

# **Compilation of Materials for Training on Risk Assessment of Chemicals**

Document for use in the SAICM QSP project

“Training on risk assessment of chemicals  
at national level in a global context”

prepared by Divna Nikolic, Martin Scheringer

International Panel on Chemical Pollution, IPCP

June 2010

The authors thank Matt MacLeod for helpful comments.

Disclaimer: This is a draft document. The final version will be distributed at the workshop in Zurich, July 7-8, 2010. The authors and the IPCP do not take any guarantees about the accuracy and completeness of the information. No legal liability or responsibility can be taken. The information is provided for informational purposes only. No part of this document may be used for any commercial purpose.

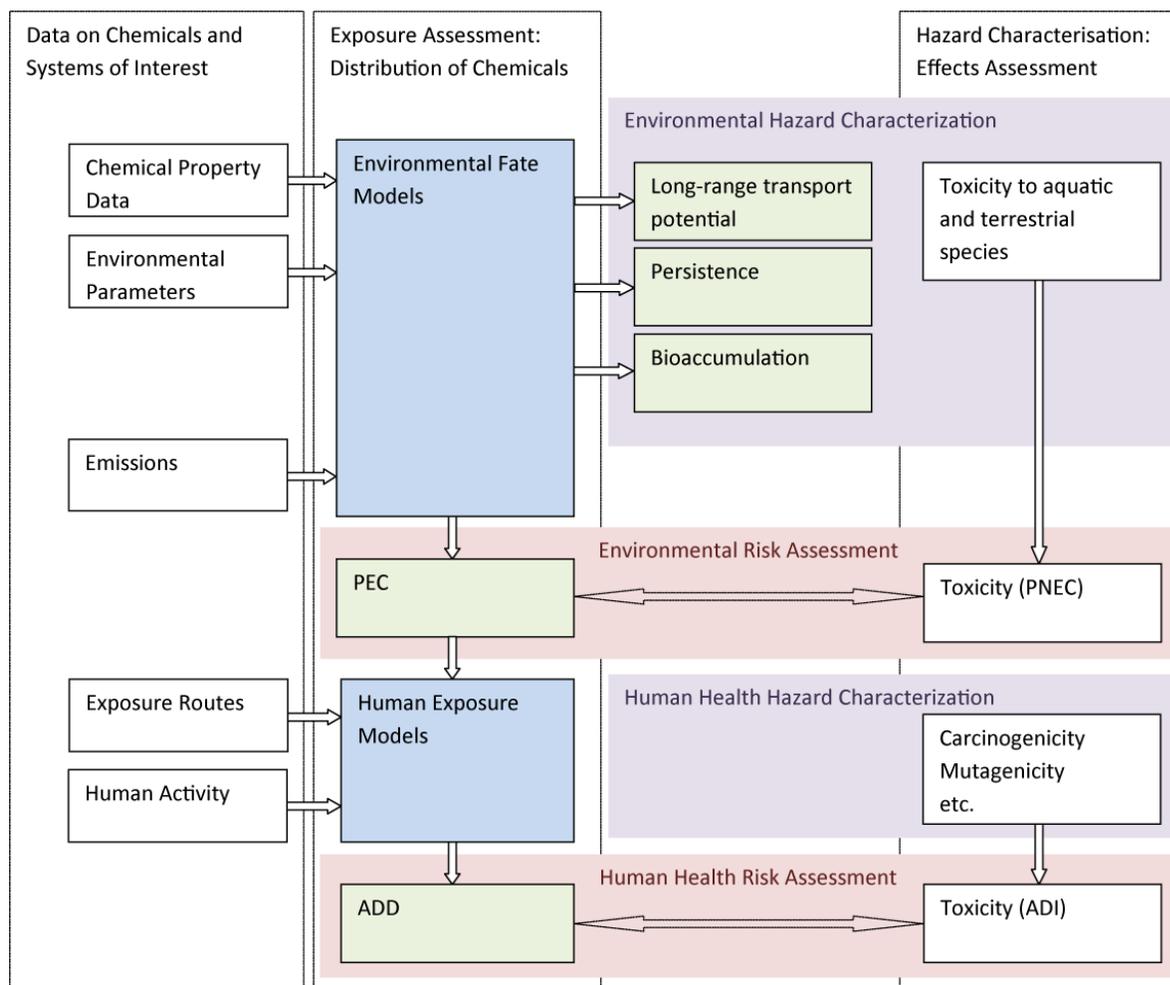
## Contents

Compilation of Materials for Training on Risk Assessment of Chemicals.....	1
Scope and Purpose of the Training Materials .....	4
Outline of the Document.....	6
Databases on Chemical Substances and Risk Assessment .....	7
Chemfinder .....	7
ChemSpider.....	7
eChemPortal.....	7
Data on hazards in general .....	8
Hazard and risk assessment reports .....	8
Test results .....	9
Classification of substances .....	10
IPCS INCHEM .....	11
Comprehensive reports .....	11
Concise documents .....	12
Information on safe handling of chemicals for readers without a technical background.....	13
European Chemical Substances Information System (ESIS).....	13
Information on chemical properties/behavior .....	13
Risk Assessment Reports .....	14
Estimation Models for Chemical Properties .....	14
Estimation Program Interface Suite (EPISuite) .....	14
US EPA PBT Profiler .....	16
Emission Estimation Tools .....	16
OECD Emission Scenario Documents.....	16
The Dioxin/Furan Toolkit.....	16

Environmental Fate Models .....	17
OECD Persistence and Long-Range Transport Screening Tool .....	17
The Canadian Centre for Environmental Modeling and Chemistry (CEMC) .....	17
The Small World Model .....	18
EUSES (European Union System for Evaluation of Substances).....	19
Manuals Related to Risk Assessment and Chemical Safety .....	20
WHO Human Health Risk Assessment Toolkit.....	20
OECD Environmental Risk Assessment Toolkit .....	20
Assessing Soil Contamination. A Reference Manual .....	20
International Chemical Control Toolkit .....	20
KEMI PRIO Tool.....	21

## Scope and Purpose of the Training Materials

The training materials in this compilation cover several different aspects of hazard and risk assessment of chemicals. To specify the purpose of individual methods and tools, it is helpful to distinguish the components of chemicals assessment shown in Figure 1.



