OR 30/2009

EnviRisk

Review of databases, modelling methods and tools for exposure assessment

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Preface

This report is a deliverable of a project ENVIRISK (Assessing the Risks of Environmental Stressors: Contribution to Development of Integrating Methodology). ENVIRISK is funded under the EU 6th Framework Programme for R & D Priority 8.1 Policy-oriented research, Contract No. SSPE-CT-2005-044232. The aim of ENVIRISK is to develop an integrated methodological framework for identification of health risks caused by exposure to environmental factors, with a view to provide useful information for prevention and targeted policy measures. The framework include the development and piloting of protocols and methodologies for exposure assessment and health impact assessment in specified areas relevant to the implementation of the European Environment & Health Action Plan (EHAP).

The ENVIRISK contains seven partners:

- Norwegian Institute for Air Research (NILU), Dr. Alena Bartonova, Project Coordinator
- National Institute for Health and Welfare (THL), Prof. Matti Jantunen, Principal Investigator
- Institute of Experimental Medicine, Academy of Science of the Czech Republic (IEM), Dr. Radim Sram, Principal Investigator
- Slovak Medical University, Research Base (SMU), Prof. Tomas Trnovec, Principal Investigator
- Regional Institute of Public Health, Kolin (ZUKOLIN), Dr. Eva Rychlikova, Principal Investigator
- Technion Israel Institute of Technology, Dr. David Broday, Principal Investigator
- University of Hertfordshire, Prof. Ranjeet Sokhi, Principal Investigator

ENVIRISK has three scientific work packages:

- WP 1-Data and techniques for realistic exposure assessment
- WP 2-Relations between exposure and health
- WP 3-Dissemination and contribution to EHIS

ENVIRISK project has two objectives for health risk assessment: one of them is to develop a general exposure and risk assessment framework and the other to apply the framework to three case studies with measured health effects. These case studies are focused on effects of exposure to PAHs and particulate matter (PM) in the Czech Republic and on effects of exposure to PCBs in Slovakia. To fulfill the first objective, the first task in ENVIRSK Work Package 1 was to review all available databases and modelling tools for exposure assessment in the areas relevant for the EC EHAP and ENHIS-2. This report described the results of this review. The data and modelling tools described in this report are not necessarily focused on the case studies alone.

For more information, please visit ENVIRISK website at http://envirisk.nilu.no or contact the coordinator Dr. Alena Bartonova, E-mail: aba@nilu.no.

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1 Introduction

Usually development of risk and/or health effect assessment starts from framing of the issue followed defining the exposure scenarios for these issues. Relevant sources, exposure media and pathways, exposed population and how they come into contact with the agent are considered when defining exposure scenarios. These facts with the used modelling methods define the input data needed for exposure calculations. Information on source emissions, environment and microenvironment characteristics, exposure media concentrations, contact activities, and population characteristics and behaviour, are needed. Facts describing the population and exposure microenvironments can be classified as general exposure factors, and this information includes time activity, ingestion, housing, land use, physiological and population size related data.

EnviRisk project has two objectives for health risk assessment: one of them is to develop a general exposure and risk assessment framework and the other to apply the framework to three case studies with measured health effects. These case studies are focused on effects of exposure to PAHs and particulate matter (PM) in the Czech Republic and on effects of exposure to PCBs in Slovakia. To fulfil the first objective, the first task in EnviRisk Work Package 1 (Data and techniques for realistic exposure assessment) was to review all available databases and modelling tools for exposure assessment in the areas relevant for the EC EHAP and ENHIS-2. Results of this review are described in this document. The data and modelling tools described in this document are not necessarily focused on the case studies alone.

2 Review of databases for exposure assessment

The exposure scenarios defining the data and modelling needs for the specific study cases in EnviRisk were developed parallel to this review. Those scenarios are described in a separate document, which will be included to the Deliverable 1.3 describing the application of the EnviRisk framework to the study cases. Those scenarios were kept in mind when reviewing the databases, so that their usability for the purposes of EnviRisk could be evaluated. For practical reasons all databases that have been reviewed are not described in more detailed here. Instead they are linked to an internet page named Platform for Exposure Assessment (http://www.ktl.fi/expoplatform/external_ui/index.php). The Platform was developed to support the framework for integrating modelling tools for human time-activity, environmental release and media dispersion of harmful agents, and the databases are described in more detail there. Features of this platform are presented in more detail in EnviRisk Deliverable 1.2 report, which describes the integrated methodology for advanced exposure assessment and modelling framework to assess the impact of alternative policy implementations on exposure and environmental health indicators and benefits.

2.1 Data for general exposure factors

Main sources of information for general exposure factors are ExpoFacts database (http://cem.jrc.it/expofacts/), which provides data for 30 European countries, and U.S. EPA's Exposure factors handbook (http://www.epa.gov/ncea/pdfs/efh/front.pdf) providing data at US level. Both these sources include data for several exposure factor categories, which are explained in more detailed in the following chapters. Third source of information is EPA's

Important exposure factors for children (http://www.epa.gov/nerl/research/data/exposure-factors.pdf), which is concentrating on the exposure for pesticides, and provides information on children's hand-to-mouth and object-to-mouth activity at US level.

2.1.1 Time activity data

Time-activity data is needed when defining the duration and frequency of exposure events. This can be the time spent in certain microenvironments (home, in traffic, work place) or it can be the duration and occurrence of certain activities (like taking shower/bath, using hygiene products, cooking) and this kind of data is usually obtained with time-activity diaries filled by persons participating in time-activity or exposure studies.

Time-activity data is quite broadly available, particularly on a country-specific level, because national level statistical centres often collect this kind of information. Furthermore, several exposure measurement studies have included time-activity questionnaires in their studies and provide this information in the form of databases and published articles.

Based on this review there is time-activity information available on a national level for several European countries, as well as in several US databases (Annex 1). Specific data for the Czech Republic is available with sufficient level of detail from ExpoFacts database, but for Slovakia there are no specific data available.

2.1.2 Ingestion data

Ingestion data can include information on ingested quantities of food, water and breast milk. Sometimes also non-dietary ingestion, mainly hand-to-mouth behaviour of children, is included under this group but may also be grouped under time activity data. Naturally ingestion data is relevant in cases where ingestion route is one of the exposure pathways. For most chemical exposures and for most of the populations ingestion is the dominant route of exposure.

Ingestion information is quite broadly collected as part of research studies and also as food related market research done by companies and by governmental institutes on national levels and usually for other purposes than for exposure science.

There are several European level databases available with the information on consumption of food items, but not so much information on water and breast milk consumption (Annex 2). The main information sources for EnviRisk are Eurostat, FAOSTAT and ExpoFacts. For both Czech Republic and Slovakia there is information available on food consumption per capita for several food items through ExpoFacts for years 1996-2001 based on information from FAO's food balance sheets and through FAOSTAT also for years 2002 and 2003. Access to most recent data in FAOSTAT requires payment for registration. In Eurostat there is consumption data for various food items available for both Czech and Slovakia with differing level of information for years 1991 to 2007. This information is provided as annual information. Besides available common databases, there is also some information collected on food ingestion by type of food and frequency by studies done in the Czech Republic and in Slovakia, and this data can be utilized for EnviRisk purposes.

For water and breast milk ingestion there is no data available, although Eurostat provides some information on how much water is consumed in different sectors per capita in both countries. Specific data for non-dietary ingestion for these two countries is not available, but there is data for other European countries, such as the United Kingdom and the Netherlands through ExpoFacts, which can be used with the assumption that there are no big differences in the behaviour of children between countries.

2.1.3 Physiological data

Physiological data includes breathing rate, body height, weight and surface area. This information is usually needed when calculating intakes for inhalation or dermal pathways.

Physiological data on people is usually collected for health purposes by government institutes and it's not so widely available. Furthermore, there are differences between counties, so data gathered in one place, e.g. USA, might not be usable in some other place, e.g. Asia.

Only one source of information with European level data was discovered by this review (Annex 3). ExpoFacts contains body weight and length information for both the Czech Republic and Slovakia on country level, but not anything else. At European level there are some body surface and breathing rates available, which might be used for EnviRisk purposes.

2.1.4 Housing data

When considering exposure in indoor environments, characteristics of housing have to be considered. This category includes a wide variety of information, such as number of dwellings, floor spaces, air exchange rates, square meter per persons or room, building age distributions, ventilation, indoor air quality etc.

For practical reasons like differences in climate, sociological and cultural patterns, this information is related to the regions, which limits its usability for other regions. There are also clear differences between countries in the level of available information. Main source of information is ExpoFacts (Annex 4), which includes quite broadly information for European countries. Unfortunately information for the Czech Republic is limited and even more limited for Slovakia.

2.1.5 Land use data

Land use data provides information about the land areas that are used for different purposes. This information can be used in exposure assessment when approximating the numbers of people exposed in certain areas or utilized for spatial analyses.

On European level land use data is available, although there are differences in the level of data between countries (Annex 5). Intelligent satellite systems have provided simpler ways to map land use at national and continental levels, and the grid size used is usually 1km x 1km.

