What is an Exposure Assessment?

OPPT's Exposure Assessmen Guidance

Specialized Priority Setting Tools

Screening Level Tools

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Glossary

Frequently Asked Questions

Estimation Program Interface (EPI) Suite

What Does EPI Suite ™ Do?

• The EPI (Estimation Programs Interface) Suite™ is a Windows®-based suite of physical/chemical property and environmental fate estimation programs developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC). EPI Suite™ uses a single input to run the following estimation programs: KOWWIN™, AOPWIN™, HENRYWIN™, MPBPWIN™, BIOWIN™, BioHCwin, KOCWIN™, WSKOWWIN™, WATERNT™, BCFBAF™, HYDROWIN™, KOAWIN and AEROWIN™, and the fate models WVOLWIN™, STPWIN™ and LEV3EPI™. ECOSAR™, which estimates ecotoxicity, is also included in EPI Suite™.
• EPI Suite™ is a screening-level tool and should not be used if acceptable measured values are available.

•A clear understanding of the estimation methods and their appropriate application is very important. Click on the Help tab in EPI Suite™ for detailed information on the methods and models in it.

How Do the Individual Models that Make up EPI Suite™ Work?

• KOWWIN™:Estimates the log octanol-water partition coefficient, log K_{OW}, of chemicals using an atom/fragment contribution method.
• AOPWIN™: Estimates the gas-phase reaction rate for the reaction between the most prevalent atmospheric oxidant, hydroxyl radicals, and a chemical. Gas-phase ozone radical reaction rates are also estimated for olefins and acetylenes. In addition, AOPWIN™ informs the user if nitrate radical reaction will be important. Atmospheric half-lives for each chemical are automatically calculated using assumed average hydroxyl radical and ozone concentrations.
• HENRYWIN™: Calculates the Henry's Law constant (air/water partition coefficient) using both the group contribution and the bond contribution methods.
• MPBPWIN™: Melting point, boiling point, and vapor pressure of organic chemicals are estimated using a combination of techniques. Included is the subcooled liquid vapor pressure, which is the vapor pressure a solid would have if it were liquid at room temperature. It is important in fate modeling.
• BIOWIN™: Estimates aerobic and anaerobic biodegradability of organic chemicals using 7 different models. Two of these are the original Biodegradation Probability Program (BPP™). The seventh and newest model estimates anaerobic biodegradation potential.
• BioHCwin: Estimates biodegradation half-life for compounds containing only carbon and hydrogen (i.e. hydrocarbons).
• KOCWIN™: Formerly called PCKOCWIN™, this program estimates the organic carbon-normalized sorption coefficient for soil and sediment; i.e. K_{OC}. K_{OC} is estimated using two different models: the Sabljic molecular connectivity method with improved correction factors; and the traditional method based on log K_{OW}.
• WSKOWWIN™: Estimates an octanol-water partition coefficient using the KOWWIN™ program, then estimates a chemical's water solubility from this value and applicable correction factors if any.
• WATERNT™: Estimates water solubility directly using a "fragment constant" method similar to that used in the KOWWIN™ program.
• BCFBAF™: Formerly called BCFWIN™, this program estimates fish bioconcentration factor and its logarithm using two different methods. The first is the traditional regression based on log K_{OW} plus any applicable correction factors, and is analogous to the WSKOWWIN™ method. The second is the Arnot-Gobas method, which calculates BCF from mechanistic first principles. BCFBAF also incorporates prediction of apparent metabolism half-life in fish, and estimates BCF and BAF for three trophic levels.
• HYDROWIN™: Estimates aqueous hydrolysis rate constants and half-lives for the following chemical classes: esters, carbamates, epoxides, halomethanes, selected alkyl halides, and phosphorus esters. Estimates rate constants for acid- and base-catalyzed hydrolysis, but with the exception of phosphorus esters, not neutral hydrolysis. In addition, HYDROWIN™ identifies a variety of chemical structure classes for which hydrolysis may be significant (e.g. carbamates) and gives relevant experimental data.
• KOAWIN: Estimates K_{OA}, the octanol/air partition coefficient, using the ratio of the octanol/water partition coefficient (K) from KOWWIN™ and the dimensionless Henry's Law constant (K) from

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HENRYWIN™. K_{OA} has multiple uses in chemical assessment.

