Overview of Exposure Assessment Tools and Models

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US EPA

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What this presentation covers

- Introductory Information
  - About the organization – what do we do?
  - OPPT tools and models – who uses them?
  - Have our workplace tools and models been peer reviewed?
  - Program requirements – when are assessments prepared?

- Workplace Exposure and Environmental Release Assessments
  - Areas of technical support and other capabilities
  - Tools and models for estimating chemical emissions and exposures
  - Activities and ideas further work on tools and models (2014 – 2016)

- General Population/ Environmental/Consumer Assessments
  - Areas of technical support and other capabilities
  - Tools and Models for estimating non-occupational exposures
  - Activities and ideas for further work on tools and models (2014 – 2016)
OPPT’s Risk Assessment Division (RAD) Focuses on Risk Assessments

- Risk assessment is the integration of qualitative and quantitative information on:
  - Hazard
    - Toxicity of chemical?
    - Types and severity of effects?
  - Dose-Response
    - Relation between an administered dose and biological response?
    - How much is bad?
  - Exposure
    - Who/what is exposed?
    - How are they exposed?
    - How much are they exposed/
OPPT Also Leads Efforts and Has Expertise In

Safer Substitutes & Cleaner Processes

- Green Chemistry
- Green Engineering
- Design for the Environment

Peer Review & Scientific Support

- Manage OPPT test guidelines development efforts
- Coordinate guidelines with other national and international organizations (including the OECD)
- Develop and implement a process of scientific peer review
Over 3,000 individuals have asked to be notified of model updates.

Who uses OPPT’s Tools & Models?

- Industry: 12%
- University/Research: 16%
- Consultants: 5%
- Fed. Government: 4%
- State/Local Gov.: 2%
- Non-OPPT EPA: 1%
- Other: 60%
## Peer Review Status

<table>
<thead>
<tr>
<th>Model</th>
<th>Application</th>
<th>Peer Review</th>
<th>Evaluation/Validation</th>
</tr>
</thead>
<tbody>
<tr>
<td>AMEM</td>
<td>Migration of chemicals through polymers</td>
<td>Letter Peer Review</td>
<td>Comparison with data</td>
</tr>
<tr>
<td>ChemSTEER</td>
<td>Worker exposure, environmental releases</td>
<td>Letter Peer Review</td>
<td>Comparison with data, publication</td>
</tr>
<tr>
<td>Chemical Safety Mapper</td>
<td>General population, environmental exposure, EJ analyses, geospatial display</td>
<td>Future</td>
<td>Enables easy comparison of monitoring data and model results</td>
</tr>
<tr>
<td>Industry Specific Generic Scenarios / Emission Scenario Documents (ESDs)</td>
<td>Worker exposure, environmental releases</td>
<td>Some received peer input from OECD EATF and industry; some reviewed by industry</td>
<td>Available data found in the literature and/or provided by industry and/or OECD; peer reviewed models are used to augment data</td>
</tr>
<tr>
<td>E-FAST</td>
<td>Consumer exposure, general population, environmental exposure</td>
<td>Letter Peer Review</td>
<td>Informal comparison with available monitoring data</td>
</tr>
<tr>
<td>EPISuite</td>
<td>P/chem properties, environmental fate and transport</td>
<td>SAB</td>
<td>Validation, publications</td>
</tr>
<tr>
<td>FIAM</td>
<td>Formaldehyde exposure from pressed wood products</td>
<td>Letter peer review</td>
<td>Evaluation with extensive monitoring data, ORD test house</td>
</tr>
<tr>
<td>GWP Approach</td>
<td>Global Warming Potential - screening</td>
<td>Future</td>
<td>Comparison with known GWP chemicals</td>
</tr>
<tr>
<td>Internet GEMS</td>
<td>General population, environmental exposure</td>
<td>Partial peer review, Future</td>
<td>Some comparison, mainstream EPA models</td>
</tr>
<tr>
<td>MCCEM and WPEM</td>
<td>Residential exposure to chemicals and wall paints, respectively</td>
<td>Letter Peer Review</td>
<td>Evaluation with extensive monitoring data, ORD test house</td>
</tr>
<tr>
<td>ReachScan</td>
<td>Exposure from drinking water, surface water</td>
<td>Future</td>
<td>Limited</td>
</tr>
</tbody>
</table>
Exposure Related Support to OPPT Program Areas

- New Chemicals (TSCA section 5)
  - Engineering Assessments (Workplace Releases and Exposures)
  - Environmental Fate and Transport Assessments
  - Consumer, Environmental, and General Population Exposure Assessments

- Existing Chemicals
  - Various types of assessments in support of TSCA sections 4, 6, and 8 of TSCA