The main source of land use information for EnviRisk is Corine land cover (CLC90 and 2000), which provides consistent information on land cover and land cover changes during the past decade across Europe. The source imagery derives from the late 1980s and early 1990s. CLC90 was compiled on the basis of Landsat and SPOT satellite imagery, using a combination of semi-automated and manual interpretation techniques. The inventory is based on computer assisted photo interpretation of satellite images divided into 44 categories, and the raw data have a spatial resolution of 25 hectares. The categories include artificial surfaces, agriculture, forest and natural areas, wetlands, water bodies etc.. The CORINE data are provided both as vector data sets, in their original form, and as a generalised raster data set, at a notional 100 meter resolution.

One other database containing information for both the Czech Republic and Slovakia is Eurostat, providing data for years 2000, 1995, 1990, 1985, 1980, 1970, 1950 as annual values.

2.1.6 Population data

Population data is needed for exposure calculations when defining the numbers of exposed people and defining subpopulations based on demographic characteristics. These kinds of data are provided by European level statistics for all EU countries. More detailed information is usually provided by national statistical centres.

Population data include demographic data such as health statistics, gender and age distributions, birth and death rates, education, employment /unemployment etc., which might be useful when performing exposure calculations or risk assessments. These data are important in determining exposure-relevant characteristics of the exposed population and any subpopulations of special concern. The reviewed sources on population data are summarized in Annex 6, and there are three (Eurostat, ExpoFacts and Gridded population of the world database) relevant data sources for EnviRisk. ExpoFacts includes some information for both the Czech Republic and Slovakia and is considered as the primary information source for EnviRisk. Gridded population of the world application provides information on population density for both countries on a grid cell basis with varying resolutions and provides useful information when defining the size of exposed populations in areas. This specified information can be used with GIS applications. Eurostat provides Census 2001 information and population can be divided between gender, education, marital status etc.

The main problem with all these databases is that information is provided only at country level. Gridded population information provides data at local level too, but the need of GIS tools makes this information more complicated to be used.

2.2 Emission data

Several kinds of data on emissions are needed in exposure assessment, although the level of data needed depends on each case. If exposure concentrations are predicted on the basis of the transport and fate of chemicals, emissions are needed for modelling. For calculation of intake fractions, total emissions or emission rates are needed. In addition to information of direct amounts of emissions, also information on emission factors or information on source profiles can be beneficial. Source profiles are used for source attribution to assess sources of the exposure.

Databases on emission related information are reviewed in this chapter and summarized in Annex 7. Data needs related to emission information are not yet defined for EnviRisk, because the modelling framework is still under consideration and data need is tightly connected with these. Nevertheless, data availability for the Czech Republic and Slovakia is separately defined with each issue and specifically data for PAHs, PM and PCBs, which are the main focus of the EnviRisk cases.

2.2.1 Air

Emissions to air are covered by several databases on European level and one reason for this is that there has been a commission decision made in 2000 on national reporting responsibilities of air pollution emissions, if set threshold limits are exceeded. Furthermore emission inventories for pollutants related to climate change, such as CO_2, CH_4, N_2O and HFCs, PFCs and SF_6 and the precursor gases CO, NO_x, NMVOC and SO_2, are targets of global interest. In addition particulate matter has gained a lot of interest because of its health effects, so there is quite a lot of data available for that also.

Main data sources for EnviRisk are European Pollutant Emission Register (EPER), RAINS emissions and EMEP data through WebDab. Data on EPER covers industrial emissions and is based on information provided by each producer, i.e. factory, whereas EMEP includes both reported and estimated values and RAINS contains only modelled values. For Czech Republic some national level data is also available through REZZO database provided by Czech Hydrometeorological Institute (CHMI).

EMEP provides information for both the Czech Republic and Slovakia and for all EnviRisk target compounds. Values are provided as national totals and can be divided between source categories. Years covered with reported data are from 1980 to 2005, although the level of information varies between years and compounds. These data can be used for EnviRisk purposes to evaluate local emissions, but obviously this produces some uncertainties to the calculations. Some of the EMEP data can be retrieved also through CEPMEIP Database.

EPER includes information for both countries, but mainly for year 2004 only. There is no information on PCBs, PAH information for the Czech Republic is available from 4 facilities and PM from 9 facilities. In principle this database provides information for local emissions, but it doesn’t provide much relevant information for our purposes.

RAINS emissions are provided as totals per country or by activity in each country. Data for both the Czech Republic and Slovakia is provided, but only on PM. Results are calculated separately each time, so it might take some time to do that. As they provide information only at national level, usability of these data for local calculations is limited.

REZZO database includes total emissions of PAHs, PCB, PCDD/Fs and heavy metals for several years for Czech Republic. There are also some emissions for total suspended particles for some regions in year 2005.

2.2.2 Water

Data on releases to water is really scarce and there was only one database found providing that kind of information on European level. This database is the same EPER database, which includes also emissions to air. Information on several pollutants for several countries is provided, and mainly for year 2004.

For purposes of EnviRisk, there are emissions of PAHs provided by two factories in the Czech Republic, but this is all, so usability of this database is minimal.

2.2.3 Soil and sediment

No European databases on emissions to soil or sediments were discovered in this review. One database for Australia was found, but naturally there's nothing useful for us in that source.

2.2.4 Emission factors

In some cases emissions can be estimated using emission factors, which are specific for each type of source. These values quantify the amount of emission per some measure describing the source. Examples are kg / animal for NH emissions, g / km of urban driving for PM emissions or kt / MJ fuel combusted in incinerator for lead emissions.

Some databases providing emission factors were discovered and these provide mainly information for PM, NO_x, SO_2 and VOCs. Various sources, such as traffic, combustion, industrial processes and agriculture are covered. Main data sources are UK Emission factor database, emission factors of CEPMEIP Database, RAINS emission factors and WebFire covering EPA's AP42 compilation of emission factors. All these databases concentrate on outdoor air, but one document listing emission factors of VOCs from building materials was also found, and this database can be linked directly to indoor air.

As data on emissions on local scale is minimal, we might need to calculate these emissions based on the emission factors, so these databases are quite useful for our purposes. RAINS emission factors are provided per country and there is information for PM in the Czech Republic. PM information is also available in all other databases mentioned too. For Czech Republic there is also available some national emission factors for cars provided by Ministry of Environment (http://www.env.cz/AIS/web-pub.nsf/$pid/MZPMSF437BOZ) and these include emission factors for PM and PAH. For PCBs only source of information is WebFire, and this information may be utilized to fill in the gaps.

2.2.5 Emission profiles

Emission profiles can be used when determining sources of emissions for some category of compounds, i.e. particulate matter, total organic carbon, VOCs or PAHs. This is based on the fact that each source is represented by emissions of certain chemicals with certain relations. These profiles can be used with source attribution modelling to provide information on how much each source is contributing to the total concentrations or exposures.

Measured emission profiles are widely published in articles, but only one database summarizing all these was found. SPECIATE database by EPA contains over 4000 emission profiles for PM and TOC covering several source categories. In EnviRisk the need for source attribution is scarce, but for the Czech Republic PM and PAH cases this might be considered. In that sense SPECIATE database might come useful for our cases too.

2.3 Data for media concentrations

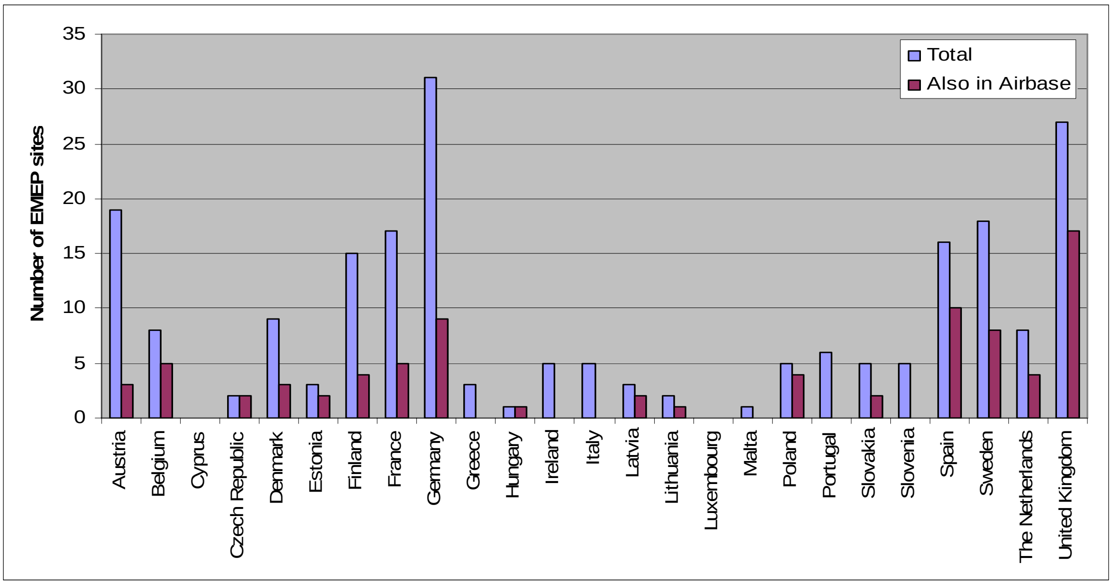
Media concentrations are one of the key values needed for exposure assessment. As mentioned earlier, media concentrations can be calculated based on the emissions with fate and transport modelling, but also directly measured concentration values can be used. This is naturally a more reliable method with smaller uncertainty than modelling. Measured concentrations can also be used to validate models.

