Designation: D3827 − 92 (Reapproved 2020)

Standard Test Method for Estimation of Solubility of Gases in Petroleum and Other Organic Liquids[1]

This standard is issued under the fixed designation D3827; 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 test method covers a procedure for estimating the equilibrium solubility of several common gases in petroleum and synthetic lubricants, fuels, and solvents, at temperatures between 0 and 488 K.

1.2 This test method is limited to systems in which polarity and hydrogen bonding are not strong enough to cause serious deviations from regularity. Specifically excluded are such gases as HCl, NH_3, and SO_2, and hydroxy liquids such as alcohols, glycols, and water. Estimating the solubility of CO_2 in nonhydrocarbons is also specifically excluded.

1.3 Highly aromatic oils such as diphenoxy phenylene ethers violate the stated accuracy above 363 K, at which point the estimate for nitrogen solubility is 43 % higher than the observation.

1.4 Lubricants are given preference in this test method to the extent that certain empirical factors were adjusted to the lubricant data. Estimates for distillate fuels are made from the lubricant estimates by a further set of empirical factors, and are less accurate. Estimates for halogenated solvents are made as if they were hydrocarbons, and are the least accurate of the three.

1.5 The values stated in SI units are to be regarded as the standard. The values in parentheses are for information only.

1.6 *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 of this standard to establish appropriate safety, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

1.7 *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]

D1218 Test Method for Refractive Index and Refractive Dispersion of Hydrocarbon Liquids

D1250 Guide for the Use of the Joint API and ASTM Adjunct for Temperature and Pressure Volume Correction Factors for Generalized Crude Oils, Refined Products, and Lubricating Oils: API MPMS Chapter 11.1

D1298 Test Method for Density, Relative Density, or API Gravity of Crude Petroleum and Liquid Petroleum Products by Hydrometer Method

D2502 Test Method for Estimation of Mean Relative Molecular Mass of Petroleum Oils from Viscosity Measurements

D2503 Test Method for Relative Molecular Mass (Molecular Weight) of Hydrocarbons by Thermoelectric Measurement of Vapor Pressure

3. Terminology

3.1 *Definitions:*

3.1.1 *Bunsen coefficient, n*—the solubility of a gas, expressed as the gas volume reduced to 273 K (32°F) and 0.10 MPa (1 atm), dissolved by one volume of liquid at the specified temperature and 0.10 MPa.

3.1.2 *Ostwald coefficient, n*—the solubility of a gas, expressed as the volume of gas dissolved per volume of liquid when both are in equilibrium at the specified partial pressure of gas and at the specified temperature.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *distillate fuel, n*—a petroleum product having a molecular weight below 300 g/mol.

3.2.2 *halogenated solvent, n*—a partially or fully halogenated hydrocarbon having a molar volume below 300 mL/mol.

3.2.3 *solubility parameter, n*—the square root of the internal energy change (heat absorbed minus work done) of vaporization per unit volume of liquid, at 298 K.

[1] This test method is under the jurisdiction of ASTM Committee D27 on Electrical Insulating Liquids and Gases and is the direct responsibility of Subcommittee D27.07 on Physical Test.

Current edition approved Nov. 1, 2020. Published November 2020. Originally approved in 1979. Last previous edition approved in 2012 as D3827– 92(2012). DOI: 10.1520/D3827-92R20.

[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.

TABLE 1 Solubility Parameters of Gaseous Solutes

Gas	M_2	δ_2 at 298 K	Fuel Factor
He	4	3.35	1.27
Ne	20	3.87	1.37
H_2	2	5.52	1.27
N_2	28	6.04	1.70
Air	29	6.67	1.44
CO	28	7.47	1.37
O_2	32	7.75	1.28
Ar	40	7.71	1.37
CH_4	16	9.10	1.42
Kr	84	10.34	1.37
CO_2	44	14.81	1.14

3.2.3.1 *Discussion*—For gases in Table 1, the liquid is hypothetical and the values were calculated from actual solubility data.

3.3 *Symbols:*

- B = Bunsen coefficient at the specified condition,
- ρ = density of liquid at 288 K (60°F), g/mL,
- ρ_t = density of liquid at specified temperature, g/mL,
- G = solubility in mg/k,
- H = Henry's law constant, MPa,
- M_1 = molecular weight of liquid, g/mol,
- M_2 = molecular weight of gas, g/mol,
- n_D = refractive index of liquid, sodium *D*-line at 298 K,
- p = partial pressure of gas, MPa,
- p_v = vapor pressure of liquid, MPa,
- T = specified temperature, K,
- L = Ostwald coefficient at T,
- X = mole fraction of gas in equilibrium solution,
- δ_1 = solubility parameter of liquid, (MPa)½,
- δ^2 = equivalent solubility parameter of gas, (MPa)½ , and
- φ_i = volume fraction of component i in a mixture of liquids.

