U.S. EPA OPPT's Screening Level Exposure Assessment Data, Tools and Models – An Overview

Cathy Fehrenbacher, Chief

Exposure Assessment Branch

EPA's Office of Pollution Prevention and Toxics

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This presentation will describe:

- Background on exposure assessment using a tiered approach
- A very brief overview of the new IUR exposure-related data
- A very brief overview of OPPT's screening level exposure assessment models
- Where you can get more information and obtain the models

Appropriate Use of Predictive Models

- Priority setting tools allow one to compare large numbers of chemicals using standardized criteria
- Screening level tools can help to screen out or eliminate chemicals of low concern and identify where additional evaluation is needed
- Higher tier tools provide more definitive, detailed analyses, often used in combination with screening level tools and available data
- Models can be helpful in filling data gaps and to supplement data

Background - Tiered Approach to Exposure Assessment

- Screening Level Assessment
  - screening chemicals for risk assessment
  - conservative (protective)
  - uses readily available data and information
- Advanced Exposure Assessment
  - focuses on higher priority exposures
  - accurate, precise exposure assessment
  - data quality standards are critical

Overview - Inventory Update Rule Amendment Data

- Site and manufacturing information is reported for chemicals manufactured/imported at or above 25,000 lb at a single site
- Use and exposure-related data is reported for chemicals manufactured in amounts of 300,000 lb or more at a single site
- Production Volume (PV)
  - Manufactured
  - Imported
- Manufacturing Information
  - Physical Forms and % of PV for each physical form
  - Number of workers potentially exposed (in range):
  - Maximum concentration (in range)

Overview - Inventory Update Rule Amendment Data

- Industrial Processing and Use Information
  - Use as described by comb. of industry, process, functional categories
  - % PV associated with each combination
  - Number of sites associated with each combination
  - Number of workers associated with each combination
- Commercial and Consumer Use Information
  - Commercial/consumer product category
  - % PV & concentration for commercial and/or consumer category
  - Used in products intended for children

Inventory Update Rule Amendment Data

- Processing and use information will help EPA, other Agencies, general public, and others to readily screen and categorize chemicals
- EPA will use the IUR data for screening and prioritizing HPV Chemicals

OPPT's Exposure Tools and Models Include:

- Methods used by OPPT for exposure assessment
- Computerized models and accompanying databases
- Default assumptions which can be modified by the user
- Online help and transparent guidance in using the models and databases
- Capability to address adults (including workers), children, and infant subpopulations
- Population data, and information on endangered species (E-FAST 2)

OPPT's Exposure Assessment Tools and Models

Priority Setting Tools:

- SRD
- UCSS

Screening Level Tools:

- **ChemSTEER**
- **E-FAST**
- **EPI Suite™**

Higher Tier Tools:

- AMEM
- Internet GEMS
- MCCEM
- **WPEM**

Physical/Chemical Properties and Environmental Fate and Transport

- EPI Suite™

Except for BioHCWIN and KOAWIN, EPI Suite™ is copyrighted by the U.S. Environmental Protection Agency

Physical/Chemical Properties and Environmental Fate and Transport

- Provides basic information on the nature and characteristics of a chemical substance
- Which gives insight into:
  - Partitioning in the environment
  - Potential for environmental exposure
  - Potential routes of human exposure
  - Toxicity and biological effects
- Can be useful in designing small molecules for biodegradability

Estimation Programs Interface (EPI Suite™)

- Reliable measured data should be used if available in preference to modeled estimates
- A clear understanding of the estimation methods and their appropriate application is very important
- Information on each method can be found in the Help tab in EPI Suite™

EPI Suite™ - How Does It Work?

- You enter the chemical structure in SMILES notation, CAS number (if available), or name via look up table
- EPI Suite™ runs chemical property and fate models sequentially
- Includes a database of p/chem fate properties for approximately 40,000 chemicals

EPI Suite™ Input Screen

EPI v3.20

File Edit Functions BatchMode ShowStructure Output Fugacity STP Other Help

PhysProp | Previous | Get User | Save User | CAS Input | CALCULATE | ClearInputField | What's New

Enter SMILES: 000050-00-0 — O=C

Chem NAME: — Formaldehyde

NameLookup

Henry LC (atm-m3/mole):

Wat Sol (mg/L):

MP:

Vap Pr (mm Hg):

BP:

Log Kow :

	River:	Lake:
Water Depth (meters):	1	1
Wind Velocity (m/sec):	3	0.5
Current Velocity(m/sec):	1	0.05

Output
- [ ] Summary
- [x] Full

The Estimation Programs Interface (EPI) Suite™ was developed by the US Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). It is a screening-level tool and cannot be used for all chemical substances. Like other such tools, it is intended for use in screening-level applications such as to quickly screen chemicals for release and exposure potential, and "bin" chemicals by priority for future work. Estimated values should not be used when experimental (measured) values are available.

Important information on the performance, development and application of the individual estimation programs within EPI Suite™ is included in the User's Guide.