**Figure 1: Components of chemical assessment. PEC: predicted environmental concentration; PNEC: predicted no-effect concentration; ADD: average daily dose; ADI: acceptable daily intake. Blue boxes: fate and exposure models; green boxes: results from fate and exposure models; red boxes: components of risk assessment; purple boxes: components of hazard assessment.**

*Hazard assessment* aims to identify properties of chemicals that are particularly problematic, such as carcinogenicity or flammability or persistence. Hazard properties of a chemical are independent of the way in which the chemical is used and the amounts used; they can be called “intrinsic” properties of a chemical. Hazard assessment can focus on environmental hazard or human health hazard. Environmental hazard is generally characterized in terms of persistence, long-range transport potential, bioaccumulation and toxicity to wildlife (top purple box in Figure 1). Hazard to human health is mainly characterized in

terms of carcinogenicity, mutagenicity, reproduction toxicity, skin sensitization, etc. (bottom purple box in Figure 1).

*Risk assessment* aims to determine whether actual effects of a chemical either in wildlife or in humans may occur. It consists of a comparison of measured or estimated levels (concentrations; doses) to which an organism is exposed with levels below which toxic effects can be excluded. To determine the exposure component of a risk assessment, information about usage and emissions of a chemical (white box on the left of Figure 1) needs to be combined with information about the chemical's distribution and transformation and degradation in the environment (so-called environmental fate, blue boxes in Figure 1). To determine the no-effect level, information from the hazard assessment (dose-response relationships, effect levels) is used and extrapolated to levels that may be assumed to be safe (predicted no-effect concentrations, PNEC; acceptable daily intakes, ADIs; white boxes on the right of Figure 1). In a simplifying way, it may be said that risk assessment combines information about hazard of a chemical with information about usage and emissions.

The goals and scope of a chemical assessment project can be different and the tools and methods needed depend on the goal and scope. In general, a risk assessment, combining information on exposure and effect, is more comprehensive than a hazard assessment, but already a hazard assessment can be adequate and helpful if, for example, many different chemicals need to be compared and priorities for further assessment or action need to be defined. Risk assessment is more appropriate and often more feasible when priority chemicals have already been identified.

In both cases, hazard and risk, the focus can be on human health or on the environment or both. If the focus is on the environment, long-range transport potential, persistence, bioaccumulation and effects in wildlife (often: aquatic species) are relevant endpoints; risk is expressed as the ratio of PEC to PNEC, which needs to be determined for different media such as freshwater, soil and sediment. If the focus is on human health, exposure via food, air and drinking water is relevant; this exposure is derived from environmental fate models and models for the transfer of chemical from environmental media to various foods (e.g. fish, meat, dairy products) and also mother's milk. Risk is then characterized in terms of doses taken up by humans compared to ADIs.

The materials in our selection do not form a toolkit that would or should be applied according to a prescribed procedure. Rather, the different methods and tools included in the compilation can be used separately or in a certain combination according to the priorities of the training process. To define priorities of the training process for each country participating in the upcoming IPCP workshop in Zurich, we will form three break-out groups. According to the needs and priorities of each country, the IPCP will aim to provide, during the training process itself, more specific guidance on the methods and tools that will be used in each country.

## Outline of the Document

This document provides links to data sources, tools and manuals for training on risk assessment of chemicals. In the first section of this document, links to **databases** containing a variety of data related to chemical assessment are provided: physical chemical property data, full risk assessment reports for existing chemicals that were performed within a national or international context (reporting also data based on which the assessment was performed), test results for different toxicological endpoints, and information about the legal context and regulations. The databases can be used in order to identify and prioritize routes of exposure and adverse effects of a considered chemical and to gather data for further investigations (e.g. modeling).

For some chemicals, quantitative data derived from measurements are available that can be used to run environmental fate or exposure models. However, often the needed input (especially the environmental half-lives but also partition coefficients etc.) is not available, and estimated values have to be used for assessing the hazards/risks. The **property estimation tools** EPISuite and PBT profiler are widely used in order to estimate partition coefficients and half-lives in the different environmental compartments. Besides estimating the properties, those tools might also be used to calculate the environmental distribution with simple environmental fate models that are integrated in the estimation tools. For more information on the underlying assumptions and limitations, see the documentation for each tool.

In the third section, a selection of **environmental fate models** that are suitable for training purposes is given. As the modeling approach (i.e. representation of the environment and organisms as “boxes” and modeling distribution and transport based on physical chemical properties and environmental parameters) are a common feature in many environmental and human health exposure models, at the Zurich workshop emphasis will be put on the application of those models. As an outlook, also the environmental fate and human health exposure model “EUSES” is presented here, however the application of this model goes beyond the scope of the Zurich workshop due to its complexity.

