CHEMICAL PROPERTIES

OVERVIEW: Chemical properties, physical properties, and the chemical structure of a substance are characteristics which identify it from other substances. In this module, the physical and chemical characteristics of the chemicals in the use cluster are detailed.

GOALS:

- Identify the physical and chemical characteristics along with the chemical structures of the chemicals in the use cluster.
- Determine a discrete appropriate name and Chemical Abstracts Service Registry Number (CAS RN), defined below for each chemical to be used throughout the assessment.
- Facilitate the identification of potential chemical substitutes with similar properties to the chemicals in the use cluster.
- Provide chemical names and/or properties to the following modules: Chemical Manufacturing Process & Product Formulation, Environmental Fate Summary, Human Health Hazards Summary, Environmental Hazards Summary, Chemistry of Use & Process Description, Process Safety Assessment, Market Information, Workplace Practices & Source Release Assessment, Exposure Assessment, Regulatory Status, Performance Assessment, and Control Technologies Assessment.

PEOPLE SKILLS: The following lists the types of skills or knowledge that are needed to complete this module.

- Knowledge of the basic concepts of chemistry, particularly physical and chemical properties.

Within a business or DFE project team, the people who might supply these skills include a chemist, chemical engineer, or an environmental scientist.

DEFINITION OF TERMS:

Boiling Point (bp): The temperature at which a liquid under standard atmospheric pressure (or other specified pressure) changes from the liquid to the gaseous state. It is an indication of the volatility of a substance. The distillation range in a separation process, the temperature at which the more volatile liquid of a mixture forms a vapor, is used for mixtures in the absence of a bp. Typical units are ^{o}C or ^{o}F.

Chemical Abstracts Service Registry Number (CAS RN): A unique identification code, up to ten digits long, assigned to each chemical registered by the Chemical Abstract Service. The CAS RN is useful when searching for information on a chemical with more than one name. Over six million chemicals have been assigned CAS RNs.

Chemical Structure: A description of how atoms in a chemical are connected and arranged, including types of bonds between atoms.

Corrosivity: As defined by EPA (40 CFR 261.22), a solid waste exhibits the characteristic of corrosivity if: (1) it is aqueous and has a pH less than or equal to 2 or greater than or equal to 12.5, as determined by a pH meter using an EPA test method (Method 9049 in EPA Publication SW-846); (2) it is a liquid and corrodes steel at a rate greater than 6.35 mm (0.250") per year when tested at 55 ^{o}C as determined by the test method specified in the National Association of Corrosion Engineers Standard TM-01-69 as standardized in EPA Publication SW-846. As defined by OSHA (29 CFR 1910.1200), a chemical is corrosive if it causes visible destruction of, or irreversible alternation in living tissue by chemical action at the site of contact.

Density: The mass of a liquid, solid, or gas per unit volume of that substance, i.e., the mass in grams contained in 1 cubic centimeter (1 ml) of a substance at 20 ^{o}C and 1 atmosphere pressure. Typical units are g/ml or lbs/in^3.

Explosive: As defined by OSHA (29 CFR 1910.1200), a chemical that causes a sudden, almost instantaneous release of pressure, gas, and heat when subjected to sudden shock, pressure, or high temperature.

Flammable: As defined by OSHA (29 CFR 1910.1200), a chemical that falls into one of the following categories:

- Flammable aerosol: An aerosol that, when tested by the method described in 16 CFR 1500.45, yields a flame projection exceeding 18 inches at full valve opening, or a flashback (a flame extending back to the valve) at any degree of valve opening.
- Flammable gas:
  - A gas that, at ambient temperature and pressure, forms a flammable mixture with air at a concentration of 13 percent by volume or less; or
  - A gas that, at ambient temperature and pressure, forms a range of flammable mixtures with air wider than 12 percent by volume, regardless of the lower limit.
- Flammable liquid: Any liquid having a flashpoint below 100 ^{o}F (37.8 ^{o}C), except any mixture having components with flashpoints of 100 ^{o}F (37.8 ^{o}C) or higher, the total of which make up 99 percent or more of the total volume of the mixture.
- Flammable solid: A solid, other than a blasting agent or explosive as defined in 29 CFR 1910.109(a), that is liable to cause fire through friction, absorption of moisture, spontaneous chemical change, or retained heat from manufacturing or processing, or which can be ignited readily and when ignited burns so vigorously and persistently as to create a serious hazard. A chemical shall be considered to be a flammable solid if, when tested by the method described in 16 CFR 1500.44, it ignites and burns with a self-sustained flame at a rate greater than one-tenth of an inch per second along its major axis.