- Voluntary Programs
  - DfE, 3M and DuPont MOUs (e.g. PFOA Monitoring)

- Enforcement
  - Biodegradation SEP (PFCs)
Workplace Releases & Exposure Assessment
Areas of Technical Support

- Areas of Technical Support
  - Occupational Exposure Assessment
  - Environmental Release Assessment
  - Industrial Hygiene (e.g. engineering controls and PPE)
  - Chemical Engineering (e.g. process related analyses)
  - On-site Treatment Systems

- Other Capabilities
  - Modeling
  - Tools Development
  - Green Engineering
Environmental Releases and Workplace Exposure Assessments

- Problem formulation
- Assessments tailored to the program/case

**Environmental Releases**
- Media: Air (stack, fugitive), Water (treatment, surface water, etc.), Land, Incineration, other (Deepwell injection)
- Amounts: Mass per time (kg/site-day)
- Frequencies (days/year)
- Locations (postal zip code, city, NPDES (discharge permit number, etc., if known)

**Workplace Exposures**
- Routes:
  - Inhalation (breathed): vapor, mist, particulate
  - Dermal (skin): liquids, solids
- Amounts:
  - Concentrations - parts per million (ppm) or mg/m³
  - Potential dose rate (mass based) – mg/day
- Frequencies (days/year)
- Populations: industrial and commercial workers

- Scope covers manufacturing, processing and use
Tools and Methods for Estimating Environmental Releases and Workplace Exposures

- Workplace scenarios
  - Industry-specific Generic Scenarios (GSs)
  - Emission Scenario Documents (ESDs)

- Chemical Screening Tool for Exposures and Environmental Releases (ChemSTEER)

- Other databases and technical documents
• What’s in a generic scenario or ESD?
  – Process description
  – Mass balance data for process / operation
  – Release and / or exposure models
  – Default values
  – Estimation equations and example calculations

• How are generic scenarios or ESD developed?
  – Literature research
  – Industry input
  – New chemical case information and data
  – OECD input and review
• OPPT RAD is an active member of OECD Task Force on Exposure Assessment

• 9 of the 30 ESDs in current published OECD ESD series are from US EPA

• Good leveraging of resources

• OECD Task Force review improves quality and enhances technical credibility of ESDs

• Examples of ESDs Published or in Progress:
  – Use of Adhesives
  – Chemical Vapor Deposition in Semiconductor manufacture
  – Use of Textile Dyes
  – Application of Radiation Curable Coatings, Inks and Adhesives
  – Use of Metalworking fluids
  – Spray Application of Coatings in Automotive Refinishing
  – Aqueous Firefighting Foam
What does ChemSTEER do and what is it used for?

- The application is used to produce screening-level estimates of workplace exposures and environmental releases.
- Its primary purpose is to support EPA’s New Chemicals Program.
- Approximately 1,000 assessments are prepared every year.
- The application can also be used to address data gaps when preparing more thorough assessments.
Running release & exposure models

- AP-42 Loading Model
- Penetration Model
- Drum Residual Model
- Solids Transfer Dust Loss Model
- Mass Balance Inhalation Model
- Models for Estimating Inhalation Exposures Based on Exposure Limits
- Models for Estimating Dermal Exposure
Other Tools & Resources

• Databases: EPA TRI and CDR; OSHA IMIS; CDC NHANES
• Other International Risk Assessments
• IH Documents
  – (e.g. Decision Logic for OPPT selection of Respirators for Chemical Substances, Guidance for Glove Permeation Testing)
• Compendium of Technical / Policy Memos
  – (e.g. Internal document, drop categories, standard assumption for efficiency of bag house/cyclone, autoclaves, incineration)
• SOP for Engineering Assessment
  – contains additional models and approaches for estimating releases and occupational exposures and information for evaluating engineering controls and some on-site treatment information
• Other Technical Guidance Documents
  – (e.g. approaches for Estimating Occupational Exposure and Environmental Releases for Nanomaterials)
• Database of Exposure Related Information for CNT/CNF

• New & Existing Chemical Programs
  – Continue effort to update/develop ESDs and program ESDs into ChemSTEER

  – Enhance ChemSTEER with a Near Field / Far Field inhalation exposure model
    • NF/FF partitions an exposure setting into two zones (near & far from emitting source)
      – Able to distinguish between exposure for Users (near) and Bystanders (far)
      – Applicable to workplace and consumer exposure scenarios

  – Compare predictive models in ChemSTEER with those in other OECD models
    • This project involves reviewing the underlying theory and assumptions behind the various models

  – For potential exposures resulting from product/article emission in workplace setting (including self-employed and contract workers)
    • Identify/develop predictive models for estimating emission rates from products/articles
    • Continue development of database of emissions and exposures from products (OECD TFEA activity)