Exposure media are defined by the exposure scenarios and this also defines the needed concentrations. Possibilities are outdoor and indoor air, water, soil and sediment, food and breast milk, dust and various consumer products. Dust and consumer products are left out from this review, because they are not relevant for our cases, but databases for other media are presented here (Annex 8).

2.3.1 Outdoor air

Outdoor air concentrations are most widely measured for ambient air quality compliance monitoring, and these results are published as reports and in internet. Nevertheless, as there are threshold limits for several pollutants legally regulated at least on EU level, there are also official measurements required with a reporting responsibility. Main pollutants measured are health based SO_2, NO_x, CO and particles. AirBase and EMEP are the two main monitoring networks with European-wide coverage. While there is some overlap between these networks in terms of the monitoring sites, the best spatial (and temporal) coverage is achieved by combining sites from both networks (Figure 1).

Figure 1. Total number of EMEP sites in the network by country (EU-25) (Also indicates the number of which are included in AIRBASE)



The EU-funded APMoSPHERE project used both the AirBase and EMEP as a basis for developing high-resolution air pollution models across the EU-15. In the APMoSPHERE project AirBase was the primary source of concentration data and additional, unique monitoring sites (where available) were obtained from the EMEP. It is proposed that a similar approach be used to acquire updated concentration data for EnviRisk.

Both AirBase and EMEP include PM data for the Czech Republic mainly for years 2004 and 2005. There are values for daily, monthly and annual means and for traffic, industrial, residiential, and background stations at least. This data is very useful for our local exposure calculations, but the timeline of the data is quite limited. Data on PAHs and PCBs are available for the Czech Republic for several years through EMEP, but for Slovakia no data on these compounds is available. For EnviRisk cases this might not be such a big problem because air is not the main exposure media for PCBs, so we may not need that information anyhow.

Use of these data in EnviRisk

The following key benefits and limitations should be considered when using these databases:
Key benefits:

- AirBase:
  - The data are free and easily accessible.
  - Large amounts of data available, especially useful for statistical purposes and detailed studies geographically and through time for each specific country (more problematic when comparing different countries, see limitations below).
- EMEP:
  - The data are also free.
  - Offers additional rural sites not included in the AirBase network, especially for ozone.
- Combined:
  - Although not all monitoring networks across Europe are included in AirBase or EMEP, taken together these databases offer basic monitoring coverage of the EU-25.

Key limitations:

- AirBase:
  - Although data are updated every year, latest input is from 2004 (July 2006).
  - Data are validated by the country of origin, resulting in some problems of intercomparability. Also increased by the lack of additional information such as meteorological data and detailed site description (number of inhabitants, traffic volume, type of industry, etc).
  - There are some important data gaps in some of the sites. Sites with low data capture (number of measurements taken during the recording period) should be excluded as per EU guidelines.
  - Data capture is provided as part of the metadata.
  - Not all European monitoring networks report their data to AirBase and therefore there are some important geographical gaps.
- EMEP:
  - Effort is required to incorporate EMEP into AirBase, in particular to ensure that duplicate records are not introduced and to reformat the data to match the AirBase format.
- Combined:
  - The AirBase and EMEP monitoring networks were designed to monitor compliance with air quality guidelines rather than for risk assessment and epidemiological studies. As a result, the spatial coverage of the combined network will likely be inadequate in some areas for assessing exposures to air pollution. To overcome this limitation, spatial modelling may be required. Should EU-wide pollution surfaces be needed for the integrated risk assessment, methods developed in the APMoSPHERE project can be explored. At the local or regional level, additional monitoring sites from local authorities may also be sourced to further facilitate modelling.

2.3.2 Indoor air

Concentrations for indoor air are not available as freely accessible databases. Nevertheless there are some measurement data available from EXPOLIS study including PM indoor concentrations in Prague. Time frame of this data is years 1996-1997, so this information might be useful for EnviRisk. For now it seems that the indoor concentrations of PAHs needed for exposure calculations have to be calculated using infiltration factors and available outdoor concentrations. EXPOLIS data might also be useful for I/O assessments.

2.3.3 Water

Contaminants in water (lakes, rivers, ground water, sea, pipe water) are quite widely measured and recorded around the world, but usually these measurements include mainly nutrients, ions and metals with biological characteristics. In some places also some organic compounds are measured but such data are very limited.

For purposes of EnviRisk it seems there are no available measured PAH and PCB data for the Czech Republic and Slovakia, so if we are going to model exposures through water pathway too, we have to try to find some local measurements or use some other data to approximate the water concentrations.

2.3.4 Soil and sediment

Chemical measurements in soil and sediment have been done for research purposes. Furthermore, for some European countries there are also limits for PAH and PCB concentrations in soils and these are legally regulated on national levels. However, this review revealed that this kind of data is not widely provided in accessible database form. Most of the soil related databases did not contain information on persistent organic pollutants, whereas those were concentrating more on soil quality.

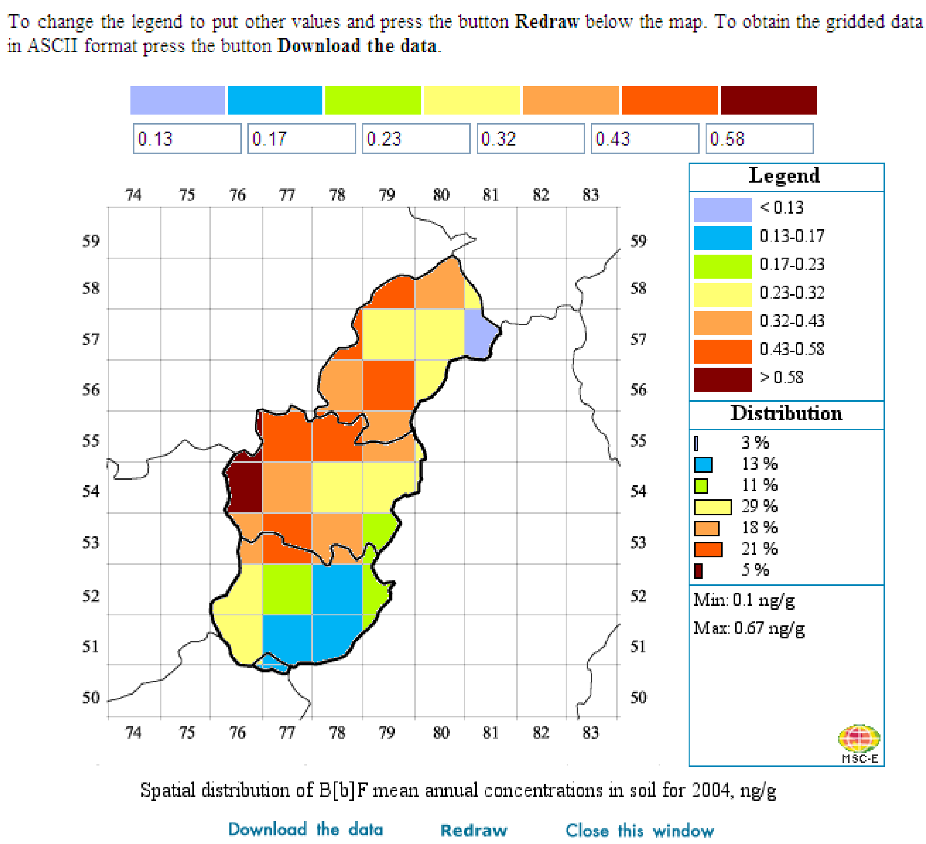
For sediments no databases were found, and for soil concentrations only one database was found to provide modelled information for PAH and PCB compounds. This database is EMEP-MSCE and it's part of the EMEP project maintained by MSCE (Meteorological Synthesizing Centre-East).