Flash Point: As defined by OSHA (29 CFR 1910.1200), the minimum temperature at which a liquid gives off a vapor in sufficient concentration to ignite when tested as follows:

- Tagliabue Closed Tester: (see American National Standard Method of Test for Flash Point by Tag Closed Tester, Z11.24-1979 [ASTM D 56-79]) for liquids with a viscosity of less than 45 Saybolt Universal Seconds (SUS) at 100 ^{o}F (37.8 ^{o}C), that do not contain suspended solids and do not have a tendency to form a surface film under test.
- Pensky-Martens Closed Tester: (see American National Standard Method of Test for Flash Point by Pensky-Martens Closed Tester, Z11.7-1979 [ASTM D 93-79]) for liquids with a viscosity equal to or greater than 45 SUS at 100 ^{o}F (37.8 ^{o}C), or that contain suspended solids, or that have a tendency to form a surface film under test.
- Setaflash Closed Tester: (see American National Standard Method of Test for Flash Point by Setaflash Closed Tester [ASTM D 3278-78].) Typical units are ^{o}C or ^{o}F.

Melting Point (mp): The temperature at which a substance changes from the solid to the liquid state. It indicates the temperature at which solid substances liquefy. Typical units are ^{o}C or ^{o}F.

Molecular Weight (MW): A summation of the individual atomic weights based on the numbers and kinds of atoms present in a molecule of a chemical substance. For polymers, this may include molecular weight distributions or average number MW (MW_n), ranges, and averages. Typical units are g/mole, daltons, or lbs/mole.

Physical State: Describes a chemical substance as a gas, liquid, or solid under ambient or other given conditions.

Reactivity: As defined by EPA (40 CFR 261.23), a solid waste is considered reactive if it exhibits any of the following properties: (1) is normally unstable and readily undergoes violent change without detonating; (2) reacts violently or forms potentially explosive mixtures with water; (3) when mixed with water, generates toxic gases, vapors, or fumes in a quantity that can present a danger to human health or the environment; (4) is a cyanide or sulfide bearing waste which, when exposed to a pH between 2 and 12.5, can generate toxic gases, vapors, or fumes in a quantity that can present a danger to human health in the environment; (5) is capable of detonation or explosive reaction if subjected to a strong initiating source or if heated under confinement; (6) is readily capable of detonation or explosive decomposition or reaction at standard temperature and pressure; or (7) is a forbidden Class A or Class B explosive as defined by the Department of Transportation (49 CFR 173). As defined by OSHA (29 CFR 1910.1200), water-reactive means a chemical will react with water to release a gas that is either flammable or presents a health hazard.

Vapor Pressure (Pv): The pressure exerted by a chemical in the vapor phase in equilibrium with its solid or liquid form. It provides an indication of the relative tendency of a substance to volatilize from the pure state. Typical units are mm Hg, torr, or in. Hg.

Water Solubility (S): The maximum amount of a chemical that can be dissolved in a given amount of pure water at standard conditions of temperature and pressure. Typical units are mg/L, g/L, or lbs/gal.

APPROACH/METHODOLOGY: The following presents a summary of the approach or methodology for obtaining chemical properties data. Methodology details for Step 6 are presented in the next section of this module.

Step 1: Prepare a list of chemical names from the substitutes tree, the Industry and Use Cluster Profile, and other pertinent documents as chemicals are identified (e.g., by the Performance Assessment or Workplace Practices & Source Release Assessment modules).

Step 2: Obtain the CAS RN and the chemical structure for each chemical on the list and identify synonyms. This will expedite the search for data on chemical properties. (Refer to Tables 5-2, 5-3, and 5-4.)

Step 3: Determine the appropriate name to be used to identify the chemical from the synonyms.