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Start | Cathy Fehrenbacher - In... | overview_screening mod... | untitled - Paint | EPI v3.20 | 2:42 PM

EPI Suite™ P/Chem Modules

- MPBPWIN™ - melting point, boiling point, and vapor pressure
- KOWWIN™ - octanol/water partition coefficient
- WS/KOWWIN™ - water solubility from Kow
- WATERNT™ – water solubility based on a fragment constant method
- HENRYWIN™ - air/water partition coefficient
- PCKOCWIN™ - ability to sorb to the organic portion of soil and sediment
- BCFWIN™ - ratio of a chemical's concentration in the tissue of an aquatic organism to the concentration in the ambient water
- HYDROWIN™ – acid and base-catalyzed hydrolysis
- AEROWIN™ – fraction of airborne substance sorbed to airborne particulates
- AOPWIN™ - atmospheric persistence
- BIOWIN™ – aerobic and anaerobic biodegradation
- BioHCWIN – biodegradation half-life for compounds containing only carbon and hydrogen (e.g., hydrocarbons)
- KOAWIN – octanol/air partition coefficient

EPI Suite™ Environmental Fate Modules

- WVOLWIN™ – rate of volatilization from rivers and lakes
- STPWIN™ – removal in a simulated sewage treatment plant
- LEVEL3EPI™ Fugacity Model – partitioning of chemicals between air, soil, sediment and water under steady state conditions for a default model "environment"

Manufacturing, Industrial & Commercial Exposures & Environmental Releases

- ChemSTEER

ChemSTEER

- Chemical Screening Tool for Exposures and Environmental Releases (ChemSTEER)
  - Estimates workplace exposures and releases resulting from manufacture or use of an industrial chemical
  - Estimates are provided in the absence of monitoring data
  - Screening level estimates
  - Uses EPA methods and models
  - Uses EPA default assumptions (worst case scenarios)

ChemSTEER – How Does It Work?

- You “build” your assessment by entering some key inputs:
  - Data on the chemical to be assessed
    - Production volume, or assessed volume, kg/year
    - P/chem properties (measured or estimated)
  - Select at least one operation (i.e., workplace); options include:
    - Pre-defined industry-specific/use-specific operation
    - User-defined operation

ChemSTEER – How Does It Work?

- Next, you “build” the releases and exposure activities
  - Select at least one release/exposure activity within each operation
  - Each source/activity is associated with default models for calculating releases and worker inhalation and dermal exposure
  - Enter mass balance and container-related data
  - Review models and model-input data

General Population, Consumer, and Environmental Exposures

- E-FAST

Exposure Estimates from Industrial Releases:

- Fugitive & Incineration Releases to Air (human)
- Releases to Landfill/Groundwater (human)
- Releases to Surface Water (human and environmental)
  - Site specific
    - Rivers/Stream flows and drinking water intakes
    - Bays/Estuaries/Ocean dilution factors
  - Receiving stream flows by industry type (generic)
    - Standard Industrial Classification (SIC) code

“Down-the-Drain” Releases of Consumer Products

- Consumer products released “down the drain” to the environment
  - Potential human exposure
  - Potential environmental exposure

E-FAST – How Does It Work?

- You “build” the exposure scenario for industrial releases:
  - Enter P/chem and fate information
  - Identify site of release by NPDES permit number, or generically (SIC Code)
  - Enter release activity, including number of sites
  - Enter release amounts and frequency
  - Removal in wastewater treatment, drinking water treatment
  - Identify population of interest, adults, children, infants, and exposure factors
  - Identify Chronic Concentration of Concern (COC) to check for exceedance for aquatic environmental exposures

E-FAST – How Does It Work?

- You “build” the exposure scenario for consumer product uses:
  - Enter the use scenario (generic or user-defined)
  - Identify the location of use
  - Enter Molecular Weight and Vapor Pressure
  - Enter weight fraction in the formulation
  - Identify population of interest, adults, children, infants, and relevant exposure factors

Designing Safer Interior Latex and Alkyd Paints by Considering Potential Exposures

- Wall Paint Exposure Model

Wall Paints Exposure Model

- Estimates potential exposure of consumers and workers to the chemicals emitted from wall paint which is applied using a roller or a brush
- Developed in EPA's Design for the Environment (DfE) Designing Wall Paints for the Indoor Environment project
- Developed in coordination and cooperation with National Paint and Coatings Association, paint manufacturers, and chemical suppliers
- Can be used to design safer interior latex and alkyd paints

WPEM – How Does It Work?

- You enter the type of paint (latex or alkyd) being assessed, density of the paint (default values available), and the chemical weight fraction, molecular weight, and vapor pressure
- Default occupancy and exposure data are included; user can input specific data

TM

Summary

- Many tools and models are available
- Use them appropriately, in the absence of data
- Most are designed for a specific purpose, but are flexible
- IUR data will be a very valuable data source for priority setting and screening

Where Can I Find More Information?

- Information on the Inventory Update Rule Amendments: http://www.epa.gov/oppt/iur/index.htm
- OPPT models and documentation are available for download from the Internet at:

  http://www.epa.gov/oppt/exposure/
- R.S. Boethling, E. Sommer, and D. DiFiore. Designing Small Molecules for Biodegradability. Chemical Reviews 107:2207-2227 (2007).