Amounts of chemicals that enter the environment and the pathway of entry (e.g. to air, water, soil) play an important role for exposure assessment. However, often the amount of a substance is not known, and sometimes neither is the pathway of entry into the environment. **Emission estimates** are very often subject to considerable uncertainties and depend on the temporal and spatial scale, the substance and type of source (e.g. point sources or diffuse sources) involved and, therefore, also other approaches than presented in this document might be suitable.

In the last section, **toolkits** or **manuals** are presented that outline the process of risk and hazard assessment and guide the user through the different steps. Notable here are the OECD Environmental Risk Assessment Toolkit and WHO Human Health Risk Assessment Toolkit, which provide an outline of the process and give information about tools and data sources that can be used. Each of these toolkits covers several individual methods and also provides detailed guidance on application and combination of individual methods.

Note that this selection of training materials is not intended to be exhaustive. Wherever possible, specific comments on the scope, purpose and applicability of data bases, methods and tools are provided.

## Databases on Chemical Substances and Risk Assessment

Chemfinder and ChemSpider provide general information on chemicals, whereas the other portals (OECD eChem, INCHEM, ESIS) contain also information on hazard and risk assessment, and related data (e.g. studies on toxicity, loads of chemicals found in the environment, full risk assessment reports). INCHEM and ESIS are listed separately in this document in order to present an overview of their contents; however they can also be accessed through the OECD eChemPortal, which is the simplest way to look for available information on a known chemical of interest. Note that also within the same database the actual information that is reported varies from substance to substance; data gaps are not unusual. Therefore the content of the databases which is indicated below represents an ideal case. Note that this is not an exhaustive list of databases.

### Chemfinder

<http://www.chemfinder.com>

A chemical search engine

NEEDED INPUT:

- Name or CAS Registry Number or Molecular Formula or Molecular Weight

OUTPUT:

- Chemical identifiers: name, molecular formula and weight, chemical structure, CAS Registry Number, SMILES etc.
- Links to other data compilations.

### ChemSpider

<http://www.chemspider.com/Search.aspx>

A chemical search engine

NEEDED INPUT:

- Name or Trade Name or CAS Registry Number or SMILES.
- Search for substances can be performed also indicating ranges of properties.

OUTPUT:

- Chemical identifiers: name, molecular formula and weight, CAS Registry Number, SMILES etc.
- Estimated Properties by EPISuite (<http://www.epa.gov/oppt/exposure/pubs/episuite.htm>)
- Links to other data compilations.

### eChemPortal

<http://webnet3.oecd.org/eChemPortal/>

eChemPortal gives access to data submitted to government chemical review programs at national, regional, and international levels. It contains information on physical chemical properties, environmental fate and behavior and (eco-)toxicity.

ESIS and INCHEM databases (which are outlined separately in this document, see below) are also accessible through the eChemPortal.

Search for chemicals entering the name or CAS-number.

The different documents and databases that can be accessed through eChemPortal are listed and explained in detail on the webpage (<http://webnet3.oecd.org/eChemPortal/ParticipatingDb.aspx>, with comments on contents, search capabilities etc.), and briefly mentioned below.

## Data on hazards in general

### *HSDB (Hazardous Substances Data Bank)*

- Comprehensive and peer-reviewed data for about 5000 chemicals on different toxicological topics (see the table of contents), e.g.
  - Human health effects
  - Emergency medical treatment
  - Animal toxicity studies
  - Metabolism/Pharmacokinetics
  - Physical chemical properties
  - Chemical safety and handling
  - Manufacturing and use

### *US EPA IRIS (Integrated Risk Information System)*

- Compilation of reports on substances found in the environment characterizing their potential to cause human health effects
  - Hazard assessment of all cancer and non-cancer endpoints
  - Some knowledge in health sciences needed
  - A standalone version of the database is also available for download (for work without internet connection) <http://www.epa.gov/ncea/iris/standal.html>

## Hazard and risk assessment reports

### *OECD SIDS (Screening Information Dataset) for High Production Volume Chemicals, maintained by UNEP*

<http://www.chem.unep.ch/irptc/sids/OECDIDS/sidspub.html>

- Initial assessment reports for over 1000 chemicals produced in large amounts (>1000 tons per year in a single OECD market) that were prioritized.
- The assessment reports contain:
  - Assessment Summary
  - Chemical identity and physical chemical properties
  - General information on exposure (human, environment, occupational etc.).
  - Environmental and human health hazards (summaries of studies and tests).
- Note that the first part of the document is the initial assessment report; followed by more comprehensive reports (e.g. IUCLID dataset, SIDS dossier), where the data based on which the assessment is done is presented.

### ***OECD Existing Chemicals Database***

<http://webnet.oecd.org/hpv/ui/Default.aspx>

- Lists of all HPV Chemicals, giving information about the status of the assessment process for the chemicals and links to data entries within OECD eChemPortal (e.g. SIDS), but no data.

