding of intermediate quantities. As far as is practicable with the calculating device, carry out calculations with the observed values exactly, and round only the final result (see E29).

6.2 Avoid calculating with reported test results (rounded and reported) and comparing these calculated values to other reported values, with the exception of obtaining the exact same calculated value.

NOTE 1—Calculations based on values that have been rounded and contain a limited number of decimal places may provide a different result than calculations based upon values that are not rounded and contain a much larger number of decimal places (e.g., up to 14 or more). Therefore, comparable, exact values will not always be calculated by the two methods. The reported value developed using un-rounded results is more precise than the value calculated off-line, e.g., in a spreadsheet program, using rounded data with a limited number of decimal places.

6.2.1 Where a composite analysis of sublots is required, whenever possible, rather than use the individual, rounded values on the individual reports to calculate a composite value, the composite analysis should be based upon the un-rounded data.

6.3 Converting from the analysis sample basis to the as-received basis (Note 2):

6.3.1 *Moisture:*

$$M_{ar} = \left[M_{ad} \times \frac{100 - ADL}{100} \right] + ADL \quad (1)$$

$$ADL = 100 \times \left[1 - (100 - M_{ar})/(100 - M_{ad}) \right] \quad (2)$$

6.3.2 *Hydrogen and Oxygen*—Inasmuch as hydrogen and oxygen values may be reported on the basis of containing or not containing the hydrogen and oxygen in water (moisture) associated with the sample, alternative conversion procedures are defined as follows:

6.3.2.1 H and Ox reported include H and Ox in water:

$$H_{ar} = \left[(H_{ad} - 0.1119 M_{ad}) \times \frac{100 - M_{ar}}{100 - M_{ad}} \right] + 0.1119 M_{ar} \quad (3)$$

$$Ox_{ar} = \left[(Ox_{ad} - 0.8881 M_{ad}) \times \frac{100 - M_{ar}}{100 - M_{ad}} \right] + 0.8881 M_{ar} \quad (4)$$

6.3.2.2 H and Ox reported do not include H and Ox in water:

$$H_{ar} = (H_{ad} - 0.1119 M_{ad}) \times \frac{100 - M_{ar}}{100 - M_{ad}} \quad (5)$$

$$Ox_{ar} = (Ox_{ad} - 0.8881 M_{ad}) \times \frac{100 - M_{ar}}{100 - M_{ad}} \quad (6)$$

6.3.3 *Other Parameters*—The equation below is applicable to all parameters, P, listed in 5.1:

$$P_{ar} = P_{ad} \times \frac{100 - M_{ar}}{100 - M_{ad}} \quad (7)$$

NOTE 2—The equations in 6.3.2 and 6.3.3 may be applied to convert analysis values from the analysis sample moisture-containing basis to any

TABLE 1 Conversion Formula Chart

Given	Wanted			
	As-Determined (ad)	As-Received (ar)	Dry (d)	Dry Ash-free (daf)
As-Determined (ad)		$\frac{100 - M_{ar}}{100 - M_{ad}}$	$\frac{100}{100 - M_{ad}}$	$\frac{100}{100 - M_{ad} - A_{ad}}$
As-Received (ar)	$\frac{100 - M_{ad}}{100 - M_{ar}}$		$\frac{100}{100 - M_{ar}}$	$\frac{100}{100 - M_{ar} - A_{ar}}$
Dry (d)	$\frac{100 - M_{ad}}{100}$	$\frac{100 - M_{ar}}{100}$		$\frac{100}{100 - A_{d}}$
Dry Ash-free (daf)	$\frac{100 - M_{ad} - A_{ad}}{100}$	$\frac{100 - M_{ar} - A_{ar}}{100}$	$\frac{100 - A_{d}}{100}$	

TABLE 2 Proximate Analysis

Sample Coal Analysis	As Determined Basis	Dry Basis	As Received Basis
Moisture, %	8.23	...	23.24
Ash, %	4.46	4.86	3.73
Volatile, %	40.05	43.64	33.50
Fixed carbon, %	47.26	51.50	39.53
Total	100.00	100.00	100.00

(Air-Dry Loss in accordance with Test Method D3302 = 16.36 %)

other moisture-containing basis (such as equilibrium capacity moisture basis) by substituting the desired moisture value for M_{ar} in the equations.