Pollutant and media in EMEP-MSCE

Form of Presentation

Three forms of data presentations are available:

- Calculated concentrations in the top soil layer (means over the country, minimum and maximum values in the country) of PCDD/Fs, B[a]P, B[b]F, B[k]F, IP for 2004; the concentrations are shown together with other data for various media in the Detailed reports for each EMEP country (an example) Data can not be downloaded for all of the countries together but may be requested (see below)
- Maps of PCDD/Fs, B[a]P, B[b]F, B[k]F, IP concentrations. The color sensitivity can be adjusted manually and the data downloaded. These maps can be accessed from each country's Detailed reports. Data can not be downloaded for all of the countries together but may be requested (see below)



(the image above is also a hyperlink for an example)

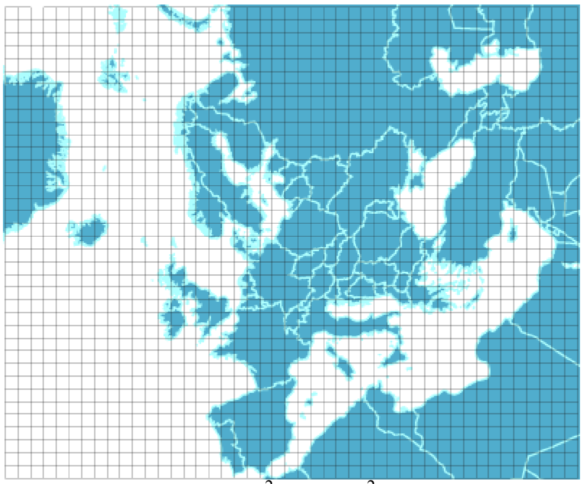
- Maps of spatial distributions of selected PCDD/Fs, B[a]P, B[b]F, B[k]F, IP in air, soil and vegetation for 2004; PCBs HCB for 1998; and gamma-HCH for 2001; **Numerical data are available by request . It's not clear whether this is true for the other presentation types as well.**

form of representation		B[a]P	B[b]F	B[k]F	IP (indeno-pyrene)	PCB	PCDD/Fs	γ-HCH	HCB
country means, max,min		yes	yes	yes	yes	?	yes	?	?
country maps		yes	yes	yes	yes	?	yes	?	?
large area maps	regional (europe)	?	?	?	?	?	?	?	?
	Hemispheric	?	?	?	?	?	?	?	?

Geographic Scale

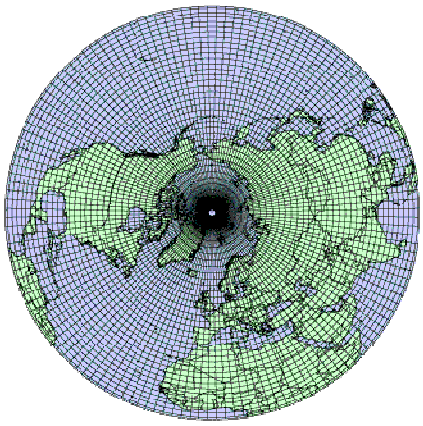
Two computation model types are available: regional and hemispheric (which is under development), with concentrations for all of the pollutants already computed for the regional model.

The regional models cover all of the area shown below with specific data available for all of Europe and on some cases extends beyond Europe and use the EMEP grid system which is based on a polar-stereographic projection. The EMEP 50x50 km^2 domain includes 132x111 points (with x varying from 1 to 132 and y varying from 1 to 111). The EMEP 150x150 km^2 domain includes 44x37 points (with x varying from 1 to 44 and y varying from 1 to 37). The Grid's minisite contains various ways to convert to and from longitude/latitude coordinates, including various (free) software and text files.



This is the 150km^{2}X150km^2 grid system
(the grid itself extends beyond protocols signees)

The Hemispheric models
In view of POP physical-chemical properties, some pollutants can be transported and accumulated in the environment on the hemispherical and global scale and so some of the calculations are available for the entire northern hemisphere. The transport model is called: "MSCE-POP-Hem transport model".



Usability of this data for EnviRisk is still unclear, because detailed numerical values have to be requested separately. The timeline for the data is mainly year 2005, so this would cause some uncertainties for the calculations.

2.3.5 Food

Food is the main exposure pathway for most persistent chemicals, so concentrations of these are measured commonly. Pesticides are naturally usually studied because of their application directly to vegetation, which increases the risk of it accumulating to food.

One global level and one national level (Ireland) were found in this review for Europe. The global level database, GEMSfood, is the only one providing information relevant for EnviRisk. There are data for PCBs in Slovakia and in several food items, and ingestion being the most important of the exposure routes in our PCB case, this information is much needed. There are also data for several years, but more detailed inventory of Slovakian data is still under its way, so it's not possible to evaluate the level of data at the moment. There was no data on PAHs found, but food is not the main medium for PAH exposure, so this might not be such a big problem for us.

3 Review of exposure assessment methods and modelling tools

3.1 Sources and media of exposure

Understanding the relationship between the source of a hazard agent and the receptor (e.g. humans) provides information about how risks may be controlled. Common source categories include point, area, line and diffuse sources, far and near field sources, indoor and personal sources; instantaneous, intermittent, continuous sources; sources that are spatiotemporally independent on the activities of the exposed (e.g. a power plant chimney), and sources that emit at the time and location of – at least some of - the exposed (e.g. street traffic, smoking),

The medium of the exposure may differ from the medium of source release, due to the agent's transport and fate properties. For example, mercury can be released into the air, but a primary route of exposure is through ingestion of fish because mercury deposits into water bodies and settles into the sediment, which are then eaten by fish and through subsequent bioaccumulation, are then ingested by humans. Another consideration in exposure modelling is that a substance may also have secondary sources, that is, they are formed not from a direct source emission, but are created through chemical or physical transformation of parent compounds. Ingestion of non-food items may be significant in some cases, such as for children who tend to put non-edible objects in their mouths, or have a great deal of hand-to-mouth behaviour. Additionally, exposure to non-contaminant agents, such as noise or electric and magnetic fields, can be modelled using the same source-to-exposure framework.

3.2 Exposure and intake modelling

Exposure models can be categorized into one or a combination of the types listed in Table 1. For policy assessments, mechanistic source-exposure models and probabilistic models are the most useful, as these allow for exploration of the effect of changes in various control strategies. Statistically-based models can also be used. The next sections go through the source-exposure pathway and describe the use of models in calculating the exposure outcomes.

Table 1: General model types

	Mechanistic	*Empirical*
Deterministic	Mathematical constructs of physical/chemical processes that predict an exposure for a set of inputs.	Statistical models based on measured input and output values (e.g. regression models that relate ambient pollutant concentrations with person exposures).
Stochastic	Mathematical constructs of physical/chemical processes that predict the probability density distribution of population exposure using full ranges of input data	Regression-based models, where model variables and coefficients are probability distributions, which represent variability and/or uncertainty in the model inputs and parameters.

Exposure incorporates the environmental concentrations that people come into contact with and the time a person spends in contact with that concentration. This contact is defined as taking place over an "exposure surface" which acts as a theoretical boundary between the environment and the internal human body. For air, exposure is merely the amount of time spent in a microenvironment with an associated agent concentration, resulting in a time-averaged exposure concentration. For ingestion or dermal exposures, it is more relevant to calculate intake.

Intake refers to the crossing of an exposure surface by the environmental agent, and thus entrance into the body. Intake can be quantified as a rate or a total mass amount. Many exposure models, especially those that deal with the ingestion and dermal pathways, include intake. Intake rates may be further specified by age, gender, and activity level. It is also possible to derive a distribution of intake rates to be used in probabilistic modelling, although a single value is sometimes used.

3.2.1 Mechanistic source-to-exposure modelling

Mechanistic exposure models are particularly suited for predicting the exposure consequences for alternative exposure scenarios, or assessing exposures in the past, therefore we describe them here first. Mechanistic models are mathematical representations of the processes between the emission of an agent to the contact of the receptor (individual or population). These models are based on the physical (and sometimes also chemical and biological) properties and processes of the agent and the surrounding media. Mechanistic source to environment, exposure and intake models can be generalised into a single framework, which, in principle, would apply for any source release, exposure pathway, and route-of-entry. One or more of the terms of the subsequent formulas are irrelevant in most model applications, but each one is crucially needed for some.

The basic term is the **concentration in contact medium**:

`Concentration = source emission x dilution x temporal decay x removal x medium transfer`

Source emission: Emission of the agent of concern from its source(s) (g, m^3, g/sec, m^3/sec)

Dilution: Physical processes which mix the agent into an increasing quantity of the dilution medium and thus reduce the concentration, but not the amount of the agent in it, i.e. 1/(dilution volume/mass between source and recipient) (m^3, g^{-1}, sec/m^3, sec/g). For multiple recipients, sources and/or time windows, the dilution term covers a whole range/distribution of values. (Recipient is either the exposed individual in the case of single medium pathway, or the second medium in case of two media pathway, e.g. water to fish, or water/soil to produce. For the case of simplicity we assume no dilution in the second medium (fish or produce in the previous examples))

Temporal decay Accounts for the chemical (e.g. oxidation) and physical (e.g. sedimentation) processes which gradually reduce the amount of the agent from the pathway medium between the point of release and the point of exposure. These processes are typically characterised by half life, $T½$, or decay constant, λ.

Removal Accounts for the "instantaneous" processes (filtration, evaporation in cooking, etc), which reduce the amount of the agent in the exposure medium between the point of release and the point of exposure.

Medium transfer Coefficient defining the discontinuous concentration change from one medium to the next (e.g. bioaccumulation of lipophilic chemical from water to fish, amplification/attenuation of minerals from soil or irrigation water to plants, or transfer of a chemical from packaging material to food)

The dimension of the concentration in contact medium is mass/vol or mass/mass

The concentration in contact medium can then be used in calculating exposure and intake:

```
Exposure = concentration x contact time
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Contact time The time (sec) the exposed subject is in contact with the medium (air, water, surface) with the given concentration. For multiple recipients there is a range/distribution of values.

The dimension of exposure is vol/vol, mass/vol or mass/mass, or any of these x time

```
Intake = concentration x intake rate
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Intake rate: Consumption of the medium with the given concentration by the exposed individual (air, water, food) (m^3, g). For dermal exposure intake equals uptake, i.e. absorption through skin. For multiple recipients and/or time windows there is a range/distribution of values for the intake term.

