
40 C.F.R. § 799.6786

TSCA water solubility: Generator column method.

(a) *Scope—(1) Applicability.* This section is intended to meet the testing requirements of the Toxic Substances Control Act (TSCA) (15 U.S.C. 2601).

(2) *Source.* The source material used in developing this TSCA test guideline is the Office of Pollution Prevention, Pesticides and Toxics (OPPTS) harmonized test guideline 830.7860 (March 1998, revised final guideline). The source is available at the address in paragraph (e) of this section.

(b) *Introduction—(1) Purpose.* (i) The water solubility of a chemical is defined as the equilibrium concentration of the chemical in a saturated aqueous solution at a given temperature and pressure. The aqueous phase solubility is an important factor in governing the movement, distribution, and rate of degradation of chemicals in the environment. Substances that are relatively water soluble are more likely to be widely distributed by the hydrologic cycle than those which are relatively insoluble. Furthermore, substances with higher water solubility are more likely to undergo microbial or chemical degradation in the environment because dissolution makes them “available” to interact and, therefore, react with other chemicals and microorganisms. Both the extent and rate of degradation via hydrolysis, photolysis, oxidation, reduction, and biodegradation depend on a chemical being soluble in water (i.e., homogeneous kinetics).

(ii) Water provides the medium in which many organisms live, and water is a major component of the internal environment of all living organisms (except for dormant stages of certain life forms). Even organisms which are adapted to life in a gaseous environment require water for normal functioning. Water is thus the medium through which most other chemicals are transported to and into living cells. As a result, the extent to which chemicals dissolve in water will be a major determinant for movement through the environment and entry into living systems.

(iii) The water solubility of a chemical also has an effect on its sorption into and desorption from soils and sediments, and on volatilization from aqueous media. The more soluble a chemical substance is, the less likely it is to sorb to soils and sediments and the less likely it is to volatilize from water. Finally, the design of most chemical tests and many ecological and health tests requires precise knowledge of the water solubility of the chemical to be tested.

(2) *Definitions.* The following definitions apply to this section.

Concentration (C) of a solution is the amount of solute in a given amount of solvent or solution and can be expressed as a weight/weight or weight/volume relationship. The conversion from a weight relationship to one of volume incorporates density as a factor. For dilute aqueous solutions, the density of the solvent is approximately equal to the density of the solution; thus, concentrations expressed in milligrams per liter (mg/L) are approximately equal to 10^{-3} g/10 g or parts per million (ppm); those expressed in micrograms per liter ($\mu\text{g/L}$) are approximately equal to 10^{-6} g/10 g or parts per billion (ppb). In addition, concentration can be expressed in terms of molarity, normality, molality, and mole fraction. For example, to convert from weight/volume to

molarity molecular mass is incorporated as a factor.

Density is the mass of a unit volume of a material. It is a function of temperature, hence the temperature at which it is measured should be specified. For a solid, it is the density of the impermeable portion rather than the bulk density. For solids and liquids, suitable units of measurement are grams per cubic centimeter (g/cm³). The density of a solution is the mass of a unit volume of the solution and suitable units of measurement are g/cm³.

Extractor column is used to extract the solute from the saturated solutions produced by the generator column. After extraction onto a chromatographic support, the solute is eluted with a solvent/water mixture and subsequently analyzed by high-pressure liquid chromatography (HPLC), gas chromatography (GC), or any other suitable analytical procedure. A detailed description of the preparation of the extractor column is given in paragraph (c)(1)(i)(D) of this section.

Generator column is used to produce or generate saturated solutions of a solute in a solvent. The column, see figure 1 in paragraph (c)(1)(i)(A) of this section, is packed with a solid support coated with the solute, i.e., the organic compound whose solubility is to be determined. When water (the solvent) is pumped through the column, saturated solutions of the solute are generated. Preparation of the generator column is described in paragraph (c)(1)(i)(A) of this section.

Response factor (RF) is the solute concentration required to give a 1 unit area chromatographic peak or 1 unit output from the HPLC recording integrator at a particular recorder attenuation. The factor is required to convert from units of area to units of concentration. The determination of the RF is given in paragraph (c)(3)(ii)(B)(2) of this section.

Sample loop is a 1/16 inch (in) outer diameter (O.D.) (1.6 millimeter (mm)) stainless steel tube with an internal volume between 20 and 50 μ L. The loop is attached to the sample injection valve of the HPLC and is used to inject standard solutions into the mobile phase of the HPLC when determining the RF for the recording integrator. The exact volume of the loop must be determined as described in paragraph (c)(3)(ii)(B)(1) of this section when the HPLC method is used.

Saturated solution is a solution in which the dissolved solute is in equilibrium with an excess of undissolved solute; or a solution in equilibrium such that at a fixed temperature and pressure, the concentration of the solute in the solution is at its maximum value and will not change even in the presence of an excess of solute.

Solution is a homogeneous mixture of two or more substances constituting a single phase.

(3) *Principle of the test method.* (i) This test method is based on the dynamic coupled column liquid chromatographic (DCCLC) technique for determining the aqueous solubility of organic compounds that was initially developed by May et al. (as described in the references listed in paragraphs (e)(5) and (e)(6) of this section), modified by DeVoe et al. (as described in the reference listed in paragraph (e)(1) of this section), and finalized by Wasik et al. (as described in the reference listed in paragraph (e)(11) of this section). The DCCLC technique utilizes a generator column, extractor column and HPLC coupled or interconnected to provide a continuous closed flow system. Saturated aqueous solutions of the test compound are produced by pumping water through the generator column that is packed with a solid support coated with the compound. The compound is extracted from the saturated solution onto an extractor column, then eluted from the extractor column with a solvent/water mixture and subsequently analyzed by HPLC using a variable wavelength ultraviolet (UV) detector operating at a suitable wavelength. Chromatogram peaks are recorded and integrated using a recording integrator. The concentration of the compound in the effluent from the generator column, i.e., the water solubility of the compound, is determined from the mass of the compound (solute) extracted from a measured volume of water (solvent).

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