StEPP™

Software to Estimate Physical Properties

An Environmental Technologies Design Option Tool™

StEPP provides design engineers with the capability to accurately predict the physical and chemical properties of contaminants.

StEPP Features:

- **Database of over 600 organic contaminants included on U.S. EPA's Title III Consolidated Chemical List**
- **Extensive parameter estimation methods to supplement the database**
- **Dependence on temperature for those properties that vary strongly with temperature**
- **Database consists of critically evaluated property values available in the literature**
- **Database includes data from the American Institute of Chemical Engineers/Design Institute for Physical Property Data - AIChE/DIPPR® (Daubert, et al., 1995)**

Classes of Compounds Available in StEPP

alkanes	aromatics
cycloalkanes	carboxylic acids
alkenes	ethers
cycloalkenes	esters
alkynes	thiols
amines	alcohols
nitriles	ketones
dioxins	aldehydes
PCBs	epoxides

Properties Available in StEPP

Vapor Pressure
Infinite Dilution Activity Coefficient
Henry's Constant
Molecular Weight
Normal Boiling Point
Liquid Density
Molar Volume at Operating Temperature
Molar Volume at Normal Boiling Point
Refractive Index
Aqueous Solubility
Octanol Water Partition Coefficient
Liquid Diffusivity
Gas Diffusivity
Water Density
Water Viscosity
Water Surface Tension
Air Density
Air Viscosity

StEPP Applications:

- **Stand-Alone Physical Property Resource Tool**
- **Air and Water Treatment**
- **Properties for Adsorption and Air Stripping**
- **Educational Resource**

StEPP Capabilities

In the process of modeling a treatment system, the most difficult task often involves accurately predicting the physical and chemical properties of the contaminants present in the system. For many treatment and control technologies, such as adsorption and packed tower aeration, models are available that can simulate such processes. However, the effectiveness of such models is severely limited when the properties of the contaminants in the system cannot be accurately determined.

Software to Estimate Physical Properties (StEPP) is designed both as a stand-alone software package to estimate physical and chemical properties and as a tool that may be directly linked to other Environmental Technologies Design Option Tools, such as air stripping and adsorption, in order to provide physical and chemical properties.

StEPP Properties

StEPP combines a reliable database of property values with structure-based estimation methods in a single software product. The list of estimation methods in StEPP is not all-inclusive, but rather focuses on the best of the validated methods found in the literature.

Methods with a theoretical basis have been chosen for StEPP because they tend to apply over a broad range of conditions and exhibit qualitatively correct behavior near physical boundaries and limits. By contrast, purely empirical equations typically have stricter limits on their applicability. The StEPP approach is to focus upon theoretical equations that suggest natural correlating expressions.

The methods within StEPP combine the idea of molecular descriptors with a theoretical model. These have the potential to represent thousands of chemicals with a parameter library containing only a few hundred molecular descriptors. Models of this type are often collectively called Quantitative Structural Activity Relationships and given the acronym "QSAR". For some environmental properties, it is not uncommon to have predictive QSAR models with accuracy approaching the average experimental error.

The temperature and pressure functionality of the QSAR models is also a key feature within StEPP. By contrast, many published estimation methods for properties that are strongly temperature dependent (i.e., Henry's law constant) typically yield a single value at a fixed temperature, and no temperature extrapolation methods are provided.

The table below shows the properties available from the StEPP database and the properties available from parameter estimation methods. Temperature-dependent properties are indicated in the table by an asterisk (*).

