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Standard Practice for Calculating Formulation Physical Constants of Paints and Coatings[1]

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1. Scope

1.1 This practice describes procedures commonly used in the paint industry to formulate paints and coating materials. It describes procedures for calculating formulation values for weight solids, volume solids, solvent content, volatile organic compound (VOC) content, and density of liquid paints and coatings. These values are calculated from basic formulation data. These calculations may be related to either as-supplied (unreduced) or as-applied (reduced) coating materials, including multicomponent types.

1.2 These calculated, formulation-based values may or may not be acceptable for VOC regulatory purposes, depending on the specific wording of the applicable regulation. Some regulations require analysis of the coating. Some rules allow the use of formulation data, however, some adjustments may be needed to the values calculated in this practice before they are used for regulatory purposes (see 4.3).

1.3 For purposes of this practice, it is assumed that volatile components evaporate and the materials that remain are identified as coating solids. For example, solvents are normally used to adjust viscosity for application and appearance of the coating. Other liquid materials, such as plasticizers, reactive diluents, etc., that are expected to be retained in the dried film to affect the final physical properties should be classified as part of the coating solids. Standards such as Test Methods D 2369, D 4758 and Guide D 2832 may be used to determine volatile or nonvolatile content of specific components. For purposes of this practice it is assumed that the blended formulation behaves as an *ideal* solution with no volume change on mixing (see 6.2).

1.4 Volatile by-products of cross-linking reactions (cure volatiles) are not considered in these calculations since the object of this practice is to define paint physical constants based on formulation information. Variations in raw materials, variations in the production processes, test methods, and test method accuracy are not taken into account in these calculations.

1.5 The values shown in this method are stated in English inch-pound units as commonly used in the United States. However, they may be readily converted into SI units, if required by the user (for example, see Note 4).

1.6 The values stated in inch-pound units are to be regarded as the standard for this specific practice. The values given in parentheses are for information only.

2. Referenced Documents

2.1 *ASTM Standards:*

D 153 Test Methods for Specific Gravity of Pigments[2]

D 1475 Test Method For Density of Liquid Coatings, Inks, and Related Products[3]

D 2369 Test Method for Volatile Content of Coatings[3]

D 2832 Guide for Determining Volatile and Nonvolatile Content of Paint and Related Coatings[3]

D 3960 Practice for Determining Volatile Organic Compound (VOC) Content of Paints and Related Coatings[3]

D 4758 Test Method for Nonvolatile Content of Latexes[2]

E 29 Practice for Using Significant Digits in Test Data to Determine Conformance with Specifications[4]

2.2 *U. S. Environmental Protection Agency Standards:*

EPA 450/3-88-018, U.S. Environmental Protection Agency Protocol for Determining the Daily Volatile Organic Compound Emission Rate of Automobile and Light Duty Truck Topcoat Operations[5]

EPA Federal Reference Method 24 —Determination of Volatile Matter Content, Water Content, Density Volume Solids, and Weight Solids, of Surface Coatings[6]

Federal Register 40 CFR 51.100 (Par.S) Def. of VOC and "Exempt Compounds"[6]

3. Terminology

3.1 *Definitions of Terms Specific to This Standard:*

[1] This practice is under the jurisdiction of ASTM Committee D01 on Paint and Related Coatings, Materials, and Applications and is the direct responsibility of Subcommittee D01.24 on Physical Properties of Liquid Paints and Paint Materials.

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[2] *Annual Book of ASTM Standards*, Vol 06.03.

[3] *Annual Book of ASTM Standards*, Vol 06.01.

[4] *Annual Book of ASTM Standards*, Vol 14.02.

[5] Available from U.S. Government Printing Office Superintendent of Documents, 732 N. Capitol St., NW, Mail Stop: SDE, Washington, DC 20401. Refer to EPA 450/3-88-018 dated December 1988. This protocol makes reference to the paint formulation physical constants for VOC and volume solids content.

[6] Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402.

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3.1.1 *formula density, n*—(see Test Method D 1475), the mass of a unit volume of material at the specified temperature.

3.1.1.1 *Discussion*—In this practice, density is expressed in pounds per U.S. gallon (lb/gal) since this is commonly used in the coatings industry. Where dry materials are concerned, actual density (not bulk density) should be determined analytically or obtained from supplier information. Use Test Methods D 153 where applicable.

3.1.2 *formula percent volume solids content, n*— the calculated volume of nonvolatile material in a formula divided by the total volume of the paint material, times 100 %.

3.1.3 *formula percent weight solids content, n*— the calculated weight of nonvolatile material in a formula divided by the total weight of the coating material, times 100 %.

3.1.4 *formula solvent content, n*—the calculated weight of the solvents in a specific volume of paint (such as pounds of solvent per gallon of paint), which is determined by totaling all solvents present.

