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Standard Practice for Calculating Formulation Physical Constants of Paints and Coatings¹

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1. Scope

- 1.1 This practice covers 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, hazardous air pollutant (HAP) 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 D2369, D4758, D5403, and Guide D2832 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 stated in inch-pound units are to be regarded as standard. The values given in parentheses are mathematical conversions to SI units that are provided for information only and are not considered standard. However, they may be readily converted into SI units, if required by the user (for example, see Note 4).
- 1.6 This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.

2. Referenced Documents

2.1 ASTM Standards:²

D153 Test Methods for Specific Gravity of Pigments

D1475 Test Method for Density of Liquid Coatings, Inks, and Related Products

D2369 Test Method for Volatile Content of Coatings

D2832 Guide for Determining Volatile and Nonvolatile Content of Paint and Related Coatings

D3960 Practice for Determining Volatile Organic Compound (VOC) Content of Paints and Related Coatings

D4758 Test Method for Nonvolatile Content of Latexes (Withdrawn 2007)³

D5403 Test Methods for Volatile Content of Radiation Curable Materials

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 & Paint Materials.

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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.

³ The last approved version of this historical standard is referenced on www.astm.org.

- E29 Practice for Using Significant Digits in Test Data to Determine Conformance with Specifications
- 2.2 U. S. Environmental Protection Agency Documents:

Code of Federal Regulations Title 40 Part 51.100 (s) Definition of VOC Clean Air Act, Section 112^{4,5}

Code of Federal Regulations Title 40 Part 63, Subpart NNNN, Table 3 (Default Organic HAP Mass Fraction for Solvents and Solvent Blends) and Subpart RRRR Table 4 (Default Organic HAP Mass Fraction for Petroleum Solvent Groups)⁴

EPA Federal Reference Method 24 – Determination of Volatile Matter Content, Water Content, Density Volume Solids, and Weight Solids, of Surface Coatings⁴

EPA Federal Reference Method 311 – Analysis of Hazardous Air Pollutant Compound in Paints and Coatings by Direct Injection into a Gas Chromatograph⁴

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 Operations⁶

3. Terminology

- 3.1 Definitions of Terms Specific to This Standard:
- 3.1.1 formula density, n—(see Test Method D1475), the calculated 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 D153 where applicable.
- 3.1.2 *formula HAP content, n*—calculated amount based on formula content (such as pounds of HAP per gallon of coating solids).
- 3.1.2.1 *Discussion*—This is a theoretical value that may be an approximation of the HAP content that would be obtained by an analytical determination, for example, EPA Reference Method 311.
- 3.1.3 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 %.
- 3.1.4 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 %.

- 3.1.5 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.
- 3.1.5.1 *Discussion*—Volatile by-products of cross-linking reactions (cure volatiles) are *not* included in the formula solvent content.
- 3.1.6 *formula volatile density, n*—the calculated density of the combined volatile composition (includes VOC, exempt solvents, water, ammonia, etc.).
- 3.1.7 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.
- 3.1.7.1 *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 E29, Guidelines for Retaining Significant Figures in Calculation and Reporting of Test Results.
 - 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:

$$D_{f} = W_{f}/V_{f} = [W_{1} + W_{2} + \dots W_{n}]/[W_{1}/D_{1} + W_{2}/D_{2} + \dots W_{n}/D_{fn}]$$

$$= [sum]W_{i}/[sum]W_{i}/D_{i}$$
(1)

where:

n = number of items in the formulation,

⁴ Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402. They are also available at the EPA website: http://www.epa.gov/ttn/atw/coat/coatingscalc.html.

⁵ A list of hazardous air pollutants (HAPs) may be found at the following website: http://www.epa.gov/ttn/atw/188polls.html. Modifications to this original list may be found at the following website: http://www.epa.gov/ttnatw01/atwsmod.html or at the Code of Federal Regulations, Title 40, Part 63, Subpart C.

⁶ Available from U.S. Government Printing Office Superintendent of Documents, 732 N. Capitol St., NW, Mail Stop: SDE, Washington, DC 20401, http://www.access.gpo.gov. 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.

= formula density, lb/gal (g/L),

= total weight of formula, lb (g),

= total volume of formula, gal (L),

= weight of ingredient, lb (g), and

= 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	Density	Volume
-	W, (lb)	D, (lb/gal)	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

 $D_f = 100/12.917 = 7.74 \text{ lb/gal}.$

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	$V_{\rm f}$

where:

 $V_{\rm f}$ = volume of total formula, gal = 100.00/7.50 = 13.3 gal,

 $V_{\rm ps}$ = volume of polymer solids, gal = 13.33 - (3.60 + 3.48)