Property	Available from Database	Available from Parameter Estimation Methods
Vapor Pressure	Yes*	No
Infinite Dilution Activity Coefficient	No	Yes*
Henry's Constant	Yes*	Yes*
Molecular Weight	Yes	Yes
Normal Boiling Point	Yes	No
Liquid Density	Yes*	Yes*
Molar Volume at Operating Temperature	Yes*	Yes*
Molar Volume at Normal Boiling Point	No	Yes
Refractive Index	Yes	No
Aqueous Solubility	Yes	Yes*
Octanol Water Partition Coefficient	Yes	Yes*
Liquid Diffusivity	No	Yes*
Gas Diffusivity	No	Yes*
Water Density	No	Yes*
Water Viscosity	No	Yes*
Water Surface Tension	No	Yes*
Air Density	No	Yes*
Air Viscosity	No	Yes*
* - Denotes temperature-dependent property		

StEPP - Chemical Properties from Database

Data sources within the StEPP database include:

(1) AIChE/DIPPR® - American Institute of Chemical Engineers/Design Institute for Physical Property Data (Daubert, et al., 1995).

(2) Research Triangle Institute (RTI)/U.S. Air Force/U.S. EPA experimental measurements (Ashworth, et al., 1988).

(3) Carl L. Yaws' book and data compilation, Thermodynamics and Physical Property Data (Yaws, 1992).

(4) EPA Superfund Public Health Evaluation Manual (1986).

The estimation algorithms and resulting software modules within StEPP are only as good as the data upon which they are based. StEPP relies largely on DIPPR data and products because strict data handling, custody protocols, and evaluation guidelines were rigorously followed when compiling AIChE/DIPPR-certified data. Statistical and thermodynamic scrutiny of modeling results is being followed in accordance with established DIPPR procedures (1986).

When data are not available through DIPPR sources, a hierarchy has been selected to make use of the secondary references noted above. For each property currently in the StEPP database, StEPP uses these methods in order of decreasing preference:

- *Vapor Pressure*: correlation from (1), (3), or discrete data from (4); correlations require temperature input
- *Henry's Law Constant*: discrete data from (2), (3), or (4)
- *Molecular Weight*: (1)
- *Normal Boiling Point*: (1)
- *Liquid Density*: correlation from (1); correlation requires temperature input
- *Molar Volume*: inverse of liquid density, multiplied by molecular weight
- *Refractive Index*: (1)
- *Aqueous Solubility*: discrete data from (3) or (4)
- *Octanol-Water Partition Coefficient*: discrete data from (4)

StEPP - Chemical Properties from Parameter Estimation Methods

To supply property estimates where data are not available, the StEPP computer software builds upon the algorithms presented by Arbuckle (1983, 1986) for calculating thermodynamic properties associated with environmental partitioning and phase equilibrium. Calculation options in StEPP currently include procedures for determining activity coefficients, Henry's law constants, aqueous solubilities, and octanol water partition coefficients.

Note that although StEPP preferentially chooses data over parameter estimation techniques in most cases, the software calculates each property from all available methods and the user can override the default property source at any time.

The infinite dilution activity coefficient, an environmental parameter of key importance in thermodynamics, is related fundamentally to several major properties and also correlates empirically with many others (Arbuckle, 1983; Arbuckle, 1986). Within StEPP, the UNIFAC (UNIversal quasichemical Functional group Activity Coefficient) model developed by Fredenslund, et al. (1975) is used to predict all properties involving vapor-liquid and liquid-liquid equilibria. Rogers (1994) gives a detailed description of the UNIFAC methods utilized in StEPP.

The original UNIFAC parameter sets for vapor-liquid (e.g. UNIFAC-VLE (Hansen, et al., 1991)) and liquid-liquid (e.g. UNIFAC-LLE (Magnussen, et al., 1981)) equilibria are available to the StEPP user in addition to a new UNIFAC parameter set (e.g. UNIFAC-ENV (Rogers, 1994)) developed especially for dilute aqueous mixtures. A set of FORTRAN routines, based on the parameter sets described above, forms the core of StEPP's partitioning and equilibrium property calculations.