3.2.2 Probabilistic modelling

Probabilistic exposure models (Table 1) are in most cases also mechanistic models. The main difference is that instead of point values, the whole distributions of input data, e.g., representing the time activity, residential sources and ambient air concentrations for entire populations, are used to estimate the whole distributions of exposure values for that population.

Parametric statistical distributions (e.g. lognormal for ambient air pollution, or beta for microenvironment/activity time allocations) may be fitted for the empirical input data, or the data may be used with no assumed distribution. To end up with realistic exposure distribution estimates, in addition to reliable and representative input parameter data, also correlations between the different input parameters need to be known.

In probabilistic modelling (or simulation) values for the different parameters in the model are randomly drawn from the available input data distributions, an (often daily) exposure estimate is generated, and the process is repeated thousands of times to generate the population exposure distributions. The most common probabilistic simulation techniques are Monte Carlo and Latin Hypercube, while @Risk, MathLab and Crystal Ball are common modelling tools. The population exposure distribution estimates may be remarkably realistic even for quite simple models, but at the price that they contain no indication about who is exposed, where and when. For population level risk assessment or comparison of risk management options, this limitation is tolerable. Unlike mechanistic modelling of average or credible worst case exposure, probabilistic modelling provides answers to questions, such as how many individuals may be exposed to a daily level exceeding X (e.g. Air quality standard value), or what is the daily exposure level exceeded by 5 % of the population.

3.2.3 Statistical modelling

Mechanistic exposure models are driven by physics – statistical models are driven by data, and are thus empirical (Table 1). A typical statistical exposure model is a best fit regression equation between measured exposure data (dependent variable) and a selection of independent variables, which are expected to affect the exposure. The independent variables may include continuous variables, such as "ambient air concentration" and "daily time spent in a car", and dummy variables, such as "current smoker" and "residence within 50 m from a busy street" (yes/no). The process of the development of a multiple linear regression exposure model also gives values for the significance (P-value) and impact (β coefficient) for each independent parameter and an estimation of how much of the exposure variation is explained by the model (r^2). Regression models never explain the whole variation, and thus they underestimate the exposure range.

Because statistical exposure models are data driven they contain also the impacts of variables and relationships which is not known to the modeller. They reflect, by definitions, the existing reality. For the same reason they should be applied for predictive modelling only with great caution, only when the model explains a high portion of the exposure variation (e.g. $r^2 \geq 0.6$), and the model is mechanistically plausible, and for conditions which closely resemble those from which the original data has been drawn. Statistical exposure models are better suited for descriptive modelling, i.e. for gaining understanding as to which parameters explain the exposure, how strongly, and much of it.

3.3 Modelling environmental concentration

In this section, we discuss methods for modelling the transport and fate processes of an agent from source emission into the environment.

Concentration = source emission x dilution x temporal decay x removal x medium transfer

3.3.1 Source emission

Source emissions are usually quantified as a rate of emission (mass per unit time) or a bulk emission (mass). There are several methods for estimating source emissions, which will not be addressed in detail in this protocol. Emission factor databases exist for any industrial processes and vehicular sources, which can be used to calculate emissions. Additionally, municipalities or countries may do emissions inventories for some pollutants from local sources. Emissions information can be determined experimentally or from measured concentration data, although often the uncertainties can be quite large in estimating real-world emissions.

3.3.2 Dilution and dispersion modelling

Once released into the environment, emitted agents undergo dilution, which refers to the time dependent mixing of an agent in a medium. The simplest representation of this is that of the mass release of an agent into a specified volume of liquid. The second law of thermodynamics ensures that this is a one way dilution process, which will eventually lead to uniform mixing ratio in the entire available mass/volume of the dilute medium. For a given mass of pollutant emitted, the longer the time from release to exposure and the larger the dilution mass/volume, the smaller the exposure to a given recipient. A variety of dispersion models for different media and capability of dealing with different levels of complexity are used to model dilution from source to exposure of the recipient (or rather a physical location).

3.3.3 Decay, removal and medium transfer (bioaccumulation)

In addition to dilution, decay and removal processes determine how much of a released agent will reach the recipient. In this protocol, time dependent processes, such as oxidation and sedimentation are called decay, and "instantaneous" processes, such as filtration, are called removal processes.

Temporal decay is proportional to the amount of an agent in the system, and can be described by a decay constant, λ. The half life of the agent in the system, assuming no other removal processes, is $\ln 2/\lambda$. A "conservative" pollutant is one where the half-life of the pollutant is much greater than the residence time of the medium in the system (e.g. the time which it takes the entire volume of air or water in the system to turn over). In this case then, temporal removal does not need to be considered in the model.

For particulate substances the important indoor decay processes are sedimentation and deposition. Outdoors, sedimentation and interception by rain and mist droplets are important for atmospheric contaminants, removal after rain and dilution into the soil decay the contaminants in the soil, and sedimentation in the water bodies. For gaseous pollutants the most important decay process indoors is sorption to surfaces and materials, although gas phase indoor chemistry may be important for some compounds and conditions. Outdoors, oxidation dominates the decay processes of chemicals in the air, hydrolysis and biological processes in soil and water. The reaction kinetics determines the rate of pollutant decay. These are often modelled as first order or pseudo-first order kinetics, allowing the use of the exponential decay function. For these reactions, the reaction constant is required. This can be calculated from the half-life of a compound. Higher order reactions may need to be calculated if the concentration of one of the reacting chemicals cannot be considered a constant.

The "instantaneous" removal mechanisms include processes such as intentional filtration of contaminants in air or water, non-intentional filtration in the entry of outdoor air particles through slits and cracks to indoor air, cookout and bake out of volatile contaminants in food preparation, etc. Most removal terms are experimentally determined.

Both decay and removal processes reduce the contaminant concentrations. In a transfer from one medium to another the contaminant concentration may decrease or increase considerably. The most exposure relevant medium transfer processes include water to fish and soil to plant. Examples of high accumulation include the bioaccumulation of methyl-mercury or PCB from lake water to fish and accumulation of the Chernobyl fallout from cities to lake bottom sediments near storm drainage release points. In the low accumulation end are many soil-to-plant transfers of soil minerals and contaminants, e.g. the very low transfer of fallout cesium to grain in potassium fertilized farming.

3.3.4 Types of models

Models can be of differing levels of complexity, and their use depends on the state of data and knowledge about the processes. The basic type of model used for environmental concentrations is a box model based on the concept of mass balance. Thus the concentration is equal to the amount entering the box, minus the amount exiting the box over the volume of the box. Emission and secondary formation are included as source terms influencing the amount entering the box, and decay and removal as well as advection define the exit processes. Box models assume that agents released are instantaneously and completely mixed (i.e. evenly distributed). Often steady state is also assumed, meaning that the inputs equal the outputs.

More complex models account for advection (e.g. wind and water flow) and diffusion (e.g. random movement from high to low concentration) as mixing processes, and go beyond the assumption of a well-mixed box. These models still follow the principles of mass balance, except in these cases, we do not examine the change in concentration in a large box, but rather at fixed points. Thus, these models are generally deterministic in nature. Dispersion describes the diffusion processes in nature which, although generally modelled as random, actually follow a complex pattern. They apply to any fluid media, although parameters may change to reflect that media. For dispersion modelling, we can define two types of coordinate grids: Eulerian, where the coordinate axes are fixed; and Lagrangian, where the coordinate axes follow the mass flow of the pollutant released. These can both be used from small to large scale (hundreds of meters to hundreds of kilometres).

The above-mentioned principles can also be applied to examine the movement of agents between a system of media, such as air, water, sediment, and soil. These multi-media models use principles of phase-transfer such as fugacity and partition coefficients.

3.4 Model descriptions by category

The following sections describe the type of models that are recommended for use in EnviRisk. The models are divided into five categories: dispersion models, time-microenvironment activity models for inhalation exposures, probabilistic intake models (generally for multi-route exposures), multi-pathway and food chain models (for modelling source-to-intake transfers), and regression models. Probabilistic intake models tend to model individual-level exposures with greater detail, while multi-pathway and food chain models tend to be on a larger scale (e.g. regional), and often are based on a compartment modelling approach.

3.4.1 Dispersion models

Model application
Three fundamentally different types of atmospheric dispersion models are described. The first two are based on physical dispersion equations and description of the ground surface topography. a) Models that estimate the dispersion/dilution of an atmospheric release in a coordinate system that moves from the point of release at the direction and speed of the wind, are called Lagrangian. They are particularly suited for elevated point sources, e.g. power plant chimneys, and exposures downwind from the source. b) Models that estimate the dispersion over a terrain in a fixed coordinate system, are called Eulerian. Such models are particularly suited for complex sources distributed over an area, e.g. road traffic, and exposures within the same area. c) Finally, statistical concentration models estimate the concentrations on the basis of a long term database of observed (empirical) release, weather and concentration data. Statistical models are particularly suitable for estimating long term concentration change resulting from a change in emission.