3.1.4.1 *Discussion*—Volatile by-products of cross-linking reactions (cure volatiles) are *not* included in the formula solvent content.

3.1.5 *formula volatile density, n*—the calculated density of the combined volatile composition (includes VOC, exempt solvents, water, ammonia, etc.).

3.1.6 *formula VOC content, n*—calculated amount based upon total formula solvent content, (such as pounds of solvent per gallon of paint) exclusive of water or solvents that are not VOC. This is a theoretical value that may be an approximation of the VOC content that would be obtained by an analytical determination, for example, EPA Reference Method 24.

3.1.6.1 *Discussion*—Solvent and VOC are not equivalent terms. See 40 CFR 51·100 (Par·S) for the current EPA definition of volatile organic compound (VOC) and description of compounds that are exempt. Ammonia and water are not VOC, as they are not organic compounds.

4. Significance and Use

4.1 Physical constants of paints and coatings are required in all aspects of their formulation, manufacture and use. This practice demonstrates standard methods agreed upon for calculating formulation values for some of these physical constants. The calculations are the same for either metric or inch/pound units.

4.2 These formula values may not be used to replace measured values required by government regulations unless specifically stated in the governing documents.

4.3 Some regulations allow compliance determination using formulation data instead of analytical data. This formulation data may not yield the same results as the required analytical method, which could be performed on a sample from any production batch of the coating. In these cases, the user may wish to compare formulation data to analytical data and develop a factor that adjusts for variability of raw materials, variability of production batches, cure volatiles, and variability of the analytical methods.

5. Calculations

5.1 Calculated values should be rounded to the appropriate number of significant digits in accordance with Practice E 29, Section 7.

5.2 *Formula Density (weight per unit volume)*:

5.2.1 The formula density (D_f) can be calculated from the total weight (W_f) and total volume (V_f) of the formulation. The formulation volume can be calculated from the weight and density of each ingredient as given by the following equation:

$$D_f = W_f/V_f = [W_1 + W_2 + ... W_n]/[W_1D_1 + W_2/D_2 + ... W_n/D_{fn}] = [sum]\, W_i/[sum]\, W_i/D_i \quad (1)$$

where:

n = number of items in the formulation,
D_f = formula density, lb/gal (g/L),
W_f = total weight of formula, lb (g),
V_f = total volume of formula, gal (L),
W_i = weight of ingredient, lb (g), and
D_i = density of ingredient.

5.2.1.1 An example would be as follows where the weight (W) and density (D) of each ingredient are known:

Ingredient	Weight W, (lb)	Density D, (lb/gal)	Volume V, (gal)
1	81.50	7.74	10.530
2	6.10	7.90	0.772
3	0.40	8.72	0.046
4	12.00	7.65	1.569
Formula	100.00	D_f	12.917

D_f = 100/12.917 = 7.74 lb/gal.

5.2.2 If the density of any one of the ingredients in a product is unknown, it can be calculated as long as the density of the paint and the other ingredients in that formulation are known. This situation may occur with a resin solution where the density and volume of the polymer solids are unknown, as in the following example:

Ingredient	Weight W, (lb)	Density D, (lb/gal)	Volume V, (gal)
Polymer solids	50.00	D_{ps}	V_{ps}
Solvent A	25.00	6.95	3.60
Solvent B	25.00	7.18	3.48
Formula	100.00	7.50	V_f

where:

V_f = volume of total formula, gal = 100.00/7.50 = 13.3 gal,
V_{ps} = volume of polymer solids, gal = 13.33 − (3.60 + 3.48) = 6.25 gal, and
D_{ps} = density of polymer solids, lb/gal = 50.00/6.25 = 8.00 lb/gal.

5.3 *Formula Solvent (Volatile) Density*:

5.3.1 The density of the solvent (volatile) portion can be calculated using the following equation:

$$D_s = [V_1D_1 + V_2D_2 + V_3D_3 + ...V_nD_n]/[V_1 + V_2 + V_3 + ...V_n] = [sum]\, V_iD_i/[sum]\, V_i \quad (2)$$

where:

D_s = density of solvent portion, lb/gal (g/L),
V_i = volume of individual solvent, gal (L),
D_i = density of individual solvent, lb/gal (g/L), and
n = number of items in the formulation.

NOTE 1—The above formula pertains to all solvents incorporated in the formulation.

NOTE 2—If the weight (W) of the solvents in the formulation is known rather than the volume, the overall solvent density can be determined using the alternative equation, as follows:

$$D_S = Sum\ W_i/Sum(W_i/D_i) \quad (3)$$

5.4 *Formula Weight Percent Solids (Nonvolatile)*:

If the weight percent solids content of each ingredient is known, the total formulation weight percent solids can be determined by summing up the weight of solids in each ingredient divided by the total weight of the paint.