Listed below are the recommendations within StEPP, in order of decreasing preference, for selecting the "best" UNIFAC parameter set in a given situation:

- *Infinite Dilution Activity Coefficient*: UNIFAC-ENV, VLE, LLE, user choice
- *Henry's Law Constant*: UNIFAC-ENV, VLE, LLE
- *Aqueous Solubility*: UNIFAC-LLE, ENV, VLE
- *Octanol-Water Partition Coefficient*: UNIFAC-LLE, VLE, (ENV not possible)

Because none of the UNIFAC parameter sets contain interaction values for all possible functional group pairs, the StEPP algorithm follows the above order until the options are exhausted, at which time an error message is displayed. At any time, the user can override the automatic choice of the parameter set.

The following paragraphs review the application of UNIFAC to specific partitioning and equilibrium calculations within StEPP that are used to determine Henry's constant, aqueous solubility, and octanol water partition coefficient.

The following additional chemical properties are available from correlations (note that they are not UNIFAC-based): molecular weight, liquid density, molar volume at the operating temperature, molar volume at the normal boiling point, liquid diffusivity, and gas diffusivity. The molecular weight is calculated from atomic structure. The liquid density is estimated by modified Schroeder group contribution method (referenced to water to account for the effect of temperature). It requires temperature input. The molar volume at the operating temperature is available as the inverse of this liquid density, multiplied by molecular weight. The molar volume at the normal boiling point is obtained from Schroeder's group contribution method (Reid, et al., 1987). Three correlations are available for calculating liquid diffusivity: the correlations of Hayduk and Laudie (1974), Wilke-Chang (1955), and Polson (1950). The Hayduk and Laudie and Wilke-Chang correlations require temperature and molar volume at the normal boiling point as input; whereas, the method of Polson requires molecular weight. The gas diffusivity is available from the Wilke-Lee modification (1955) of the Hirschfelder-Bird-Spotz method (1949). It requires molecular weight, molar volume at the normal boiling point, normal boiling point, temperature, and pressure as input parameters.

StEPP - Physical Properties of Air and Water

The following commonly-used properties of air and water are available from correlations: water density, water viscosity, water surface tension, air density, and air viscosity. Water density is found from a correlation developed from a polynomial fit of data given in McCabe and Smith (1976). The water viscosity is calculated using a correlation presented in Yaws, et al. (1976). The water surface tension is available from a correlation presented in Cummins and Westrick (1983). The air density is calculated using the ideal gas law. Air viscosity is found from a correlation presented in Cummins and Westrick (1983).

All five air and water properties available in StEPP require temperature input. Air density also requires pressure as an input parameter.

StEPP – Sample Program Results

Sample results from running the StEPP program for trichloroethylene at 10.0°C and 101325 Pa are provided. The table below shows the complete listing of chemical properties available from StEPP for trichloroethylene in this case.

Complete List of Data Available from StEPP for Trichloroethylene at 10.0 °C and 101325 Pa