### ***HPVIS (High Production Volume Information System by USEPA)***

<http://www.epa.gov/hpvis/>

- Screening level hazard characterization for over 1000 HPV chemicals on the US market, with data on:
  - Physical/chemical properties (e.g., melting point, vapor pressure)
  - Environmental fate and pathways (e.g., biodegradation, stability in soil)
  - Ecotoxicity (e.g., fish toxicity, toxicity to aquatic plants)
  - Mammalian health effects (e.g., reproductive toxicity, developmental toxicity)

### ***CESAR (Canada's Existing Substances Assessment Repository)***

<http://www.chemicalsubstanceschimiques.gc.ca/about-apropos/assess-eval/caes-ecse/index-eng.php>

- Risk assessment reports of chemical substances, considering risk to environment and human health in a Canadian context
- Reports may include (depending on the considered chemical)
  - Physical chemical properties
  - Use patterns and sources, environmental fate
  - Environmental hazards
  - Human health exposure characterization
  - Potential adverse effects on humans/environment
  - Risk characterization

### ***NICNAS (Australian National Chemicals Notification and Assessment Scheme) Priority Existing Chemical Assessment Reports***

<http://www.nicnas.gov.au/Publications/CAR/PEC.asp>

- Assessments reports for priority chemicals (PDF files), some are full risk assessment reports, other focus on a specific aspect, region of conditions for risk characterization.
  - Physical chemical properties
  - Uses, exposure, kinetics, metabolism
  - Effects on experimental animals
  - Human health effects
  - Environmental release/fate/effects
  - Risk characterization

### **Test results**

#### ***CHRIP (Chemical Risk Information Platform)***

[http://www.safe.nite.go.jp/english/kizon/KIZON\\_start\\_hazkizon.html](http://www.safe.nite.go.jp/english/kizon/KIZON_start_hazkizon.html)

- Results of biodegradation and bioconcentration tests
- See also “Total search system for chemical substances” on the bottom of the document, which provides links to other data sources on the considered chemical.

### ***EnviChem (Data bank on Environmental Properties of Chemicals)***

<http://www.ymparisto.fi/default.asp?contentid=141944&lan=en>

- Database containing test results on ca. 3000 chemicals, related to environmental hazard/risk assessment:
  - Physical chemical properties
  - Degradation, metabolism, bioaccumulation
  - Effects on aquatic and terrestrial ecosystems
- Interpretation of the data needs a background in environmental hazard assessment/chemistry

### ***JECDB (Japan Existing Chemical Data Base)***

[http://dra4.nihs.go.jp/mhlw\\_data/jsp/SearchPageENG.jsp](http://dra4.nihs.go.jp/mhlw_data/jsp/SearchPageENG.jsp)

- Reports on the results of toxicity tests, performed under the Japanese existing chemicals safety programme
- Abstracts summarizing the test results are available in english
  - Single-dose toxicity
  - 28-day repeated-dose toxicity
  - Reproductive/developmental/mutagenicity tests
- Interpretation of the data needs a background in environmental hazard assessment/chemistry

## **Classification of substances**

Classification of chemical substances according to hazardous properties have been done by several countries based on the “Globally Harmonized System of Classification and Labeling of Chemicals” (GHS). See [http://www.unece.org/trans/danger/publi/ghs/ghs\\_welcome\\_e.html](http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html) for an introduction to the GHS and [http://www.unece.org/trans/danger/publi/ghs/ghs\\_rev03/03files\\_e.html](http://www.unece.org/trans/danger/publi/ghs/ghs_rev03/03files_e.html) for the report on classification categories.

### ***GHS-J (Result of the Globally Harmonized System Classification by the Japanese Government)***

[http://www.safe.nite.go.jp/english/ghs\\_index.html](http://www.safe.nite.go.jp/english/ghs_index.html)

- Classification of ca. 1500 chemicals, according to the GHS
- Data is provided as EXCEL-files (volume: ca. 15'000 KB). Query for substances can be done through the eChemPortal, however in order to retrieve the data the EXCEL file has to be downloaded. Data is reported for:
  - Chemical/physical hazards
  - Environmental hazards (often lack of information)
  - Health hazards
- See the manual ([http://www.safe.nite.go.jp/english/pdf/ghs\\_manual\\_e.pdf](http://www.safe.nite.go.jp/english/pdf/ghs_manual_e.pdf)) for detailed information on the classification categories and procedure

## ***HSNO CCID (New Zealand Hazardous Substances and new Organisms Chemical Classification Information Database)***

<http://www.ermanz.govt.nz/hs/compliance/chemicals.html>

- Database of chemicals classified by their hazardous properties based on HSNO Classification Criteria and according to GHS
- The hazard classifications of the chemicals indicating numbers (see <http://www.ermanz.govt.nz/resources/publications/pdfs/GHS%20and%20NZ%20HSNO%20HAZARD%20CLASSES%20AND%20CATEGORIES.pdf> for the criteria relating to the numbers). For some chemicals data on which the classification is based is also reported.

## **IPCS INCHEM**

<http://www.inchem.org/>

This portal provides peer-reviewed information on chemical risks and sound management of chemicals. Fulltext search and search for chemicals by name or CAS Number is available, browsing the documents is also possible.

In some cases a query through the Google search engine returns more specific results than the fulltext search (search for results within a webpage of interest using the “advanced search” option).

Note that at the bottom of the documents that are displayed as web pages you can find links to other documents on the considered chemical within INCHEM.

The different documents/databases and its contents are listed and explained here (<http://www.inchem.org/pages/about.html>), a selection is briefly mentioned below.