Model application criteria

a) The most used Lagrangian atmospheric dispersion models, the Gaussian models, predict short term ground level concentration fields downwind from the source (point, line or area), which can be extended to long term average ground level concentration fields and concentration probability distributions. To predict ambient concentration fields for extended periods Gaussian dispersion models require extensive meteorological, topographical, source location and emission time series data.

b) Eulerian atmospheric dispersion models predict dynamic high resolution concentration fields, which can be averaged for long term average ground level concentration fields. To predict ambient concentration fields for extended periods Lagrangian dispersion models require extensive meteorological, topographical, source location and emission time series data.

c) Statistical (empirical) atmospheric concentration models predict long term average atmospheric concentration changes due to changing source emissions, urban structure and/or climate. Statistical models require long term emission data for each grid cell and source category, concentration data from monitoring locations within this grid, and long term city wide meteorological statistics.

Description of model type

a) Gaussian dispersion models (x-axle is the wind direction and centreline of the release plume) are mechanistic, based on turbulent eddy mixing theory, and predict for each model run a downwind ground (xy) level concentration field of the emitted pollutant.

b) Eulerian dispersion models are mechanistic, based on fluid dynamics, and predict a ground level concentration field on a geographically fixed xy coordinate system.

c) Statistical dispersion models are empirical, based on the best fit multiple regressions of the measured concentrations vs. emission and meteorological data, and predict long term average ground level concentrations.

Modelling Specifics

a) Model coordinates fixed to the moving air mass: Source emissions are given in the form of release height (z) and emission rate. Wind direction and plume centreline (after thermal and/or kinetic plume rise) define the x-axle. For point sources Gaussian dispersion models also require source emission flow rate, velocity and temperature. In its basic form a Gaussian dispersion model computes the progression of the concentration field on a 2D y-z plane (assuming Gaussian distribution along both y and z axles). Advanced Gaussian modelling tools predict both short (downwind from the source) and long term (around the source) ground level concentration fields. Other types of sources (line, area), are treated as expansions of the point source model. Physical and chemical decay processes are also incorporated in the more advanced Gaussian dispersion models.

b) Model coordinates fixed to the ground: Source emissions are given in the form of release coordinates (xyz) and emission rates (and times). A basic Eulerian dispersion model applies fluid dynamics to compute the mixing of a point release into a turbulent air mass that moves over a terrain. The mixing is forced by characteristics of the emission, the local topography, and the wind field and thermal layering of the lower atmosphere. Other types of sources (line, area), receptors (concentration fields, mobile receptors), and times up to a year are treated as expansions of the short term point source model. Physical and chemical decay processes of the released agent are incorporated in more advanced Lagrangian dispersion models.

c) Statistical models: Source emissions are given as emission rates. For a city a simple polar grid structure with the city centre forming the central cell is often used. Long term average dilution is predicted from the long term average emission-concentration ratio specific for each source and target grid cell and source category. The effects of any atmospheric decay (and also secondary pollutant formation!) phenomena are accounted for in the empirical emission-concentration data.

Model examples are summarized in Annex 9.

3.4.2 Time-microenvironment activity models (inhalation only)

Model application

Time microenvironment activity (TMA) models combine concentrations in specific locations (microenvironments) and data on the locations, the time spent in these locations, and in some situations the activities that individuals perform in these locations. Microenvironments are defined as a space in which contaminant concentrations can be considered to be spatially uniform during some specific interval (typically a room, car, back yard, etc.). These models represent total personal exposure, and are used for inhalation exposures. Similar modelling approaches for other exposure pathways are addressed in the section on Probabilistic Intake Models. Concentration inputs to TMA models come from measured data or other models, such as dispersion models. Some TMA models also have the ability to further calculate intake and dose using physiologically based pharmacokinetic (PBPK) models.

The major benefit in comparison with ambient air quality models is that the effects of spending time (i) indoors and (ii) in traffic are separately accounted for. The role of these special microenvironments depends naturally on the type of pollutants studied, i.e. indoor environments on the other hand lower the experienced levels of ambient pollutants but increase – sometimes substantially – levels generated by indoor sources. Pollutant levels in traffic often resemble ambient levels for pollutants of remote origin but are high for traffic emission components.

Output capabilities

- Personal exposure or intake concentrations for individuals and populations over a specified period of time
- Outcomes can be in distributional form

Input data requirements

- Probabilistic models require inputs (not necessarily all) to be distributions
- Microenvironmental concentration distributions (e.g. inside homes, in workplaces, in vehicles, etc.)
- Time-activity patterns for the population of interest (e.g. children, elderly, adults, etc.)

- Contact times
- Inhalation rates
- Physiological parameters (if dose is of interest)

Limitations

- Continuously variable concentrations are described as averages during the stay in each microenvironment.
- TMA models must be able to account for longitudinal patterns, however, most data used are based on daily dairies or surveys, which account only for a 24 or 48 hour periods during weekdays.

Description of model type

TMA models are typically stochastic, using Monte Carlo techniques and input data probability distributions to describe exposure distributions within the target populations. The major benefit in comparison with ambient air quality models is that the effects of spending time (i) indoors and (ii) in traffic are separately accounted for. The role of these special microenvironments depends naturally on the type of pollutants studied, i.e. indoor environments on the other hand lower the experienced levels of ambient pollutants but increase – sometimes substantially – levels generated by indoor sources. Pollutant levels in traffic often resemble ambient levels for pollutants of remote origin but are high for traffic emission components.

Modelling Specifics

TMA models address exposure specifically, including the time spent in contact with the contaminated medium across a person's exposure time.

Exposure = time-weighted average exposure over microenvironments visited

Or in the notion used in the other fact sheets:

Exposure = Σ (concentration x contact time or rate)

Exposure is then the concentration to which an individual comes into contact with in a particular microenvironment multiplied by the fraction of total time (over a time frame of interest, be it a lifetime or a shorter period) spent in the microenvironment. For models that can calculate dose, absorption coefficients and partition coefficients for the different physiological compartments would be required.

The microenvironment model uses average concentrations experienced and times spent in each microenvironment as inputs, typically described as probability density distributions of the average concentrations, and times spent in the same microenvironments, typically from time-activity diaries. The concentrations can be obtained from measurements or using ambient air quality models and models of indoor air quality. The exposure times in each microenvironment can be obtained from time-activity diaries, and are also typically expressed as probability density distributions. Classification of microenvironments into indoor and outdoor locations is an important modifier of exposures to ambient and indoor generated pollution.

- ambient concentrations
- infiltration of ambient pollution indoors
- indoor sources

Some TMA models also incorporate 2-stage Monte Carlo simulation, allowing for propagation of both variability and uncertainty through the model. In these models, uncertainty distributions for model parameters would need to be included.

Model examples are summarized in Annex 10.

3.4.3 Probabilistic intake models

Model application

Models for exposure to consumer products (including pesticides, personal care products, cleaning products, etc.) must usually account for multiple exposure pathways. Dermal and ingestion, particularly non-dietary ingestion, are important routes of exposure. Inhalation may also be considered. These models may vary greatly in their approach to modelling exposure or intake/dose.

Output capabilities

- Absorbed dose
- Intake
- Exposure concentration

Input data requirements

- Source emissions
- Time-activity patterns for the population of interest (e.g. children, elderly, adults, etc.)
- Contact times and behaviour
- Intake rates
- Transfer coefficients
- Physiological parameters

Limitations

- Ingestion and dermal contact rates are very heterogeneous within and across populations - quantification of this information is time and resource intensive to collect, therefore they are not widely available. Rates in children and workers tend to be better studied than in other populations.
- Transfer coefficients and absorption rates are not well quantified for many substances. QSAR has been used in some cases, but the relationships have not been established as robust yet.

Description of model type
Consumer products exposure models can be deterministic or stochastic. Generally several scenarios may be investigated by a model. These scenarios involve different applications of a product. The product distribution in the environment and contact media is modelled or derived from measured concentrations and subsequent contact frequency and duration data are used to calculate exposure. Inhalation applications may or may not include inhalation rates, while intake is calculated for ingestion and dermal exposure. Some models may also include dosimetry calculations.
Modelling Specifics Consumer product models may calculate exposure or intake. Intake is most likely if the exposure routes are ingestion or dermal uptake. Models account for exposure or intake during specific use scenarios, and may treat multiple pathway exposure either in sum or separately. Default source values and parameters are possible in some models if user does not have further information.

Model examples are summarized in Annex 11.