Step 4: Collect measured and/or estimated data for all of the terms listed in the Definition of Terms, when applicable. Many sources of data can be searched by CAS RN. Data are generally available from suppliers of the chemicals. (See material safety data sheets [MSDSs], described in the Process Safety Assessment module.)

Step 5: Use standard or accepted mathematical models or computer programs to estimate the data. (See Table 5-2: Mathematical Models Used to Estimate Chemical Properties.)

Step 6: Provide pertinent chemical properties to the appropriate modules (see Methodology Details below).

METHODOLOGY DETAILS: This section presents the methodology details for completing Step 6 in the above section.

Details: Step 6, Providing Pertinent Chemical Properties to the Appropriate Modules

Table 5-1 lists examples of data that the Chemical Properties module transfers to other modules in a CTSA.

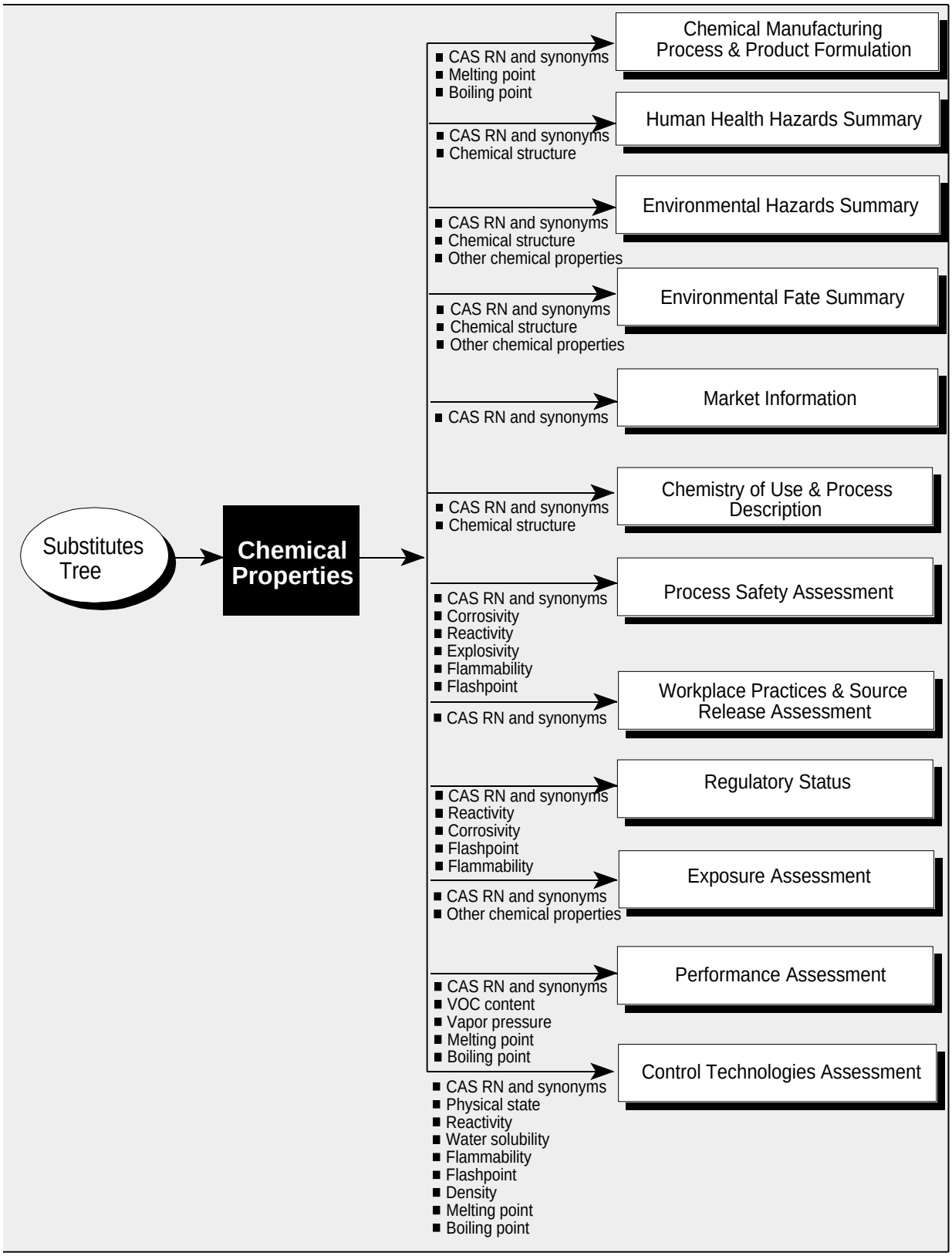
TABLE 5-1: DATA TRANSFERRED FROM THE CHEMICAL PROPERTIES MODULE

Module	Data Transferred
Chemical Manufacturing Process & Product Formulation	CAS RN, synonyms, mp, bp
Human Health Hazards Summary	CAS RN, synonyms, chemical structure
Environmental Hazards Summary	CAS RN, synonyms, chemical structure, S.

TABLE 5-1: DATA TRANSFERRED FROM THE CHEMICAL PROPERTIES MODULE	
Module	**Data Transferred**
Environmental Fate Summary	CAS RN, synonyms, chemical structure, Pv, S, mp, bp, physical state, MW
Market Information	CAS RN, synonyms
Chemistry of Use & Process Description	CAS RN, synonyms, chemical structure
Process Safety Assessment	CAS RN, synonyms, corrosivity, reactivity, explosivity, flammability, flashpoint
Workplace Practices & Source Release Assessment	CAS RN, synonyms
Regulatory Status	CAS RN, synonyms, reactivity, flammability, flashpoint, corrosivity
Exposure Assessment	CAS RN, synonyms, chemical structure, Pv, S, physical state
Performance Assessment	CAS RN, synonyms, Pv, bp, flashpoint
Control Technologies Assessment	CAS RN, synonyms, physical state, reactivity, S, flammability, flash point, mp, bp, density