## **Comprehensive reports**

### ***EHC (Environmental Health Criteria) Monographs***

- Documents published for 250 substances/substance classes on:
  - Physical/chemical properties, analytical methods
  - Sources of human/environmental exposure and environmental fate
  - Kinetics and metabolism
  - Effects on organisms in the environment, test animals and man
  - Evaluation of human health risks and effects on the environment
- Documents outlining concepts, principles related to risk assessment (e.g. EHC 214: Human Health Exposure Assessment)

### ***JMPR (Joint Meeting on Pesticide Residues) - Monographs and Evaluations***

- Toxicological information and evaluation of pesticides, produced by "WHO/FAO Joint Meeting on Pesticide Residues (JMPR)", based on scientific data:
  - Biochemical aspects (e.g. uptake, distribution, transformation, and elimination in test organisms)
  - Toxicological studies (e.g. acute/long-term toxicity, genotoxicity etc.)
  - Toxicological evaluation (ADI (Acceptable Daily intake), ARfD (Acute Reference Dose) derived where possible)

- Note that some pesticides were evaluated several times; the most recent monographs are at the end of the list. See also the "Inventory of IPCS and other WHO pesticide evaluations and summary of toxicological evaluation performed by the Joint Meeting on Pesticide Residues" (<http://www.inchem.org/documents/jmpr/jmpeval/jmpr2006.pdf>) for an overview of the existing reports and evaluations.

### ***JECFA (Joint Expert Committee on Food Additives) - Monographs and Evaluations***

- Toxicological information on/evaluation of food additives, contaminants, and of residues of veterinary drugs in food, produced by the "Joint WHO/FAO Expert Committee on Food Additives JECFA".
- The documents provide information (where available) on:
  - biological aspects (e.g. occurrence, distribution, transformation, elimination in test organisms)
  - toxicological studies (e.g. acute/long-term toxicity)
  - toxicological evaluation (ADI values)
- Note that first all monographs (which contain the actual information) are listed, then the very short evaluation summaries.

### **Concise documents**

#### ***CICADs (Concise International Chemical Assessment Documents)***

- Brief summaries of scientific information on potential effects of chemicals upon human health and environment, published for ca. 75 substances/substance classes
- Based on selected national/international evaluation documents or EHCs.

#### ***IARC (International Agency for Research on Cancer) Monographs - Summaries and Evaluations***

- (Qualitative) summaries of evaluation of the available evidence on carcinogenicity for agents (e.g. chemical substances) to which humans are known to be exposed. The documents may be helpful when assessing if a substance is known to pose a risk of cancer.
- The documents are based on the "IARC Monographs on the Evaluation of Carcinogenic Risks to Humans" and give very short information about the conclusions drawn from evaluating scientific data on carcinogenicity to humans and experimental animals. The (original) Monographs (reviewing scientific data) are published for single chemicals and mixtures, reviewing scientific studies on carcinogenicity. Some of them can be downloaded as PDF files (<http://monographs.iarc.fr/ENG/Monographs/PDFs/index.php>).
- Lists of agents (e.g. chemical substances) that are classified by the IARC Monographs: <http://monographs.iarc.fr/ENG/Classification/index.php>

#### ***PDs (Pesticide Documents)***

- The WHO Recommended Classification of Pesticides by Hazard and Guidelines to Classification:
  - A document describing the classification scheme tables of active ingredients of pesticides that have been classified according to the outlined scheme. The hazard classification is mainly based on the LD<sub>50</sub> for rat.
- Pesticide Datasheets:
  - Basic and concise information (e.g. physical/chemical properties, use, toxicity, regulations, disposal) on some widely used and/or toxicologically relevant pesticides

## Information on safe handling of chemicals for readers without a technical background

### *HSGs (Health and Safety Guides)*

- Summaries in non-technical language for decision-makers (e.g. occupational health services, ministries, governmental agencies etc.) aimed to assist the application of international guidelines concerning chemical safety on a national level
- Available for over 100 chemicals, summarizing information with the focus on human health hazards
  - Chemical identity, analytics, exposure and effects (based on corresponding EHCs)
  - Human health/environmental hazards, prevention/protection and emergency action (e.g. spillage)
  - Chemical safety information related to handling of chemicals based on IPCS International Chemical Safety Cards.
  - Regulations, guidelines, standards (on e.g. exposure limits, packaging, waste disposal) based on IRPTC (International Register of potentially Toxic Chemicals) and other UN sources

### *ICSC (International Chemical Safety Cards)*

- Summarize health and safety information on chemical substances in a clear way intended to be understandable for workers dealing with chemical substances.
  - Symptoms after acute exposure
  - Prevention
  - First aid measures

## European Chemical Substances Information System (ESIS)

<http://ecb.jrc.ec.europa.eu/esis/>

ESIS is a portal that provides lists of chemical data related to EU legislation. A selection of lists and compilations of data are provided below. Notable are especially the IUCLID Datasets that contain physical chemical properties (for use in fate and exposure models).

Search by CAS number or chemical name or browse the lists. If looking for information on a particular chemical, look first for the “ESIS-Datasheet” (<http://ecb.jrc.ec.europa.eu/esis/>) that summarizes the information available at ESIS on a particular chemical. Note that if you click on the EC-Number of a chemical in any of the lists on ESIS, this datasheet will appear.

## Information on chemical properties/behavior

### *IUCLID (International Uniform Chemical Identification Database) Chemical Data Sheets.*

- Extract of data from the IUCLID on High Production Volume Chemicals. The data sheets contain:
  - Physical chemical properties
  - Environmental Fate and Pathways
  - Ecotoxicity
  - Toxicity

- The data sets are still being developed; therefore many fields for several chemicals are empty!
- Data sets can be downloaded as PDF files as well as IUCLID 5 export files (for use within the IUCLID5 software).