3.4.4 Multimedia and food chain models

Model application
Output capabilities Food chain models, also known under the name of dietary exposure models, explicitly focus on the exposure via ingestion and, thus, are applicable for the prediction of chemical exposure originating from a wide range of sources, such as industry and agriculture. Ingestion involves the two main substrates food and drinking water. For some contaminants, i.e. heavy metals, the source of the latter rather stems from the distribution system, such as pipes, than from the source of drinking water (World Health Organisation, 1992; Becker et al., 1997). This may be different for other chemicals, e.g. organic pollutants, for which water treatment is not very efficient (Versteegh et al., 2001; European Commission, 2003a). The output of a food exposure model generally is an exposure concentration. But in practice, exposure via the ingestion pathway often includes estimates of ingested dose. Food chain modelling results can therefore be used as individual/population exposure estimates. With regard to the temporal scope of exposure modelling ingestion exposure through the media (fresh) water and soil as well as partly exposure through the medium air, i.e. dry and wet atmospheric deposition onto leafy plants, is most dominant in the intermediate to long term and is highly relevant with respect to sustainable development especially in terms of intergenerational equity. **Input data requirements** (Multimedia) food chain models are based on transfer factors, uptake rates, such as the rate of food intake, partitioning or bioconcentration factors, and environmental concentrations of contaminants. Individual components of an exposure pathway within the food chain can be

estimated on the basis of measured or predicted data. For example, the bioconcentration of organic pollutants in fish is often based on empirical bioconcentration factors or on an estimation equation based on observed correlations between the bioconcentration factor and the octanol-water partition coefficient (Mackay and Boethling, 2000). The bioaccumulation factor, however, also can be modelled, taking into account factors, such as the trophic level, growth dilution, and biomagnification (Campfens and Mackay, 1997). For heavy metals, respective food chain models require the input of measured transfer and partitioning factors while for organic chemicals, these transfer and partitioning factors are often predicted by simple correlations. The use of such estimation methods is convenient because it allows for the assessment of many chemicals for which detailed empirical data do not exist.

Limitations

The subsequent exposure assessment for ingestion is more complex than for inhalation due to both the variety of food items to which human beings and/or animals of concern might be exposed and the spatial distribution of the food production (Bachmann, 2006). Even with respect to national and/or international trade whose contribution may be a homogenizing effect on the concentration of food items between or within countries (Spadaro and Rabl, 2004) ingestion exposure assessment remains extremely complex. Thus, the exposure via food does not exclusively lead to exposure of people living or staying in the contaminated environment.

The consideration of exposure routes due to ingestion implies the coverage of longer time horizons in order to fully assess the effects of long-lived substances, e.g. heavy metals. For those substances, this leads to the question how effects that occur at a very distant point in time can be valued in terms of the present value of money which is an important matter in monetisation methods where it is principally known as discounting. In any case, the uncertainty about the predictability of the future is an issue that needs to be kept in mind when it comes to exposure via ingestion.

Description of model type

An established type of food chain models is the group of integrated multimedia fate and exposure models that calculate the distribution of a chemical among different environmental compartments and the transfer of chemicals through various exposure routes to a species of interest, e.g. humans. These models usually treat environmental media, such as air, surface water and sediments as uniformly mixed (Hertwich et al., 2002). Moreover, transport processes are basically described by simple elementary models that use measured or, more commonly, estimated partitioning constants and intermedia transport rates for processes, such as rainfall and runoff.

Regarding human exposure, these models calculate a potential dose or individual dose fraction which is indicative of the level of the expected impact (Hertwich et al., 1998). For exposure to ecosystems, these models either calculate environmental compartment concentrations or potential doses for animals at different levels of the food chain (Jolliet, 1996; Huijbregts, 1999).

Modelling Specifics

From the three main routes of exposure, i.e. the routes by which a substance enters the human body (United States - Environmental Protection Agency, 1992; World Health Organisation, 2000; European Commission, 2003b)

- inhalation (absorption through the lungs),
- ingestion (absorption from the digestive tract), and
- dermal absorption (penetration through the skin)

the most important exposure route through (fresh) water and soil is ingestion noting that dermal exposure due to bathing and soil contact might principally also play a role (Mileson et al., 1999).

Within food chain modelling not only exposure to humans may be taken into account but also exposure to aquatic and terrestrial ecosystems. Whereas in human health risk assessment, as mentioned above, generally only intake via ingestion is essential, for exposure to ecosystems methods like the critical loads concept have been established to estimate impacts and damages, respectively (Schütze, 1999; de Vries and Bakker, 1998). Additionally, for both human and ecosystem exposure also external exposure (International Atomic Energy Agency, 2001), i.e. the exposure due to staying in the vicinity of contaminated environmental media, may be considered due to its important role when it comes to specific contaminants, such as radionuclides.

3.4.5 Model examples are summarized in Annex 12.

3.4.6 Regression models

Model application

Output capabilities

Regression analysis examines the dependence of a variable, called a dependent or response variable, on other variables, called independent variables or predictors. The mathematical model of their relationship is the regression equation. Regression models can be used in source-exposure analysis for producing estimation about which parameters best explain the variation in exposure. Furthermore, result of the regression modelling (regression equations) can be used for predictive purposes in situations where parameters are known, but the exposure is unknown.

Input data requirements

When studying the relations of exposure and the predictors, you need measured values for both exposure and predictive parameters. In case of using regression equations for prediction, you need measured data only for the predictive parameters.

Limitations

Main limitations of the regression models are the demand of preliminary knowledge about what parameters might have effect to the level of exposure to produce models that really can explain some of the variations of exposure. Furthermore, applicability of regression equations for predictive purposes is limited only to situations which are similar enough with the situation for which the regression equations are based on. Also collinearity and its effects have to be kept in mind when using regression models.

Description of model type

Well-known types of regression models are linear regression, the logistic regression for discrete responses, and nonlinear regression. Regression models are classified as deterministic models, although they can also be used with probabilistic models. Furthermore regression models can be either mechanistic or empirical depending on the way of their use. Parametric regression is classified as mechanistic models, since it demands some knowledge about the relationships between explaining factors and exposure and also an assumption of the underlying distribution in the population. However nonparametric regression is a form of regression analysis in which the predictor does not take a predetermined form but is constructed according to information derived from the data. Nonparametric regression requires larger sample sizes than regression based on parametric models because the data must supply the model structure as well as the model estimates. Selection between parametric and non-parametric regression has to be done case-by-case, based on the data.

In principle regression models can be used for individual and population level modelling and also for environmental exposure approximation (now and estimating the future) with all exposure pathways and medias.

Modelling Specifics

In practice regression models are basically used for relating levels of exposure to some explaining parameters, and since regression models in themselves do not include any treatment of source emission, dilution or removal, some other applications have to be used prior to regression modelling for those parts of the calculations. Anyhow, regression models can be used for examining the relationship between various physical parameters as predictors of concentrations (Dimopoulos et al. 2003, Zota et al. 2005,) or to determine source rates (Reiss 1995), which can be regarded as source emission estimation, but these models are always case specific and cannot be regarded as general source emission or dilution models.

Regression models are mainly used for relating exposures to health effects (exposure-response) and for source attribution purposes (described in source attribution fact sheets). In source-exposure applications regression models could be used in any situation where you have data that you want to relate to each other. For example, you can relate indoor air concentrations of PM to the outdoor measured values, and look at how different descriptors can explain the variations (Levy et al. 2002) or you can try to explain concentrations of PCDD/F levels in serum relating those with age, gender, food consumption etc. (Chen et al. 2003). Results from a regression analysis can be used to determine exposure proxies (e.g. proximity to traffic as a substitute for traffic pollution) and also to evaluate the effect of different parameters to the level of intake fraction.

Examples of regression models used for exposure assessment are summarized in Annex 13.

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4 Annexes

Annex 1. Summary table for time-activity databases

Name	Source	Description	Other comments
ExpoFacts	http://cem.jrc.it/expofacts	Contains time activity data from 30 European countries: Austria, Belgium, Bulgaria, Cyprus, the Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, The Netherlands, Norway, Poland, Portugal, Romania, the Slovak Republic, Slovenia, Spain, Sweden, Switzerland, and United Kingdom. Not updated regularly.	Includes wide variety of time activity data which is needed for exposure assessment, but there are great variation in the level of data and time frame between countries; usability is strongly dependable on the case.
HETUS	https://www.testh2.scb.se/tus/tus/Default.htm	Harmonised European time use surveys (HETUS) includes time activity data for Finland, France, Germany, Italy, Norway, Sweden, Spain and UK. There are pre prepared tables for mean time spent on Main and Secondary activities and Participation rates for Main activities during an average day, by Sex and Country and addition to that, user can create tables for his own interest. There are also links to the time-use statistics of above listed countries provided.	At least part of the data can also be found from ExpoFacts database. There are links provided to the web pages of statistics for all eight participating countries, where the most recent information can be retrieved.
Exposure Factors Handbook	http://www.epa.gov/ncea/pdfs/efh/front.pdf	This is not actually a database, but there are references and tables from several studies for population related data, which can be used for average values. Includes information for example time spent in household works, for personal hygiene, in various locations in home and in traffic.	Data is mainly based on U.S. data, so usability for EU level might be low. Data may also be outdated, as it is published 1997
CHAD	http://www.epa.gov/chadnet1/	Consolidated Human Activity Database (CHAD) contains data obtained from pre-existing human activity studies that were collected at city, state, and national levels. CHAD is a master database providing access to other human activity databases using a consistent format. This facilitates access and retrieval of activity/and questionnaire information from those databases that EPA currently has access to-and-uses-in its various regulatory analyses undertaken by program offices	Includes only U.S. level data. Data is presented as individual answers to time activity questionnaires, and there are no summaries available, so usability is quite complex. Might be useful in some case, where other data are not available