6.4 Converting from the analysis sample basis to the dry basis (Note 3):

6.4.1 *Hydrogen and Oxygen:*

$$H_d = (H_{ad} - 0.1119M_{ad}) \times \frac{100}{100 - M_{ad}} \quad (8)$$

$$Ox_d = (Ox_{ad} - 0.8881M_{ad}) \times \frac{100}{100 - M_{ad}} \quad (9)$$

6.4.2 *Other Parameters*—The equation below is applicable to all parameters, *P*, listed in 5.1:

$$P_d = P_{ad} \times \frac{100}{100 - M_{ad}} \quad (10)$$

NOTE 3—The equations in 6.4.1 and 6.4.2 may be applied to convert analysis values from any moisture-containing basis to the dry basis by substituting the appropriate moisture value for M_{ad} in the equations. If *H* and *Ox* values reported on the moisture-containing basis do not include *H* and *Ox* in the moisture (as illustrated in the last column of Table 3), the equation in 6.4.2 is applicable.

6.5 For converting data from the as-determined basis to the dry or moist, mineral matter-free basis, see procedures in Classification D388.

7. Conversion Formula Chart

7.1 To convert any of the analysis values for the parameters listed in 5.1 from one basis to another, multiply the given value by the value shown in the appropriate wanted column in Table 1.

7.2 The chart is applicable to conversion of hydrogen and oxygen values only when the given values do not include the hydrogen and oxygen in the associated moisture. If the given hydrogen and oxygen values include the hydrogen and oxygen in associated water, refer to 6.3.2.1 or 6.4.1.

8. Sample Calculations

8.1 An example of a proximate analysis reported on three different bases is shown in Table 2.

8.2 An example of ultimate analysis data tabulated for a hypothetical coal on various bases is shown in Table 3.

9. Report

9.1 To avoid ambiguity and to provide a means for conversion of data to other than the reported basis, it is essential that, except for data reported on a dry basis, an appropriate moisture content be given in the data report.

9.2 It is recommended that if hydrogen or oxygen data are reported on the as-received basis (or any other moist basis) a footnote or some other means be employed in the report to indicate whether the values reported do or do not include the hydrogen and oxygen in the moisture associated with the sample.

10. Weight Average Calculations

10.1 It is not unusual for data from one (sub)sample to be weight-averaged with data from another (or more) (sub) sample(s) to calculate the result that would represent the combined mass of the material represented by the individual (sub)samples. Example: individual sublot sample analyses are weight-averaged to obtain a mathematical composite analysis, representing the entire consignment.

Because the mathematical composite test results do not include any additional sample division variance that would be found in the production of the physical composite test sample prepared from the various (sub)samples, the weight-averaged result (mathematical composite) of multiple samples is often a more reliable value.

Note that Practice D2013, section 10, "Preparation of Composite Samples to Represent Lot-Size (or Consignment-Size) Quantities of Coal," discusses additive and non-additive parameters or analytes. It is possible to use weight-average calculations to calculate a mathematical composite for additive analytes; however, non-additive analytes must be tested as a physical composite. Non-additive analytes include Hardgrove grindability and ash fusibility results.

Whenever performing weight-average calculations, both the mass represented by the (sub)sample and the analyte determined on the (sub)sample must be on the same moisture-content basis for the calculation to be correct.

10.2 *Samples Representing Sublots in a Trade Transaction*—Most trade transactions are based upon as-received moisture basis. The moisture basis on which weight-averaging takes place most normally would be the as-received moisture basis. Convert the as-determined analytical data to the as-received moisture basis and perform the weight averaging. Weight-averaged results are then reported on the as-received, wet tons basis. Once the as-received weight-averaged test results are calculated, the calculation of the weight-averaged values to other moisture-content bases may be accomplished in the normal fashion utilizing these as-received results.

10.3 *Sieve Analysis or Washability Analysis Samples*—Sieve and washability testing are typically conducted on the air-dried samples; mass data and analysis data are usually obtained on an air-dried basis (i.e., usually on an as-determined basis). Use the as-determined mass and the as-determined analytical data to perform the weight averaging. Weight-averaged results are then reported on the as-determined tons basis, which can then be converted to dry basis analytical data and dry basis mass data. Once the dry weight-averaged test results are calculated, the calculation of the weight-averaged values to other moisture-content bases may be accomplished in the normal fashion.

10.3.1 Alternatively, convert the air dried (as-determined) analytical data and the air dried (as-determined) mass data to

TABLE 3 Ultimate Analysis Data

Test Parameter	As-Determined	Dry Basis	As-Received Basis	
	Hydrogen and oxygen include *H* and *Ox* in sample moisture (M_{ad})		Hydrogen and oxygen include *H* and *Ox* in sample moisture (M_{ar})	Hydrogen and oxygen do not include *H* and *Ox* in sample moisture (M_{ar})
Carbon, weight %	60.08	66.02	46.86	46.86
Hydrogen, weight %	5.44	4.87	6.70	3.46
Nitrogen, weight %	0.88	0.97	0.69	0.69
Sulfur, weight %	0.73	0.80	0.57	0.57
Ash, weight %	7.86	8.64	6.13	6.13
Oxygen, weight % (by difference)	25.01	18.70	39.05	13.27
Total %	100.00	100.00	100.00	70.98
Total moisture, weight % (as-received)	...	...	(29.02)	29.02
Moisture weight % (sample as-determined)	9.00	...	...	Total % 100.00

(Air-Dry Loss in accordance with Test Method D3302 = 22.00 %)

the dry basis and perform the weight averaging. Weight-averaged results are then reported on the dry tons basis. Once the dry weight-averaged test results are calculated, the calculation of the weight-averaged values to other moisture-content bases may be accomplished in the normal fashion.