In order facilitate administration data within the scope of EU Legislation (REACH), IUCLID5 (<http://iuclid.echa.europa.eu/>) was developed. This is a software tool for entering, storing and maintaining data on intrinsic and hazard properties of chemical substances. For further information/documentation on the software see <http://iuclid.echa.europa.eu/index.php?fuseaction=home.support>

## **Risk Assessment Reports**

### ***ORATS (Online European Risk Assessment Tracking System)***

- Access to the European Union Risk Assessment Reports for substances belonging to priority lists (because of their potential effects on humans or environment). The assessment reports cover:
  - Physical/chemical properties
  - Production/Use
  - Environmental/human hazard and risk assessment including studies and data used to perform the evaluation

### ***Lists of chemicals without further information on physical/chemical properties and behavior***

#### ***BPD (Biocidal Products Directive)***

- List of substances that are allowed for use in biocidal products within EU. Assessment Reports (containing e.g. physical chemical properties, risk assessment summary etc.) and legal context can be retrieved.
- List of substances to be phased out. No further information on chemical properties available.

#### ***PBT (Persistent, Bioaccumulative, Toxic)***

- List of existing substances that have been evaluated regarding their PBT properties. Summary reports of the PBT evaluation (that cover some information on the chemicals needed for evaluation) and the concluding statement (i.e. fulfilling the PBT-criteria or not) are available.

#### ***C&L (Classification and Labeling)***

- Recommended Risk Phrases for chemicals packaging.

## **Estimation Models for Chemical Properties**

Where *no* physical chemical property data or information on toxicity is available from measurements, the tools below can be used in order to make an estimation of those properties. Note that the estimates obtained are subject to considerable uncertainty and give reasonable results only for certain chemical substances (see the tools' documentation for further information).

### **Estimation Program Interface Suite (EPISuite)**

<http://www.epa.gov/oppt/exposure/pubs/episuite.htm>

A tool for screening-level estimates of physical/chemical and environmental fate properties. This tool should only be used if no acceptable measured values are available. Note that the estimated values are subject to considerable uncertainties. EPISuite consists of several different models for estimating various properties. Simple environmental fate models are also included.

#### NEEDED INPUT:

- Chemical structure in SMILES notation (or CAS Number)

SMILES can be obtained from Chemfinder, ChemSpider or directly within the EPISuite program (with the SMILECAS database, containing 112'000 entries) indicating the CAS number.

#### OUTPUT:

Estimates of different properties and, where available, also experimental values are given. The environmental fate models can be run within EPISuite with estimated values or by adjusting them to more accurate values if available.

#### Partitioning

- KOWWIN: octanol-water partition coefficient
- HENRYWIN: Henry's Law constant (air-water partition coefficient)
- KOCWIN: organic carbon-normalized sorption coefficient for soil and sediment
- KOAWIN: octanol-air partition coefficient
- AEROWIN: fraction of airborne substance sorbed to airborne particulates

#### Reactivity

- AOPWIN: gas phase reaction rate constant, atmospheric half-lives.
- BIOWIN: Probability of biodegradation (fast/not fast), timeframes of ultimate and primary biodegradation.
- BIOHCWIN: Biodegradation half-lives for hydrocarbons (only H and C atoms).
- HYDROWIN: Aqueous hydrolysis rate constants and half-lives for the following chemical classes: esters, carbamates, epoxides, halomethanes, selected alkyl halides, and phosphorus esters.

#### Other properties

- MPBPWIN: Melting point, boiling point, vapor pressure, subcooled liquid vapor pressure
- WSKOWWIN and WATERNT: water solubility, two different methods.

#### Toxicity related values

- BCFBAF: Bioconcentration factor, biomagnification factor, biotransformation rate constant for fish.
- ECOSAR: Acute (EC50 or LC50) and chronic (ChV) toxicity of aquatic invertebrates and algae
- DERMWIN: dermal permeability coefficient

#### Environmental fate models included in EPISuite

- STP: Sewage treatment plant model. For a short description: <http://www.trentu.ca/academic/aminss/envmodel/models/STP211.html>
- Fugacity: Level III (i.e. steady state) multimedia model (i.e. for the environmental compartments air, water, soil, sediments and aquatic biota). For a short description see: <http://www.trentu.ca/academic/aminss/envmodel/models/L3280.html>
- WVOLNT: Calculates the half-life of volatilization of a chemical from a river and lake

## US EPA PBT Profiler

<http://www.pbtprofiler.net/>

Online risk-screening tool that predicts a chemical's potential to persist in the environment, bio-concentrate in animals, and be toxic (to fish). This tool should only be used if no experimental data on persistence, bioaccumulation and toxicity is available. It is not a regulatory but a research tool that helps to identify chemicals that need further evaluation of their Persistence, Bioaccumulation and Toxicity potential. The outcome is also compared to the US EPA criteria of Persistence, Bioaccumulation and Toxicity. See also which chemicals should *not* be profiled: <http://www.pbtprofiler.net/Chemicals.asp>

NEEDED INPUT:

- CAS number

CAS Number can be obtained through Chemfinder, Chemspider, Wikipedia or by entering “chemical name CAS” in any search engine.

OUTPUT:

For definitions of the output values see: <http://www.pbtprofiler.net/details.asp>

For the methodology and underlying assumptions see: <http://www.pbtprofiler.net/Methodology.asp>

### **Persistence**

- Half-lives in air, water, soil, sediment.
- Percentage of the chemical in the different media

### **Bioaccumulation**

- BCF (Bioconcentration Factor)

### **Toxicity**

- Fish ChV (Chronic Value)

## Emission Estimation Tools

### OECD Emission Scenario Documents

[http://www.oecd.org/document/46/0,3343,en\\_2649\\_34373\\_2412462\\_1\\_1\\_1\\_37465,00.html](http://www.oecd.org/document/46/0,3343,en_2649_34373_2412462_1_1_1_37465,00.html)

Emission Scenario Documents describe sources, production processes and use patterns for several industrial sectors. The documents may help to identify pathways of chemical entry into the environment. However, use patterns and industrial processes might differ from country to country and adjustment of the default values might be necessary. When you are dealing with emissions on a regional scale it might be useful to consider trade, use or application statistics for deriving estimates rather than single processes.