FLOW OF INFORMATION: The Chemical Properties module is the basic starting point for many of the other modules in the CTSA. The Chemical Properties module receives chemical names from the substitutes tree and other sources and transfers data to the Chemical Manufacturing Process & Product Formulation, Human Health Hazards Summary, Environmental Hazards Summary, Environmental Fate Summary, Market Information, Chemistry of Use & Process Description, Process Safety Assessment, Workplace Practices & Source Release Assessment, Regulatory Status, Exposure Assessment, Performance Assessment, and Control Technologies Assessment modules. Example information flows are shown in Figure 5-1.

FIGURE 5-1: CHEMICAL PROPERTIES MODULE: EXAMPLE INFORMATION FLOWS



ANALYTICAL MODELS: Table 5-2 presents references for analytical models that can be used to estimate chemical properties.

TABLE 5-2: MATHEMATICAL MODELS USED TO ESTIMATE CHEMICAL PROPERTIES

Reference	Type of Model
Hunter, R.S. and F.D. Culver. 1992. *MicroQSAR Version 2.0: A Structure-Activity Based Chemical Modeling and Information System.*	Personal computer-based system of models. Uses quantitative structure-activity relationships to estimate chemical properties and aquatic toxicity values.
Syracuse Research Corporation (SRC). Continually Updated. Estimation Programs Interface (EPI©).	A shell program used to access a series of models used to estimate S, mp, bp, Pv, and environmental fate properties.
Syracuse Research Corporation (SRC). Updated Periodically. MPBVP©.	This program estimates the mp, bp, and Pv of organic compounds.

Note: References are listed in shortened format, with complete references given in the reference list following Chapter 10.

PUBLISHED GUIDANCE: Table 5-3 presents a reference for published guidance on chemical and physical properties and the use of estimation models for these properties.

TABLE 5-3: REFERENCES FOR CHEMICAL AND PHYSICAL PROPERTIES

Reference	Type of Guidance
Lyman, W.J., et. al. 1990. *Handbook of Chemical Property Estimation Methods.*	Methods for estimating density, Pv, S, and other chemical properties relevant to the Chemical Properties module.

Note: References are listed in shortened format, with complete references given in the reference list following Chapter 10.

DATA SOURCES: Table 5-4 lists sources of chemical and physical property data.