Property:	Hierarchy - Source:	Value:	Units:	Temperature:
Vapor Pressure	*1* - DIPPR801	4.69E+03	Pa	10.0 °C
Activity Coefficient[a]	*1* - UNIFAC	8.12E+03	(-)	10.0 °C
Henry's Constant[a]	*1* - Regression of Data Points	0.230	(-)	10.0 °C
	2 - UNIFAC Fit with Data Points	0.232	(-)	10.0 °C
	3 - UNIFAC at Operating T	0.292	(-)	10.0 °C
	4 - Database (RTI)	0.231	(-)	9.9 °C
	Database (RTI)	0.282	(-)	15.0 °C
	Database (RTI)	0.349	(-)	20.1 °C
	Database (RTI)	0.414	(-)	25.0 °C
	Database (RTI)	0.515	(-)	29.9 °C
	5 - UNIFAC at Database T	0.291	(-)	9.90 °C
	UNIFAC at Database T	0.338	(-)	15.0 °C
	UNIFAC at Database T	0.390	(-)	20.1 °C
	UNIFAC at Database T	0.444	(-)	25.0 °C
	UNIFAC at Database T	0.504	(-)	29.9 °C
Molecular Weight	*1* - Group Contribution Method	131.38	kg/kmol	
Normal Boiling Point	*1* - Database (DIPPR801)	87	°C	
Liquid Density	*1* - Database (DIPPR801)	1.48E+03	kg/m^3	10.0 °C
	2 - Group Contribution Method	1.43E+03	kg/m^3	10.0 °C
Molar Volume at Operating T	*1* - Database (DIPPR801)	0.0886	$m^3/kmol$	10.0 °C
	2 - Group Contribution Method	0.0917	$m^3/kmol$	10.0 °C
Molar Volume at NBP	*1* - Schroeder's Method	0.102	$m^3/kmol$	
Refractive Index	*1* - Database (DIPPR801)	1.4750	(-)	
Aqueous Solubility[a]	*1* - UNIFAC Fit with Data Point	821	PPMw	10.0 °C
	2 - UNIFAC at Operating T	906	PPMw	10.0 °C
	3 - Database (Yaws)	1100	PPMw	25.0 °C
	4 - UNIFAC at Database T	1180	PPMw	25.0 °C
log Octanol Water Partition Coeff.	*1* - UNIFAC at Operating T	Not Available		
	2 - Database (SUPERFUND)	2.38	(-)	25.0 °C
	3 - UNIFAC at Database T	Not Available		
Liquid Diffusivity	*1* - Hayduk & Laudie	6.44E-10	m^2/sec	10.0 °C
	2 - Wilke-Chang	6.41E-10	m^2/sec	10.0 °C
	3 - Polson	5.39E-10	m^2/sec	10.0 °C
Gas Diffusivity	*1* - Wilke-Lee	7.89E-06	m^2/sec	10.0 °C

[a]UNIFAC Parameter Set = UNIFAC-ENV
(-) - Denotes Dimensionless Units

The properties of air and water available at 10.0°C and 101325 Pa (1 atm) are shown in the table below.

Complete List of StEPP Data for Properties of Air and Water at 10.0 °C and 101325 Pa

Property	Hierarchy - Source	Value	Units	Temperature
Water Density	*1* - Data Correlation	999.75	kg/m^3	10 °C
Water Viscosity	*1* - Yaws (1976)	1.31E-03	kg/m/sec	10 °C
Water Surface Tension	*1* - Cummins & Westrick (1983)	0.0742	N/m	10 °C
Air Density	*1* - Ideal Gas Law	1.25	kg/m^3	10 °C
Air Viscosity	*1* - Cummins & Westrick (1983)	1.72E-05	kg/m/sec	10 °C

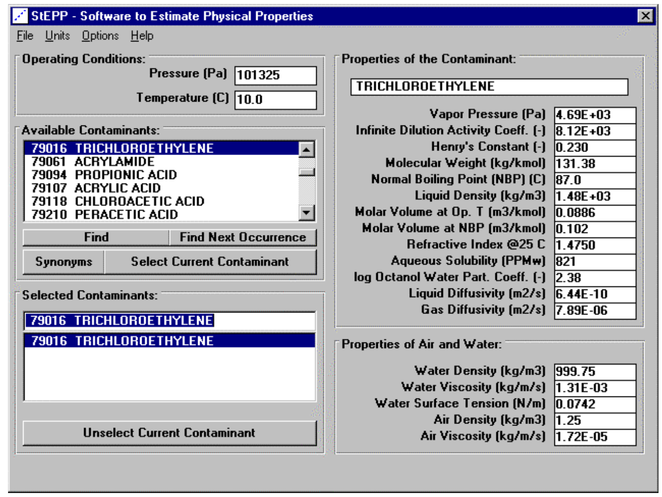
StEPP contains a built-in hierarchy in order to preferentially select a value when more than one source of values is available for a property. This hierarchy is shown in the sample result tables by the italicized numbers that precede the sources for each property. For example, the table for the properties of trichloroethylene shows that the hierarchy for aqueous solubility is as follows: (1) UNIFAC Fit with Data Point, (2) UNIFAC at Operating T, (3) Database, and (4) UNIFAC at Database T.