10.4 *Example Calculations*—The below are several examples that compare the results of proper weight averaging and the results of improper weight averaging.

10.4.1 Scenario 1: Trade Transaction; Mass and Total Moisture are on the As-Received Basis and Ash Values (and As-Determined Moisture) are on the As-Determined Basis.

Step 1		Step 2	Step 3		Step 4	Step 5
Sublot	AR Tons	AR Moisture, %	AD Moisture, %	AD Ash, %	D Ash, %	AR Ash, %
1	950	5.15	1.52	5.37	5.45	5.17
2	1020	4.92	1.38	4.95	5.02	4.77
3	1060	5.21	1.46	5.64	5.72	5.43
4	980	5.06	1.47	5.27	5.35	5.08
5	990	4.87	1.51	5.13	5.21	4.95
Composite	5000	5.04				5.08

Step 6				Incorrect; Step 6A		Incorrect; Step 6B	
	AR Tons and AR Ash			AR Tons and AD Ash		AR Tons and D Ash	
AR Tons	AR Ash, %	AR Tons * AR Ash, %	AR Ash, %	AR Tons * AD Ash, %	AR Ash, %	AR Tons * D Ash, %	AR Ash, %
950	5.17	4913.46		5101.50		5180.24	
1020	4.77	4867.76		5049.00		5119.65	
1060	5.43	5750.89		5978.40		6066.98	
980	5.08	4976.42		5164.60		5241.65	
990	4.95	4905.44		5078.70		5156.56	
5000	5.08	25413.97	5.08	26 372.20	5.27	26 765.09	5.35

10.4.1.1 *Step 1*—Record the wet tons represented by each sublot sample (the as-received tons).

10.4.1.2 *Step 2*—Record the total moisture as as-received data. At this point, the as-received total moisture weight-averaged (mathematical composite) value may be calculated.

10.4.1.3 *Step 3*—Record analysis data.

NOTE 4—It is not possible to calculate the mathematical composite/weight-averaged air-dried/as-determined moisture or ash because the as-determined/air-dried mass has not been calculated for each tonnage fraction.

NOTE 5—It is not possible to calculate the mathematical composite/weight-averaged dry-basis ash because the dry-basis mass has not been calculated for each tonnage fraction.

10.4.1.4 *Step 4*—Calculate dry basis analytical data as a precursor to converting as-determined data to dry data and then to as-received data.

NOTE 6—It is not necessary to convert to dry basis data as an intermediary process; one may calculate directly from as-determined data to as-received data. However, it is often advantageous to compare lab-to-lab analyses on a dry basis (to minimize the effect of moisture on data comparisons); thus, having the dry data available may be helpful in the long run.

10.4.1.5 *Step 5*—Calculate dry basis analytical data to as-received data.

10.4.1.6 *Step 6*—Calculate the weight averaged as-received ash value (mathematical composite), using as-received tons and as-received ash values.

10.4.1.7 *Incorrect, Step 6A*—The results of erroneously using as-received tons and as-determined ash values.

10.4.1.8 *Incorrect, Step 6B*—The results of erroneously using as-received tons and dry ash values.

10.4.2 Scenario 2: Sieve Analysis; Mass, Ash, and Moisture are all on the air-dried or as-determined basis.

Step 1		Step 2		Step 3	Step 4
Sieve Fraction	AD kg	AD Moisture, %	AD Ash, %	AD Ash, %	D kg
+50 mm	1.1	0.65	7.37	7.42	1.1
50 mm × 25 mm	35.4	1.38	5.95	6.03	34.9
25 mm × 10 mm	52.7	1.46	4.64	4.71	51.9
10 mm × 5 mm	49.2	3.47	7.27	7.53	47.5
-5 mm	23.7	5.51	9.13	9.66	22.4
Composite	162.1	2.64	6.40	6.57	157.8

Step 5		Incorrect; Step 5A		Incorrect; Step 5B	
D kg and D Ash		AD kg and D Ash		D kg and D Ash	
D kg * D As, %	D Ash, %	AD kg * D Ash, %	D Ash, %	D kg * AD Ash, %	D Ash, %
8.11		8.16		8.05	
210.63		213.58		207.72	
244.53		248.15		240.96	
357.68		370.54		345.27	
216.38		229.00		204.46	
1037.33	6.57	1069.43	6.60	1006.47	6.38

10.4.2.1 *Step 1*—The sample to be sieved is air-dried and then sieved; record the air-dried kg in each sieve fraction (the as-determined kg).