= 6.25 gal, and

 $D_{\rm ps}$ = density of polymer solids, lb/gal = 50.00/6.25 = 8.00

- 5.3 Formula Solvent (Volatile) Density:
- 5.3.1 The density of the solvent (volatile) portion can be calculated using the following equation: ards/sist/ccd8a79e

$$D_{s} = [V_{1}D_{1} + V_{2}D_{2} + V_{3}D_{3} + \dots V_{n}D_{n}]/[V_{1} + V_{2} + V_{3} + \dots V_{n}]$$

$$= [sum]V_{i}D_{i}/[sum]V_{i}$$
(2)

where:

 $D_{\rm s}$ = 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

= 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:

$$D_{S} = Sum W_{i}/Sum(W_{i}/D_{i})$$
 (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:

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

$$= (\Sigma(W_iS_i))/W_f$$

where:

 S_W = formula weight percent of solids (nonvolatile), %,

 W_f = total weight of formula, lb. (g), W_i = weight of ingredient, lb. (g), and

= 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 solvent. Calculate percent of solids by volume using one of the following equations, depending on available informa-
- 5.5.1 Calculate volume percent solids by subtracting the volume of solvents from the total volume of paint, as follows:

$$S_{v} = ((total\ vol\ of\ paint - vol\ of\ solvents)/(total\ vol\ of\ paint)) \times 100$$
(5)

where:

 S_{ν} = volume percent of solids (nonvolatile)

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

$$S_{\rm v} = \text{(volume of solids)/(total volume of paint)} \times 100$$
 (6)

 S_{v} = volume percent of solids (nonvolatile)

- 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: 61/251m-
- 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) :

$$V_{:} = W_{:}/D_{:} \tag{7}$$

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

$$V_f = \Sigma V_i \tag{8}$$

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:

$$S_{vf} = \left(\Sigma \left(S_{vi} V_i\right)\right) / V_f \tag{9}$$

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

Ingredient	Weight W, (lb.)	Density D, (lb./gal)	Total Volume	Volume Solids, %	Volume of Solids
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

 $S_v = (total\ vol\ of\ solids,\ gal)/(total\ vol\ of\ paint,\ gal) \times 100\ (10)$

where:

 S_{v} = volume percent of solids (nonvolatile).

5.6 Formula Total Solvent Content and VOC Content (see 3.1.7)—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:

or

$$VOC = \frac{(W_v - W_w - W_{ex})(D_c)}{100\% - (W_w)(D_c/D_w) - (W_{ex})(D_c/D_{ex})}$$
(11)

where:

or

VOC = VOC content in g/L of coating less water and exempt volatile compound,

 W_{ν} = weight of total volatiles, % (100 % - weight % nonvolatiles),

 W_{w} = weight of water, %,

 W_{ex} = weight of exempt volatile compound, %,

 D_c = density of coating, g/L at 25°C,

 D_w = density of water, g/L at 25°C (0.997 × 10³), and D_{ex} = density of exempt volatile compound, g/L at 25°C.

Note 3—See Practice D3960, Appendix X2, Two or More Exempt Solvents, 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:

 $VOC = (100 - wt \% solids) \times density of coating/100$

 $VOC = \frac{(W_{v})(D_{c})}{100\%}$ (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:

$$VOC = ((100 - wt \% solids - wt \% water - wt \% exempt volatile$$
 (13)

compound) × formula density)/volume % solids

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:

= (100 - wt % solids)/volume % solids

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

5.6.3.1 General Expression:

$$VOC = ((100 - wt \% solids - wt \% water - wt \% exempt volatile$$
 (15)

compound) × formula density)/weight % solids

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) = (16)

(100 - wt % solids)/weight % solids

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:

$$VOC(lbs/gal) = ((100 - wt \% solids - wt \% water (17))$$

-wt % exempt volatile compound) × formula density)/100

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 5.6.4.1 simplifies to:

including water and exempt volatile compounds) = $((100 - wt \% solids) \times formula density)/100$

5.7 Formula HAP Content—In this practice, HAP content is expressed in three ways: (1) Mass of HAP per unit volume of coating, (2) Mass of HAP per unit mass of coating solids, and (3) Mass of HAP per unit volume of coating solids. The following equations may be used to calculate HAP content.

Note 5—Very few materials used in paint formulations are pure substances. To accurately assess the HAP content of a paint formulation the HAP content of each ingredient must be determined. Sources for this information include supplier Material Safety Data Sheets (MSDS), technical data sheets, material specification sheets and supplier contacts. Solvent Blends are often listed on MSDS or other product data sheets only by their name or Chemical Abstract Services (CAS) number with no information about their HAP components. If this information is not available, see Code of Federal Regulations Title 40, Part 63, Subparts NNNN and RRRR, Tables 3 and 4 for default values established by the EPA. Note that the HAP content of materials from different suppliers may not be the same.

5.7.1 HAP Content Expressed as Mass of HAP per Unit Volume of Paint:

5.7.1.1 General Expression:

$$HAP_{w} = \Sigma(HAP \ content)/total \ vol \ of \ coating = \Sigma(W_{i}H_{i})/V_{f}$$
 (19)