TABLE 5-4: SOURCES OF CHEMICAL AND PHYSICAL PROPERTIES DATA

Reference	Type of Data
Aldrich Chemical Company, Inc. 1990. *Catalog Handbook of Fine Chemicals*.	Commercial catalog containing over 27,000 organic and inorganic chemicals (mostly for research and development). Entries list the chemical name, CAS RN, structure, MW, and possibly the mp or bp, density, refractive index, a Beilstein reference, and other data (e.g., "hygroscopic, irritant, or moisture sensitive").
Beilstein. Beilstein on-line data base. Updated Periodically.	Data base containing data on known organic compounds. Its unique feature is its ability to define reactants in products. It is an extensive collection of physical properties and chemical reactions.
Buckingham, J. 1982. *Dictionary of Organic Compounds*.	Five volume set (plus supplements) with molecular formula and name index. Lists, with references, synthesis, spectra, physical properties, and derivatives for a large number of organic compounds.
Chemical Abstracts Systems. 1994.	Data base containing CAS RNs and chemical and physical properties.
Farm Chemicals Handbook '87. 1987.	A commercial "magazine" of registered agricultural herbicides, fungicides, and pesticides. Contains measured values of Pv, S, and many others. Usually listed by the agricultural trade name.
Handbook of Chemistry and Physics (CRC). 1992-1993.	Handbook containing CAS RNs and chemical and physical properties.
Hawley, Gessner G., et. al., Ed. 1981. *Condensed Chemical Dictionary*.	A compendium of technical data and descriptive information covering many thousands of chemicals, including their industrial uses. Also includes trademark names.
HSDB®. Hazardous Substances Data Bank (HSDB). Updated Periodically.	On-line data base containing CAS RNs, synonyms, and chemical and physical properties.
Merck Index. 1989.	Handbook containing chemical and physical properties and CAS RNs.
Perry's Chemical Engineering Handbook. 1984.	Handbook containing chemical and physical data.

TABLE 5-4: SOURCES OF CHEMICAL AND PHYSICAL PROPERTIES DATA

Reference	Type of Data
RTECS®. Registry of Toxic Effects of Chemical Substances. 1995.	An on-line data base that contains chemical identity information such as chemical name, CAS RN, synonyms, molecular formula, MW, and others. Also included are toxicity and mutagenicity information.
Sax, N. Irving and Richard J. Lewis, Sr. 1987. *Hazardous Chemicals Desk Reference*.	Handbook containing CAS RNs and chemical and physical properties as well as synonyms, hazard ratings, and current standards for exposure limits.
Syracuse Research Corporation (SRC). 1994. Environmental Fate Data Bases (EFDB©).	Data base containing CAS RNs and chemical and physical property information.
Syracuse Research Corporation (SRC). Updated Periodically. Water Solubility Data Base.	A compilation of measured S data, as well as data on other physical property values for over 4,000 (and growing) chemicals stored on a searchable computer data base (ChemBase v.1.4). It currently contains referenced data from the Arizona data base, the Syracuse data base, the Merck Index, on-line Beilstein, other pertinent literature, and journal articles.
U.S. Department of Health and Human Services. 1985. CHEMLINE: Chemical Dictionary Online.	An on-line interactive chemical dictionary file containing one million chemical substance records. The data elements consist of CAS RNs, molecular formula, synonyms, ring information (part of the structure of some chemicals), and a locator to other on-line data bases that would contain further information on that compound.
U.S. Environmental Protection Agency. 1995d. *Integrated Risk Information System (IRIS®).*	An on-line data base that contains information and data on numerous chemical substances. Information includes substance identification (name and CAS RN) and physical properties such as color/form, odor, bp, mp, MW, density, vapor density, Pv, solubilities, flash point, and others.
Verschueren, K. 1983. *Handbook of Environmental Data on Organic Chemicals.*	An extensive text compiling information on organic chemicals. The data given include formula, physical appearance, MW, mp, bp, Pv, and solubility.

TABLE 5-4: SOURCES OF CHEMICAL AND PHYSICAL PROPERTIES DATA	
Reference	**Type of Data**
Worthing, Charles R. and S. Barrie Walker. 1987. *Pesticide Manual*.	An index of agricultural pesticides which contains chemical names and physical properties, such as mp or bp, Pv, S, and other useful measured values.

Note: References are listed in shortened format, with complete references given in the reference list following Chapter 10.