• AEROWIN™: Estimates the fraction of airborne substance sorbed to airborne particulates, i.e. the parameter phi (φ), using three different methods. AEROWIN™ results are also displayed with AOPWIN™ output as an aid in interpretation of the latter.
• WVOLWIN™: Estimates the rate of volatilization of a chemical from rivers and lakes; and calculates the half-life for these two processes from their rates. The model makes certain default assumptions with respect to water body depth, wind velocity, etc.
• STPWIN™: Using several outputs from EPI Suite™, this program predicts the removal of a chemical in a typical activated sludge-based sewage treatment plant. Values are given for total removal and three processes that may contribute to removal: biodegradation, sorption to sludge, and air stripping. The program assumes a standard system design and set of default operating conditions.
• LEV3EPI™: This program contains a level III multimedia fugacity model and predicts partitioning of chemicals among air, soil, sediment, and water under steady state conditions for a default model "environment". Some (but not all) system default values can be changed by the user.
• ECOSAR™: Estimates the toxicity of chemicals discharged to water. ECOSAR™ predicts toxicity to fish, aquatic invertebrates and algae using an extensive set of structure-activity relationships (SARs). The program estimates a chemical's acute (short-term) toxicity and, when available, chronic (long-term or delayed) toxicity.

What Do I Need to Use EPI Suite™?

• EPI Suite™ requires only a single input, a representation of the chemical structure in SMILES notation. SMILES means "Simplified Molecular Information and Line Entry System." A description of this system is available with the EPI Suite™ program. Entry of SMILES via a linked file of CAS numbers (the SMILECAS file) is also possible; as is entry by chemical name using the Name Lookup function.

How Are EPI Suite™ Data Used?

• EPI Suite™ provides users with screening-level estimates of physical/chemical and environmental fate properties. These properties are the building blocks of exposure assessment. Before using EPI Suite™, users should first determine whether any suitable data are available from the literature (e.g., Merck Index, Beilstein). This is facilitated by a database of >40,000 chemicals (called PHYSPROP©) that is included in the EPI Suite™ software. Dermwin™, a program that estimates the dermal permeability coefficient K_p, is included in EPI Suite™. ECOSAR™ is a program that predicts aquatic toxicity and is included in EPI Suite™. ECOSAR™ can also be downloaded as a separate program from the ECOSAR home page.

Has EPI Suite™ been peer reviewed?

Individual estimation programs and/or their underlying predictive methods and equations have been described in numerous journal articles in peer-reviewed technical journals. The full reference citations are given in the Help files for the individual programs. In addition, EPI Suite™ has undergone detailed review by a panel of EPA's independent Science Advisory Board (SAB) (http://yosemite.epa.gov/sab/sabpeople.nsf/WebCommittees/BOARD), and the September 2007 report can be downloaded from http://www.epa.gov/sab/panels/epi_suite_review_panel.htm.

PLEASE NOTE: the items mentioned at this page are in Adobe's Portable Document Format (PDF). To view or print them you will need to have the Adobe Acrobat Reader program installed on your computer. The Reader can be downloaded and used with no charge; for more information at EPA about PDF files.

Citing EPI Suite™

Full reference citations for the individual programs are given in the Help files for the individual programs. Cite the software itself as follows:
US EPA. [2009 or insert current year]. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.00 or insert version used]. United States Environmental Protection Agency, Washington, DC, USA.

What Type of Computer System Do I Need?

EPI Suite v4.00 runs on Windows NT®, Windows XP/XP Professional®, and Windows Vista®. All of the individual programs and help files also work correctly on Windows 95® and 98® when opened from within the EPI Suite folder, but users of the interface program may encounter error messages.

Users of Windows Vista: please see the special instructions on the download page

What's New?

• Description of Updates for EPI Suite Version 4.00 (January, 2009)

Download EPI 4.00

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Who Can I Call for More Information?

For more information about the model, please contact:

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