5.4.1 Calculate percent of solids by weight as follows:

$$S_W = (Sum(wt\ of\ solids)/(total\ wt\ of\ coating)) \times 100 \quad (4)$$

$$= (Sum(W_iS_T)/W_f) \times 100$$

where:

S_W = formula weight percent of solids (nonvolatile), %
W_f = total weight of formula, lb. (g)
W_i = weight of ingredient, lb. (g)
S_T = weight percent solids of ingredient, %

5.5 *Formula Volume Percent Solids (Nonvolatile)*:

Generally the volume solids content is calculated by subtracting the volume of all solvent from the total volume, since the volume of the solvent portion is usually more readily available than the volume of solid materials. The volume of the solvent portion may be obtained directly from the formula data or determined by dividing the weight (W) by the Density (D) of each. Calculate percent of solids by volume using one of the following equations, depending on available information.

5.5.1 Calculate volume percent solids by subtracting the volume of solvents from the total volume of paint, as follows:

$$S_v = ((total\ volume\ of\ paint - volume\ of\ solvents)/(total\ volume\ of\ paint)) \times 100 \quad (5)$$

where:

S_v = volume percent of solids (nonvolatile)

or

5.5.2 Calculate volume percent solids directly if the volume of solids and volume of paint are known:

$$S_V = (\text{volume of solids})/(\text{total volume of paint}) \times 100 \quad (6)$$

where:

S_v = volume percent of solids (nonvolatile)

or,

5.5.3 When the volume solids of each ingredient in a formulation is known, the volume solids of the formulation can be calculated by totaling the volumes and volume solids of each ingredient as follows:

5.5.3.1 Calculate the volume (V_i) of each ingredient from the formula weight (W_i) of each ingredient, divided by its density (D_i):

$$V_i = W_i/D_i \quad (7)$$

5.5.3.2 Determine the total volume (V_f) of the formula from the sum of the volumes of the individual ingredients:

$$V_f = [[sum]]\ V_i \quad (8)$$

5.5.3.3 Formula volume solids content (S_{vf}) is calculated in the following manner. The volume of each ingredient (V_i) is multiplied by the volume percent solids of that ingredient (S_{vi}) and the sum of these volume solids is divided by the total volume of the formula to give formula volume solids. This is shown symbolically as follows:

$$S_{vf} = ([[sum]](S_{vi} \times V_i))/(v_f) \quad (9)$$

5.5.3.4 An example would be as follows:

Ingredient	Weight W, (lb.)	Density D, (lb./gal)	Total Volume	Volume Solids, %	Volume of Solids
1	7.35	8.00	0.92	31.0	0.29
2	22.41	7.96	2.82	21.5	0.61
3	52.85	8.24	6.41	23.8	1.53
4	5.98	7.16	0.84	0.0	. . .
5	6.13	9.27	0.66	100.00	0.66
6	0.28	7.17	0.04	0.0	. . .
7	5.00	8.14	0.61	33.6	0.20
	100.00		12.30		3.29

$$S_V, \% = (total\ volume\ of\ solids, gal)/(total\ volume\ of\ paint, gal) \times 100$$
$$= (3.29)/(12.30) \times 100$$
$$= 26.7\ \% \quad (10)$$

where:

S_v = volume percent of solids (nonvolatile).

5.6 *Formula Total Solvent Content and VOC Content (see* 3.1.6*)*:

In this practice VOC content is expressed in four ways: (1) Mass of VOC per unit volume of coating less water and less exempt volatile compounds, (2) Mass of VOC per unit volume of coating solids, (3) Mass of VOC per unit mass of solids, and (4) Mass of VOC per unit volume of coating including water and exempt volatile compounds. The following equations may be used to calculate VOC content.

5.6.1 *VOC Content Expressed as the Mass of VOC per Unit Volume of Coating Less Water and Exempt Volatile Compounds*:

5.6.1.1 *General Expression*:

$$VOC = ((100 - wt\ \%\ solids - wt\ \%\ water - wt\ \%\ exempt\ volatile\ compound)(density\ of\ coating)\ (100\ \% - (volume\ \%\ water - volume\ \%\ exempt\ volatile\ compounds)) \quad (11)$$

where:

volume % water = wt % water (formula density/water density)
volume % exempt volatile compound = wt % exempt volatile compound (formula density/density exempt volatile compound)

NOTE 3—See Practice D 3960, Appendix X2, Section X2.2 when there is more than one exempt volatile compound.

5.6.1.2 If all of the volatile in the formulation is considered to be VOC for regulatory purposes, then the general expression in 5.6.1.1 simplifies to:

$$VOC\ (mass\ of\ VOC\ per\ unit\ volume\ of\ coating\ less\ water\ and\ less\ exempt\ volatile\ compounds) = ((100\ wt\ \%\ solids) \times density\ of\ coating) \times density\ of\ coating)/100 \quad (12)$$

NOTE 4—Solvent content and VOC content values may be converted

from pounds per (U.S.) gallon (lb/gal) to grams per litre (g/L) by multiplying by 119.84.