NOTE 7—After air-drying, the total mass of the sample prior to sieving is normally recorded. If there is an unacceptably high loss of material, a root cause investigation may be undertaken. If agreed with the client and noted during the work order review, any material loss during sieving may be attributed as being "dust loss" and assigned to the finest sieve fraction. Note, however, that, if the material loss is, in part, moisture loss, or, in part, material loss, or both, from the other sieve fractions, this assignment of loss to the finest sieve fraction could result in error.

10.4.2.2 *Step 2*—Record the analysis data from each sieve fraction as as-determined data; while only as-determined ash is given in this example, "sulphur", "calorific value," "volatile matter," etc. are equally valid.

10.4.2.3 *Step 3*—Calculate the dry basis ash.

10.4.2.4 *Step 4*—Calculate the dry basis mass, kg.

10.4.2.5 *Step 5*—Calculate the weight-averaged (mathematical composite) dry ash value, using dry kg and dry ash values.

NOTE 8—Since determining the mass per sieve fraction wet and determining the ash on each wet sieve fraction was not practicable, one cannot calculate the weight-averaged as-received ash content. Note that, if a separate chemical test sample had been collected simultaneously with the sieve analysis sample, the total moisture and the as-received ash contents of that chemical test sample could be stipulated as being the same as the sieve analysis sample.

10.4.2.6 *Step 5A*—The results of erroneously using dry ash and air-dried/as-determined masses.

10.4.2.7 *Step 5B*—The results of erroneously using dry kg and as-determined ash values.

10.4.3 Scenario 3: Washability Testing of 10 mm x 25 mm sieve fraction; Mass, Ash, and Moisture are all on the air-dried or as-determined basis.

Step 1		Step 2		Step 3	Step 4
SG Fraction	AD kg	AD Moisture, %	AD Ash, %	AD Ash, %	D kg
+1.65 SG	1.1	0.65	7.37	7.42	1.1
1.50 SG × 1.65 SG	35.4	1.38	5.95	6.03	34.9
1.40 SG × 1.50 SG	52.7	1.46	4.64	4.71	51.9
1.30 SG × 1.40 SG	49.2	3.47	7.27	7.53	47.5
-1.30 SG	23.7	5.51	9.13	9.66	22.4
Composite	162.1	2.64	6.40	6.57	157.8

Step 5		Incorrect; Step 5A		Incorrect; Step 5B	
D kg and D Ash		AD Tons and D Ash		D kg and D Ash	
D kg * D As, %	D Ash, %	AD kg * D Ash, %	D Ash, %	D kg * AD Ash, %	D Ash, %
8.11		8.16		8.05	
210.63		213.58		207.72	
244.53		248.15		240.96	
357.68		370.54		345.27	
216.38		229.00		204.46	
1037.33	6.57	1069.43	6.60	1006.47	6.38

10.4.3.1 *Step 1*—The sample to be washability tested is air-dried and then subjected to washability testing; record the air-dried kg in each SG sieve fraction (the as-determined kg).

NOTE 9—After air-drying, the total mass of the sample prior to washing is normally recorded. If there is an unacceptably high loss of material, a root cause investigation may be undertaken. If agreed with the client and noted during the work order review, any material loss during washing may be attributed as being moisture loss.

10.4.3.2 *Step 2*—Record the analysis data from each SG fraction as as-determined data; while only as-determined ash is given in this example, "sulphur," "calorific value," "volatile matter," etc. are equally valid.

10.4.3.3 *Step 3*—Calculate the dry basis ash.

10.4.3.4 *Step 4*—Calculate the dry basis mass, kg.

10.4.3.5 *Step 5*—Calculate the weight-averaged (mathematical composite) dry ash value, using dry kg and dry ash values.

NOTE 10—Since determining the mass per SG fraction wet and determining the ash on each wet sieve fraction was not practicable, one cannot calculate the weight-averaged as-received ash content. Note that, if a separate chemical test sample had been collected simultaneously with the washability analysis sample, the total moisture and the as-received ash contents of that chemical test sample could be stipulated as being the same as the washability analysis sample.

10.4.3.6 *Step 5A*—The results of erroneously using dry ash and air-dried/as-determined masses.

10.4.3.7 *Step 5B*—The results of erroneously using dry kg and as-determined ash values.

11. Keywords

11.1 as-determined; coal; coke