When a component is selected in StEPP, calculations are performed to determine all the values that are available for that compound. However, only the "best" available value (as determined by the hierarchy) appears in the main StEPP window as the recommended value for each particular property. Each value source that is preferentially chosen by StEPP for a property is indicated by a *1* in the *Hierarchy* column in Tables 1.3 and 1.4.

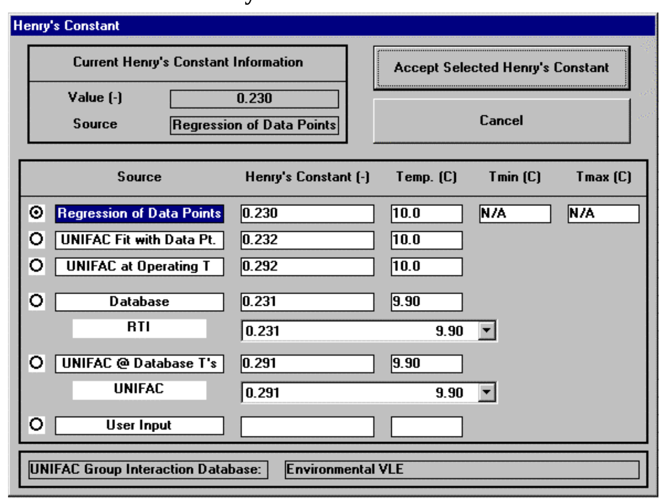
When a particular value source is not available from StEPP, the next value in the hierarchy will be chosen by StEPP to appear in the main StEPP window. For example, for the aqueous solubility (see hierarchy shown above), if no value is available from the UNIFAC Fit with a Data Point (hierarchical choice 1), then the value from UNIFAC at the Operating T (hierarchical choice 2) is shown in the main StEPP window as the recommended value. If UNIFAC is unable to calculate this value, then the value from the Database (hierarchical choice 3) will appear in the main StEPP window. If no value is available in the Database, then no value will be available for UNIFAC at the Database T (hierarchical choice 4) and a "Not Available" message will appear in the main StEPP window in the column for aqueous solubility.

The following figure shows the main StEPP window for trichloroethylene with the values selected according to the hierarchy presented in the earlier tables. It should be noted that even though this hierarchy is used when a compound is initially selected, the user may override the hierarchy and choose any available value for a property to appear in the main StEPP window as the currently selected value. In addition, it is possible for the user to input a value for any or all properties. The final figure shows the Henry's constant window for Trichloroethylene at 10 °C and 101325 Pa (1 atm).

Main StEPP Window for Trichloroethylene at 10.0°C and 101325 Pa



Henry's Constant Window for Trichloroethylene at 10.0°C and 101325 Pa



Graphical User Interface

ETDOT is designed for the Microsoft Windows environment with a graphical user interface (GUI) to maximize user-friendliness. Making use of the Microsoft Windows interface, with its built-in file and hardware control features, frees the engineer from concerns over printer drivers and other "machine" issues and allows more attention to the computational algorithms. The GUI consists of a Microsoft Visual Basic front-end shell that calls FORTRAN subroutines to perform the calculations.

System Requirements

The minimum ETDOT system requirements are as follows:

- English-language version of Microsoft Windows 95, Microsoft Windows 98, or Microsoft Windows NT 4.0; in the case of Microsoft Windows NT 4.0, Service Pack 3 or more recent is required
- 50 MB of hard disk space
- 32 MB of RAM is recommended
- A Pentium or more recent processor is recommended
- A graphic VGA or more recent video display
- A mouse or other pointing device is recommended

Product Information

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