### The Dioxin/Furan Toolkit

<http://chm.pops.int/Programmes/ToolKit/Overview/tabid/372/language/en-US/Default.aspx>

The Toolkit was developed for identification and quantification of dioxin and furan releases under the Stockholm Convention. Ongoing projects to improve the Toolkit in order to cover the situation in

developing countries can be accessed here:

[http://www.chem.unep.ch/pops/pcdd\\_activities/projects/default.htm](http://www.chem.unep.ch/pops/pcdd_activities/projects/default.htm)

## Environmental Fate Models

### OECD Persistence and Long-Range Transport Screening Tool

[http://www.oecd.org/document/17/0,3343,en\\_2649\\_34373\\_40754961\\_1\\_1\\_1\\_1,00.html](http://www.oecd.org/document/17/0,3343,en_2649_34373_40754961_1_1_1_1,00.html)

A screening-level tool for organic chemicals (MS Excel document). A steady-state model consisting of three different environmental compartments (i.e. air, oceanic surface water, soil) is used to calculate overall persistence ( $P_{OV}$ ) and long range transport potential (LRTP) for the comparative assessment of environmental hazard properties. The tool was designed to identify potential POPs (Persistent Organic Pollutants)/PBTs (Persistent, Bioaccumulative, Toxic) according to persistence and long-range transport.

#### NEEDED INPUT

Chemical property data:

- Partition coefficients (air-water and octanol-water)
- Degradation half-lives (in air, water, and soil)

If no measured values of chemical properties can be found from literature, values can be estimated with EPISuite (KOWWIN (octanol-water partition coefficient), HENRYWIN (air-water partition coefficient), AOPWIN (atmospheric half-lives), BIOWIN (biodegradation, for deriving soil and water half-lives)). As the BIOWIN output has first to be converted into quantitative half-lives, it is easier to use the PBT Profiler Output for half-lives in air, water, soil, sediment (which are also based on the AOPWIN and BIOWIN results). See chapter on persistence in <http://www.pbtprofiler.net/Methodology.asp> on how quantitative half-lives that can be used in the model are derived from the EpiSuite BIOWIN 3 Output.

#### OUTPUT

##### **Persistence**

- Overall Persistence ( $P_{OV}$ )

##### **Long Range Transport Potential**

- Characteristic Travel Distance (CTD)
- Transport Efficiency (TE)

See also the manual (<http://www.oecd.org/dataoecd/54/28/40719272.pdf>) for further information.

### The Canadian Centre for Environmental Modeling and Chemistry (CEMC)

<http://www.trentu.ca/academic/aminss/envmodel/models/models.html>

Several environmental fate models that can be downloaded for free but cannot be changed. For an introduction of the modeling approach (e.g. the fugacity approach, Level I-III) and a description of the models see the manual (<http://www.trentu.ca/academic/aminss/envmodel/CEMReport200501.pdf>). As many environmental fate models are based on these principles, this manual can provide valuable

information on environmental fate modeling in general. A case study for practice is included in the appendix.

The needed input values and output parameters are listed on the webpage of each of the models.

## The Small World Model

<http://tinyurl.com/3a6d5or> (MS Excel sheet for calculation)

A global-scale model that calculates the distribution of chemicals in different environmental media (i.e. air, water, soil). The basic principles of the model are the same as for the OECD Persistence and Long-Range Transport Screening Tool and the CEMC environmental fate models, but this particular model allows the user to adjust all the model parameters (e.g. properties of the environmental media, transport coefficients, emission rates to different environmental compartments) and to calculate time-dependent loads of chemicals in the different compartments (i.e. Level IV, dynamic solution of the mass balance equations).

Calculations can be done for different assumptions/cases:

- Level I (i.e. distribution of chemical in the environment assuming equilibrium. The distribution does not depend on transport processes between the environmental compartments, only on partitioning properties of the chemical and the environmental compartments properties)
- Level III (i.e. distribution of chemicals in the environment assuming steady state, constant emission rates)
- Level IV (i.e. time-dependent distribution of chemicals in the environment, time-dependent or constant emission rates)

### NEEDED INPUT

Only chemical property data is mandatory (and emission rates for quantitative assessments), other data is optional (i.e. default values can be used).

#### Level I:

Chemical property data:

- Partition coefficients (air-water and octanol-water)
- Half-lives (in air, water, and soil)

Bulk environmental properties:

- Dimensions (i.e. heights and areas) of the different compartments (air, water, soil)

Environmental sub-compartment properties (or use default values):

- Volume fractions of solids, air, water in the different compartments (air, water, soil)
- Fraction of organic carbon in solids
- Densities of solids, air, water.

#### Level III:

In addition to properties mentioned above:

Mass transfer coefficients:

- Transfer of mass between the different compartments
- Transfer of mass to/out of the whole system
- Constant emission rates to air, water, soil

**Level IV:**

In addition to properties mentioned above:

- Initial load of chemical in air, water, soil
- Time-dependent emission rates to air, water, soil

The default environmental properties of the Small World Model correspond to global averages, but they can also be adjusted to represent a regional environment.