4. Summary of Test Method

4.1 The solubility of gases in petroleum and other organic liquids may be calculated from solubility parameters of the liquid and gas.[3] The parameters are given for several classes of systems and their use illustrated. Alternative methods for estimation of solubility parameters are described.

5. Significance and Use

5.1 Knowledge of gas solubility is of extreme importance in the lubrication of gas compressors. It is believed to be a substantial factor in boundary lubrication, where the sudden release of dissolved gas may cause cavitation erosion, or even collapse of the fluid film. In hydraulic and seal oils, gas dissolved at high pressure can cause excessive foaming on release of the pressure. In aviation oils and fuels, the difference in pressure between take-off and cruise altitude can cause foaming in storage vessels and interrupt flow to pumps.

6. Procedure

6.1 Obtain the value of δ_1 for the liquid by the appropriate one of the following options:

6.1.1 If the liquid is a nonhydrocarbon, obtain δ_1 from Table 2. If it is not listed there, and the structure is known, calculate δ_1 by the method of Fedors.[4]

6.1.2 If the liquid is refined petroleum or a synthetic hydrocarbon, determine ρ by Test Method D1218 or equivalent. If ρ is 0.885 g/mL or less, calculate δ_1 as follows:

$$\delta_1 = 12.03\rho + 7.36 \quad (1)$$

6.1.3 If the liquid is refined petroleum or a synthetic hydrocarbon with ρ = 0.886 g/mL or more, or a nonhydrocarbon of unknown structure, determine n_D by Test Method D1218, and calculate as follows:

$$\delta_1 = 8.63 n_D^2 + 0.96 \quad (2)$$

NOTE 1—Values of δ_1 from Table 2 or ρ are accurate to ±0.2 unit, but those from n_D may be in error by as much as ±1.0 unit.

6.1.4 For mixtures of liquids with solubility parameters δ_a, φ_b ... δ_i in volume fractions φ_{a}, $_b$ ... φ_i, calculate δ_1 as follows:

$$\delta_1 = \varphi_a\delta_a + \varphi_b\delta_b \ldots + \varphi_i\delta_i \quad (3)$$

6.2 Obtain the value of δ_2 from Table 1.

6.3 Calculate the Ostwald coefficient for a lubricant as follows:

$$L = \exp[(0.0395(\delta_1 - \delta_2)^2 - 2.66)(1 - 273/T) - 0.303\delta_1 - 0.0241(17.60 - \delta_2)^2 + 5.731] \quad (4)$$

6.4 Calculate the Ostwald coefficient for a distillate fuel or halogenated solvent as in 6.3, then multiply by the fuel factor from Table 1.

6.5 Calculate the Bunsen coefficient as follows:

$$B = 2697(p - p_v)L/T \quad (5)$$

NOTE 2—For most lubricants, p_v is less than 10 % of p and can be neglected. For fuels, solvents or oils contaminated with solvents and fuels, or at very high temperatures, p_v is important.

6.6 For mixtures of gases, calculate the individual Ostwald coefficients as in 6.3, calculate a Bunsen coefficient for each and add them together.

6.7 For hydrocarbon oils, obtain ρ_t as follows:

$$\rho_t = \rho(1 - 0.000595(T - 288.2)/\rho^{1.21}) \quad (6)$$

NOTE 3—The constants 0.000595 and 1.21 are an empirical approximation of the calculations involved in Guide D1250.

6.8 For nonhydrocarbon liquids, obtain ρ_t by one of the following methods, listed in decreasing order of preference:

6.8.1 Determine it directly, using Test Method D1298 or equivalent.

6.8.2 Obtain suitable data from the supplier of the liquids.

6.8.3 Obtain ρ by one of the above, and adjust it as follows, using *dd/dT* from Table 2:

$$\rho_t = \rho - (T - 288.2)d\rho/dT \quad (7)$$

6.8.4 Obtain both ρ and *dρ/dT* from Table 2 and combine as in 6.8.3.

6.9 Obtain M_2 from Table 1, and calculate the solubility in mg/kg:

[3] Beerbower, A., "Estimating the Solubility of Gases in Petroleum and Synthetic Lubricants," *ASLE Trans*, Vol 23, 1980, p. 335.

[4] Fedors, R. F., "A Method for Estimating Both the Solubility Parameters and Molar Volumes of Liquids," *Polymer Engineering and Science*, Vol 14, 1974, p. 147.