5.6.2 *VOC Content Expressed as the Mass of VOC per Unit Volume of Coating Solids (Nonvolatiles)*:

5.6.2.1 *General Expression*:

$$VOC = ((100 - wt\ \%\ solids - wt\ \%\ water - wt\ \%\ exempt\ volatile\ compound) \times formula\ density)/volume\ \%\ solids \quad (13)$$

5.6.2.2 If all of the volatile in the formulation is considered to be VOC for regulatory purposes, then the general expression in 5.6.2.1 simplifies to:

$$VOC\ (mass\ of\ VOC\ per\ unit\ volume\ of\ coating\ solids) = (100 - wt\ \%\ solids)/volume\ \%\ solids \quad (14)$$

5.6.3 *VOC Content Expressed as the Mass of VOC per Mass of Solids*:

5.6.3.1 *General Expression*:

$$VOC = ((100 - wt\ \%\ solids - wt\ \%\ water - wt\ \%\ exempt\ volatile\ compound) \times formula\ density)/weight\ \%\ solids \quad (15)$$

5.6.3.2 If all of the volatile in the formulation is considered to be VOC for regulatory purposes, the general expression in 5.6.3.1 simplifies to:

$$VOC\ (mass\ of\ VOC\ per\ mass\ of\ solids) = (100 - wt\ \%\ solids)/weight\ \%\ solids \quad (16)$$

5.6.4 *VOC Content Expressed as the Mass of VOC per Unit Volume of Coating Including Water and Exempt Volatile Compounds*:

5.6.4.1 *General Expression*:

$$VOC\ (lbs/gal) = ((100 - wt\ \%\ solids - wt\ \%\ water - wt\ \%\ exempt\ volatile\ compound) \times formula\ density)/100 \quad (17)$$

5.6.4.2 If all of the volatile in the formulation is considered to be VOC for regulatory purposes, then the general expression in 5.6.4.1simplifies to:

$$VOC\ (mass\ of\ VOC\ per\ unit\ volume\ of\ coating\ including\ water\ and\ exempt\ volatile\ compounds) = ((100 - wt\ \%\ solids) \times formula\ density)/100 \quad (18)$$

5.7 *Paints Reduced for Application*:

5.7.1 The calculations and examples shown in 5.2-5.6 are for as-supplied materials intended for use without further reduction. Similar calculations can be used for determining the formula density, percent weight solids content, percent volume solids content, and solvent (VOC) content of materials that have been reduced for application. It is only necessary to know the amount of reduction (volume or weight) and the density of the reducing solvent. The reducing solvent then becomes an additional ingredient in the paint formulation.

5.7.2 Each of the following examples is based on the equation:

$$D = W/V \quad (19)$$

where:

D = density,
W = weight, and
V = volume.

5.7.2.1 *Density of Reduced Material Knowing Percent Reduction by Volume*:

(1) The paint material described in the example in 5.2.1.1 is reduced 20 % by volume with reducing thinner having a density of 7.20 lb/gal as follows:

	Volume, gal	Density, lb/gal	Weight, lb
Unreduced material	1.00	7.74	7.74
Reducing thinner	0.20	7.20	*W*

where (reducing thinner), weight = volume × density,

or

$$W = 0.20 \times 7.20 = 1.44\ lb. \quad (20)$$

(2) The density of the reduced material is obtained by adding the volume and weight of each component, and dividing the total weight by the total volume:

	Volume, gal	Weight, lb
Unreduced material	1.00	7.74
Reducing thinner	0.20	1.44
	1.20	9.18

where:

density of reduced paint = 9.18/1.20 = 7.65 lb/gal.

5.7.2.2 *Formula Volume Solids of Reduced Paint Knowing Percent Reduction and Unreduced Volume Solids*:

Using the information from the previous example and assuming an unreduced volume solids of 50 % and a volume reduction of 20 % thinner, the reduced formula volume solids content (S_{vr}) is calculated as follows:

	Volume, gal	Solids, gal
Unreduced material	1.00	0.50
Reducing thinner	0.20	0.00
	1.20	0.50

formula volume solids, reduced = (0.50)/(1/20) = 0.42 gal,
or S_{vr}= 42.0 %.

6. Precision and Bias

6.1 No statement is made about either the precision or bias of this practice for calculating formulation physical constants since the results are obtained strictly by mathematical calculations and will be related to the accuracy of the data used and conformance to the prescribed calculations.

6.2 A bias toward slightly smaller volumes and higher densities may result from non-ideal solution behavior (see 1.3, (2)).

7. Keywords

7.1 density; formulation; physical constants; solids content; (VOC); volatile organic compound

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