• New & Existing Chemical Programs (cont’d)
  – Continue development of Waste Treatment Information Search Tool
    • Explore use of tools in new and existing chemicals assessments
    • Explore use of tools in ESDs development

  – Nano-related Guidances and Databases
    • Update Interim Guidance on Approaches for Assessing and Controlling Workplace Releases and Exposures to New and Existing Nanomaterials
    • Guidance for Exposure Monitoring of Nanomaterials

  – Develop approaches for estimating cumulative exposures in workplace settings.
Consumer, General Population, and Environmental Exposure Assessments
Areas of Technical Support

• Areas of Technical Support
  • Environmental Fate and Transport Assessment
  • Environmental Exposure Assessment
  • General Population Exposure Assessment
  • Consumer Exposure Assessment
  • Database and Model Development

• Other Capabilities
  • CREM
  • Exposure Assessment Guidelines, Exposure Factors Handbook, Peer Review Guidelines
  • OECD Exposure Assessment Task Force, WPMN SG 3, 4, 8
Overall Assessment Approach

• Problem Formulation

• Assessments tailored to the program/case
  – Fate and transport – all endpoints
  – Consumer, General Population, Environmental Exposure – inhalation, dermal, ingestion (water)
    • All media (for releases assessed)
    • All uses (provided or identified by OPPT)
    • Frequency, duration, magnitude (e.g., mg/kg-day)
    • LADD, ADD based on health endpoint
    • Exceedance of COC for ecotox
    • Locations (SIC code, generic SIC)
    • Populations (including children, EJ, etc.)
Non-Occupational Exposure Assessment Tools and Models

Screening Level Tools:
- EPI Suite™
- E-FAST

Higher Tier Tools:
- AMEM
- IGEEMS/CSM
- ReachScan
- VVWM
- MCCEM
  - WPEM
  - FIAM

www.epa.gov/oppt/exposure/
Except for BioHCWIN and KOAWIN, EPI Suite™ is copyrighted by the U.S. Environmental Protection Agency
EPI Suite® v4.11

EPI Suite - Welcome Screen

PhysProp | Previous | Get User | Save User | Search CAS
---|---|---|---|---

Input CAS #: 236391-76-7
Input Smiles: CCC(=O)CCC(=O)OC(C)C1CC(C)(C)CCC1
Input Chem Name: Romandolide

Henry LC: atm-m/mole
Melting Point: Celsius
Boiling Point: Celsius
Water Solubility: mg/L
Vapor Pressure: mm Hg
Log Kow:
River Water Depth: 1 meters
Lake Water Depth: 1 meters
Wind Velocity: 5 meters/sec
Current Velocity: 0.05 meters/sec

The Estimation Programs Interface (EPI) SuiteTM 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, intended for use in applications such as to quickly screen chemicals for release potential and “bin” chemicals by priority for future work. Estimated values should not be used when experimental (measured) values are available.

EPI Suite® cannot be used for all chemical substances. The intended application domain is organic chemicals. Inorganic and organometallic chemicals generally are outside the domain.

Important information on the performance, development, and application of EPI Suite® and the individual programs within it can be found under the Help tab. Copyright 2000-2011 United States Environmental Protection Agency for EPI Suite® and all component programs except BioHCWIN and KOAWIN.
Environmental Fate and Transport

- Provides
  - Basic information on the behavior of a chemical substance when released to the environment
- 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
General Population and Environmental Exposure

- E-FAST – screening
- IGEMS/Chemical Safety Mapper – higher tier, GIS
- ReachScan – drinking water
- VVWM – under development
EFAST2 Exposure Modules

- Suite of models and databases
- Four modules: General Population and Ecological Exposure; Down the Drain; Consumer Exposure Module; and stand-alone PDM
- Default exposure factors which can be changed
- User builds the scenario to be assessed
• Predicts release concentrations to surface water, air, and landfills
  – Aquatic concentrations
  – Human exposure doses

• When combined with toxicity data, can be used to determine if release may pose risk to humans or the aquatic environment

• Used routinely for new chemical assessments, but also for existing chemicals as appropriate

• Ongoing update of model
• Capability to upload monitoring data, use multimedia models in IGEMS, and display results geospatially with Environmental Justice (EJ) data
• Internet-based system of EPA regulatory models and data combined with EJ, graphics, and Geographic Information System (GIS) capabilities
• Estimates general population and environmental exposures via air, surface water, soil, and ground water
• Beta development complete
General Population and Environmental Exposure: ReachScan