TABLE 2 Constants for Synthetic Nonhydrocarbons

Compound	δ_1	M_1	ρ	$d\rho/dT$
Di-2-ethylhexyl adipate	18.05	370	0.928	0.00075
Di-2-ethylhexyl sebacate	17.94	427	0.916	0.00073
Trimetholylpropane pelargonate	18.48	459	0.962	0.00070
Pentaerythritol caprylate	18.95	540	1.002	0.00065
Di-2-ethylhexyl phthalate	18.97	390	0.986	0.00075
Diphenoxy diphenylene ether	23.24	440	1.178	0.00079
Diphenoxy triphenylene ether	23.67	520	1.205	0.00076
Polychlorotrifluoroethylene	15.47	600	1.925	0.00166
Polychlorotrifluoroethylene	15.55	700	1.942	0.00154
Polychlorotrifluoroethylene	15.71	1 000	1.998	0.00152
Dimethyl silicone	15.14	10 000	0.969	0.00093
Methyl phenyl silicone	18.41	5 000	1.063	0.00080
Perfluoropolyglycol	14.30	1 000	1.914	0.00180
Tri-2-ethylhexyl phosphate	18.27	467	0.923	0.00090
Tricresyl phosphate	18.82	368	1.158	0.00090

$$G = 44.6BM_2/\rho_t \quad (8)$$

NOTE 4—The equation in 6.9 is based on the assumption that the *liquid* in definitions 3.1.1, 3.1.2, and 3.1.3 has the same volume and density as the oil. That is a good approximation, except for gases more soluble than CH_4. Furthermore, the laborious corrections required to render this more rigorous are not justified in light of the precision shown in Section 7.

6.10 Obtain the value of M_1 by the appropriate one of the following options:

6.10.1 For synthetic nonhydrocarbons, locate in Table 2 or calculate directly.

6.10.2 For refined petroleum or synthetic hydrocarbons, estimate M_1 by Test Method D2502.

6.10.3 For nonhydrocarbons of unknown structure, determine M_1 by Test Method D2503. Despite the limitations implied in its scope, that method will serve this purpose.

6.11 Calculate the solubility as mole fraction as follows:

$$X = 10^{-6}\, GM_1/M_2 \quad (9)$$

6.12 Calculate the Henry's law constant as follows:

$$H = (p - p_v)/X \quad (10)$$

7. Precision and Bias[5]

7.1 *Precision*—The precision of this test is not known to have been obtained in accordance with currently accepted guidelines (for example, in Committee D02 Research Report RR:D02-1007, Manual on Determination of Precision Data for ASTM Methods on Petroleum Products and Lubricants).

7.1.1 *Lubricants:*

7.1.1.1 The gases for which reliable data were available are listed in Table 3. The nature of the correlation was such that solubilities calculated from the corresponding parameters in Table 1 will have an average precision of less than 3 %.

7.1.1.2 In this correlation, 257 data points from 9 sources were included. The breakdown by gases is shown in Table 3. Overall, the standard error of estimate was 21 %. At the 95 % confidence level, this predicts a maximum error of ±42 % from the true value.

7.1.2 *Distillate Fuels:*

7.1.2.1 The gas parameters were adjusted to give less than 1 % precision on distillate fuels. When δ_2 had been adjusted for lubricants, the fuel factor was set empirically. If both were free, the fuel factor was set at 1.37 and δ_2 adjusted.

7.1.2.2 With this correlation, 176 data points gave a standard error of 18 %, or at the 95 % confidence level, a maximum error of 36 % from the true value.

7.1.3 *Halogenated Solvents:*

7.1.3.1 No attempt was made to remove precision from the solvent estimates, and the fuel parameters were used. The precision was – 13 %; the details are shown in Table 3.

7.1.3.2 With the fuel correlation used on solvents, the standard error was 44 %, or at 95 % confidence level, ±88 % from the true value maximum error. Details are shown in Table 3 on these 64 data points.

7.2 *Bias*—No general statement is made for bias by Test Method D3827 since the data used to determine the condition cannot be compared with accepted reference material.

8. Keywords

8.1 gases; liquids; organic liquids; petroleum liquids; solubility

[5] Supporting data have been filed at ASTM International Headquarters and may be obtained by requesting Research Report RR:D02-1104.

TABLE 3 Precision of Estimate with Various Gases

Gas	Lubricant Points	Standard Error, %	Fuel Points	Standard Error, %	Solvent Points	Mean Bias, %	Standard Error, %
He	34	5	16	17	8	–25	35
Ne	—	—	16	12	8	–30	43
H_2	19	18	8	10	5	+ 10	51
N_2	89	32	13	15	6	–19	37
Air	44	8	55	12	—	—	—
CO	—	—	6	18	4	+ 4	64
O_2	32	7	18	17	7	–24	50
Ar	—	—	15	17	9	–7	46
CH_4	—	—	8	42	5	–13	50
Kr	—	—	15	25	6	–11	75
CO_2	39	11	6	54	—	—	—