If no measured values of chemical properties can be found from literature, values can be estimated with EpiSuite (KOWWIN (octanol-water partition coefficient), HENRYWIN (air-water partition coefficient), AOPWIN (atmospheric half-lives), BIOWIN (biodegradation, for deriving soil and water half-lives)). As the BIOWIN-Output has first to be converted into quantitative half-lives, it is easier to use the PBT Profiler output for half-lives in air, water, soil, sediment (which are also based on the AOPWIN and BIOWIN results). See chapter on persistence in <http://www.pbtprofiler.net/Methodology.asp> on how quantitative half-lives that can be used in the model are derived from the EpiSuite BIOWIN 3 Output.

**OUTPUT****Level I:**

- Relative distribution of the chemical in air, water soil

**Level III:**

- Amounts, fugacities and relative distribution of the chemical in air, water, soil
- Mass flows into, out of and between the compartments (air, water, soil)

**Level IV:**

- Time-dependent amounts, fugacities and relative distribution of the chemical in air, water, soil

**EUSES (European Union System for Evaluation of Substances)**

<http://ecb.jrc.ec.europa.eu/Euses/>

EUSES is developed for quantitative risk assessment in order to support decision-making by risk managers. With its default parameter values, it can be used for screening-level assessments. On the basis of this screening it can be decided if a refined assessment is necessary where the default values have to be replaced with more accurate data.

The model consists of several modules accounting for the entire life cycle of a chemical, (i.e. emission rates, environmental distribution, exposure levels (human and environment) and compares the outcome to the estimated/extrapolated no-effect values in order to characterize the risk for human health and environment.

**NEEDED INPUT**

- Molecular weight
- Octanol-water partition coefficient
- Water solubility
- Vapor pressure

Depending on the availability of data and assessment type, additional parameters might also be required.

**OUTPUT**

Risk characterization:

- Environment: Ratio of PEC/PNEC (Predicted Environmental Concentration, Predicted No-Effect Concentration)
- Human health: MOS (Margin of Safety)

## Manuals Related to Risk Assessment and Chemical Safety

### WHO Human Health Risk Assessment Toolkit

[http://www.who.int/ipcs/methods/harmonization/areas/ra\\_toolkit/en/index.html](http://www.who.int/ipcs/methods/harmonization/areas/ra_toolkit/en/index.html)

Work in progress, final version of the report will be available at the Zurich workshop in July 2010.

The Toolkit is a manual that explains the human health risk assessment procedure and supports the user to perform an assessment by:

- providing roadmaps for conducting chemical risk assessment,
- identifying information that must be gathered to complete an assessment,
- listing, describing, and providing URLs to international resources of information and methods essential to risk assessment.

Illustrative case studies are also included in the manual.

### OECD Environmental Risk Assessment Toolkit

[http://www.oecd.org/document/54/0,3343,en\\_2649\\_34373\\_44909430\\_1\\_1\\_1\\_1,00.html](http://www.oecd.org/document/54/0,3343,en_2649_34373_44909430_1_1_1_1,00.html)

A web page describing the workflow of environmental risk assessment and related tools, focusing on products developed within the OECD Environment, Health and Safety Programme.

### Assessing Soil Contamination. A Reference Manual

<http://www.fao.org/docrep/003/x2570e/x2570e00.htm> (available also in French, Spanish)

The aim of this tool is to determine if a pesticide spill (e.g. as a consequence of inappropriate storage of obsolete pesticides) may cause groundwater or soil contamination and if there is any risk to human health. This web-based manual guides the user through the relevant questions that have to be answered and how to make concluding statements about the posed risk. Fact sheets containing information on several pesticides are included in the appendix.

### International Chemical Control Toolkit

[http://www.ilo.org/legacy/english/protection/safework/ctrl\\_banding/toolkit/icct/index.htm](http://www.ilo.org/legacy/english/protection/safework/ctrl_banding/toolkit/icct/index.htm)

This tool is designed for small and medium-size companies in developing countries, outlining a scheme of protection against harmful, dangerous chemical substances at the work place (e.g. storage, protective equipment, and disposal).

## KEMI PRIO Tool

[http://www.kemi.se/templates/PRIOEngframes\\_4144.aspx](http://www.kemi.se/templates/PRIOEngframes_4144.aspx)

This tool relates to EU and Swedish legislation; however it also may help in getting information on hazard properties, possible environmental and health criteria, and supporting decision-making with the aim to reduce risks. The tool comprises the following parts:

- **PRIO database:** The PRIO database comprises a selection of labeled or classified substances (related to EU and Swedish legislation). Enter chemical name or CAS-Number, or browse for chemicals by specifying hazardous properties (e.g. environmentally hazardous, carcinogenic) and/or substance groups (e.g. chlorinated solvents, dioxins). The database contains (a selection of) chemicals that are identified as being of concern indicating:
  - Prioritization Level (according to Swedish/EU Legislation)
  - PRIO Criteria (e.g. environmentally hazardous, carcinogenic etc. Hazardous properties of the substance that determine the prioritization level)
  - Reference (legal context, e.g. multilateral agreements )
- Priority setting guide for prioritizing chemical substance risks in articles and products. The prioritization is based on having one substance you want to know more about; the guide is set up as a decision tree. The guide helps to:
  - find out what substances are contained in a chemical product or article.
  - assess the environmental and health properties of substances.
  - prioritize which properties of the substance to which you should pay particular attention.
  - structure the work on replacing hazardous substances.
- Chemicals in practical use: Information on good chemical management strategies for professionals dealing with chemical products. The different sections give information about how to deal with chemical issues and what should be considered in dealing with chemicals in different professional roles.