- Estimates surface water concentrations and populations served by drinking water utilities downstream from industrial facilities
- Robust model with GIS capabilities; web-based to retrieve data from primary sources
- Rebuilding old model based on ICWater model
- Partnership with Department of Defense, U.S. Geological Service and EPA’s Office of Water
General Population and Environmental Exposure: VVWM

- Desire for a higher tier model to calculate benthic concentrations in existing and new chemicals
- EXAMS (Exposure Analysis Modeling System)
  - Calculates concentrations of chemical of concern in the benthic and aquatic zone and evaporative losses (suspended particles, water phase, sediment and pore water)
  - Three components needed: Chemical Information, Release scenario, Environmental data
  - EXAMS model results have been compared to environmental data for ponds and rivers in the scientific literature
- VVWM (Variable Volume Water Body Model)
  - Models mostly the same fate processes as EXAMS
  - Reduced complexity of the model, use of a GUI
Consumer Exposures

- E-FAST - screening
- AMEM – migration of chemicals through polymers
- MCCEM (activity patterns, multichamber exposure)
  - WPEM wall paints
  - FIAM formadehyde
• AMEM is being redeveloped; estimates chemical migration through certain polymers
• E-FAST predicts human exposure from using consumer products
  – Ongoing redevelopment of consumer model
  – Inhalation and Dermal (Skin) Exposure Predictions
    • LADD, ADD and ADR dose concentrations
    • Pre-set scenarios defined by EPA
    • Option of user defined scenarios
Consumer Exposure Pathway:
MCCEM, WPEM, FIAM

- MCCEM – multi-chamber model, activity patterns,
  - WPEM; Wall Paint formulation
  - FIAM; formaldehyde in pressed wood products; IGEMS platform
Consumer Product Scenarios

- Developed by EPA in 1986; multiyear effort; reflective of consumer lifestyles at that time
- Published in two volumes
- Information culled from literature reviews, reference texts, trade association guides, consumer surveys, coupled with professional judgment as appropriate

- 8 Categories of products, 44 total scenarios
- Data for each scenario:
  - Formulation data
  - Weight fractions of functional components
  - Air exchange rates
  - Mixing factors
  - Room volumes
  - Inhalation rates
  - Exposed skin surface area
  - Annual frequency and duration
Consumer Products Database

• Based on formulation-related data for consumer and commercial products available
  – U.S. Inventory Update Rule (IUR) and Chemical Data Reporting (CDR), U.S. New Chemicals program, U.S. Design for the Environment (DfE), U.S. Source Ranking Database

• Confidential Business Information

• Currently Includes U.S. EPA data for about 5000 chemicals

• Undergoing internal review; intend to release public version in future
EPA-Expo-Box (A Toolbox for Exposure Assessors)

EPA’s EXPOSure toolBOX (EPA-Expo-Box) is a toolbox created to assist individuals from within government, industry, academia, and the general public with assessing exposure. It is a compendium of exposure assessment tools that links to guidance documents, databases, models, reference materials, and other related resources. Exposure assessment resources are organized into 6 Tool Sets, each containing a series of modules that you can access from the table below. In addition, links to resources on other over-arching topics can be accessed from the Quick Finder menu at the top of the homepage. Searching the toolbox (click the link to the right) allows you to quickly identify relevant resources by key words or topics.

EPA-Expo-Box also contains an Exposure Factors module which has been designed to improve the accessibility and usability of data from

Top Three Questions
1. How do I use EPA-Expo-Box?
2. When was EPA-Expo-Box developed and how often is it updated?
3. How can I find out about updates to EPA-Expo-Box?

More Frequent Questions

Popular Downloads
- EPA-Expo-Box Fact Sheet (PDF) (1 pg., 176KB, About PDF)
- Highlights of the Exposure Factors Handbook 2011 (PDF) (72 pp., 3.5MB, About PDF)

In the news
- EPA’s Blog: EPA-Expo-Box
Some Future Plans

- New & Existing Chemical Safety Programs
  - E-FAST
    - Update air model to AERScreen
    - Update water databases
    - Add land application
    - Update down the drain and consumer modules
    - Compile data on test methods for measuring emission rates from products/articles (OECD TFEA activity)
  - IGEMS/CSM
    - Ongoing development
  - ReachScan
    - Complete development and release public version
  - VVWM
    - Complete development, release public version

- New & Existing Chemical Safety Programs, cont’d
  - EPI Suite™
    - Ongoing development of web-based version
    - Update methods periodically
  - AMEM
    - Complete development and release public version
  - Consumer Scenarios
    - Continue to develop/update, release public versions (could be an OECD TFEA activity)
  - Consumer Product Database
    - Complete development, release public version
  - Internationally Harmonized Functional Use Codes
    - Proposed new OECD TFEA activity