Name	Source	Description	Other comments
MTUS	http://www.timeuse.org/mtus/	Multinational Time Use Study (MTUS) describes total time spent per day in 41 activities. Encompasses over 50 datasets from 19 countries, and incorporates recent data from the HETUS, ATUS, and other national level time use projects. Data is provided from EU and US.	Data is provided in SPSS form and there is free registration demanded. Some of the data is restricted and use of it may be prohibited.
AHTUS	http://www.timeuse.org/ahtus/	The American Heritage Time Use Study, a database of national time-diary samples collected over five decades, includes harmonised background, activity, location, mode of transport and who else were present variables. The AHTUS is suitable for a wide range of investigative purposes. Data is freely available to the research community.	ONLY U.S. data, which includes data from NHANES and ATUS studies. Data is in SPSS files, so you have to have a program to open them.
Time use studies	http://www.timeuse.org/information/studies/	Web page that contains references to available time use studies, and provides a short description of them with possible links to the data source. Some of the data are included in other databases, like HETUS and AHTUS, but this provides good overall look for the time use studies completed.	Web page that contains references to available time use studies, and provides a short description of them with possible links to the data source. Some of the data are included in other databases, like HETUS and AHTUS, but this provides good overall look for the time use studies completed.
UK time use survey 2000 and 2005	http://www.statistics.gov.uk/statbase/Product.asp?vlnk=9326	The main aim of the Time Use survey (TUS) is to measure the amount of time spent by the UK population on various activities. Data is divided to 28 tables for year 2000 and to 16 tables for year 2005.	Data only for U.K.
Dutch Time Use Survey (TBO)	http://www.scp.nl/onderzoek/tbo/english/default.htm	In the Time Use Survey several thousand respondents fill in a diary during one week. The survey was first carried out in 1975. The last survey was in 2000. It provides a unique insight in the way how the Dutch plan and spend their time. How much time is spent on work, education, care, travel, sleep and meals? How much leisure time is left, and in what way is it spent? User can create own tables based on data, time spend in each activity is presented as hours/week.	Data for several years, but only for Netherlands. Time use is presented only as hours/week.

Name	Source	Description	Other comments
Finnish time use survey	http://www.stat.fi/tk/el/kva_ajankaytto_en.html	The Time Use Survey has been carried out three times. The first survey was made in autumn 1979 and the next one in 1987/1988. The latest survey, 1999/2000, is part of the European Time Use Survey harmonised (HETUS). The first two surveys were based on individual samples. In the newest survey the data were collected from all over 10-year-old members of the household. Household samples also allow study of intra-household time use. The material contains more than 10,000 survey days. The primary and secondary activities as recorded by the respondents themselves were coded according to a 185-category activity classification.	Data only for Finland.

Annex 2. Summary table for ingestion databases

Name	Source	Description	Other comments
ExpoFacts	http://cem.jrc.it/expofacts	Contains data from 30 European countries: Austria, Belgium, Bulgaria, Cyprus, the Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, The Netherlands, Norway, Poland, Portugal, Romania, the Slovak Republic, Slovenia, Spain, Sweden, Switzerland, and United Kingdom. Ingestion data for food and water and also information on non-dietary ingestion.	Level of information and time frame is variable between countries and data.
Eurostat	http://epp.eurostat.ec.europa.eu/portal/page?_pageid=1090,30070682,1090_30298591&_dad=portal&_schema=PORTAL	Various statistics are maintained by Eurostat and are freely available for download from the website, although the site demands registration. There are some predefined tables provides, and addition to that user can make own queries with several options for data retrieval. Data is divided to several sub-categories including information for food and water consumption. Availability of actual ingestion data unclear.	There is large variation of data available and for several years and countries. Usability of data is quite complex and you have to do quite a lot work to find the data necessary.
FAOSTAT	http://faostat.fao.org/site/346/default.aspx	Food and Agriculture Organization of the United Nations maintains FAOSTAT database that provides access to over 3 million time-series and cross sectional data relating to food and agriculture. FAOSTAT contains data for 200 countries and more than 200 primary products and inputs. Data starts from year 1990. Food consumption data is presented as the amount of food quantities divided for several commodities. Database enables various ways to search data.	Years 1990-2005, updated yearly
Food Consumption and Other Exposure Data	http://www.foodrisk.org/exposure_food_consumption.cfm	This page lists extensively links to food consumption information provided as tables, documents, databases etc.	Large amount of data, laborious to find relevant information.

Annex 3. Summary table for physiological databases

Name	Source	Description	Other comments
ExpoFacts	http://cem.jrc.it/expofacts	Contains data from 30 European countries: Austria, Belgium, Bulgaria, Cyprus, the Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, The Netherlands, Norway, Poland, Portugal, Romania, the Slovak Republic, Slovenia, Spain, Sweden, Switzerland, and United Kingdom. Physiological related data includes body lengths and weights and breathing rates.	Level of information and time frame is variable between countries and data.

Annex 4. Summary table for databases related to housing

Name	Source	Description	Other comments
ExpoFacts	http://cem.jrc.it/expofacts	Contains data from 30 European countries: Austria, Belgium, Bulgaria, Cyprus, the Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, The Netherlands, Norway, Poland, Portugal, Romania, the Slovak Republic, Slovenia, Spain, Sweden, Switzerland, and United Kingdom. Housing data includes ventilation rates, number of dwellings, some information on indoor air quality etc.	Level of information varies considerable between countries.

Annex 5. Summary table for land use databases

Name	Source	Attribute / Description	Scale / Geography	Time period	Geographic extent	Other comments
CORINE Land Cover (CLC2000) - Version 8/2005	http://dataservice.eea.europa.eu/dataservice/metadetails.asp?id=822	44 classes	1:100,000; 100m grid	1999-2002	EU25	
CORINE Land Cover (CLC90) - Version 12/2000	European Environment Agency	44 classes	1:100,000; 100m grid	1986-1996	EU25 (excluding Sweden, Cyprus, and Malta)	
Global Land Cover 2000 (GLC2000)	http://dataservice.eea.europa.eu/dataservice/metadetails.asp?id=955	23 classes	1km grid	2002	EU25	
PELCOM grid	http://www.geo-informatie.nl/projects/pelcom/public/index.htm	14 classes	1km grid	1996-1997	EU25	
FAOSTAT	http://faostat.fao.org/site/418/default.aspx	10 classes		1961-2004		Difficulty finding all the details about the database
EUROSTAT	http://epp.eurostat.ec.europa.eu/portal/page?_pageid=1996,45323734&_dad=portal&_schema=PORTAL&screen=welcomeref&open=/&product=EU_MASTER_environment&depth=2	40 classes	1 km grid	1950-1980, then updated ever five years onwards	EU-15 and EU-25, EU-Candidate Countries (Bulgaria, Romania and Turkey), the EEA-Countries (EU25 and Norway, Iceland, Liechtenstein), Switzerland, Japan and the United States	Difficulty finding all the details about the database

Annex 6. Summary table for population related data

Name	Source	Description	Other comments
Eurostat	http://epp.eurostat.ec.europa.eu/portal/page?_pageid=1090,30070682,1090_30298591&_dad=portal&_schema=PORTAL	Various statistics are maintained by Eurostat and are freely available for download from the website, although the site demands registration. There are some predefined tables provides, and addition to that user can make own queries with several options for data retrieval. In addition to CENSUS data, data for population includes also information for education, health etc.	There is large variation of data available and for several years and countries. Usability of data is quite complex and you have to do quite a lot work to find the data necessary.
ExpoFacts	http://cem.jrc.it/expofacts	Contains data from 30 European countries: Austria, Belgium, Bulgaria, Cyprus, the Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, The Netherlands, Norway, Poland, Portugal, Romania, the Slovak Republic, Slovenia, Spain, Sweden, Switzerland, and United Kingdom. Includes population data with information on employment, births, deaths etc.	Level of information and time frame is variable between countries and data
Gridded Population of the World (GPV)	http://sedac.ciesin.columbia.edu/gpw/index.jsp	* Common geo-referenced framework, produced by the Center for International Earth Science Information Network (CIESIN) of the Earth Institute at Columbia University. Globally consistent. * Gridded Population of the World, version 3 (GPWv3): distribution of human population across the globe including population estimates to 2015 * Global Rural-Urban Mapping Project (GRUMP): GRUMP builds on GPWv3 by incorporating urban and rural information	Available for several years and in several spatial distributions

Annex 7. Summary table for databases related to emissions

Name	Source	Description	Other comments
WebDab	http://webdab.emep.int/	Emission database for air pollutions based on the information obtained from 37 European countries. Information is gathered for Main Pollutants, Heavy Metals, Persistent Organic Pollutants and Particulate Matter as totals/sectors and as gridded emissions both for officially reported data and expert estimates. Officially reported emission data is available for the years 1980 to 2005 and projections for 2000, 2005, 2010, 2015 and 2020.	Air only
EPER	http://www.eper.cec.eu.int/eper/	EPER is the European Pollutant Emission Register in which member states have to produce a triennial report on the emissions of industrial facilities into air and waters. The report covers 50 pollutants which must be included if the separately indicated threshold values are exceeded. The first reporting year was 2001 and the second reporting year was 2004 and data were provided by the Member States in June 2006.	Air and water. Data are available as national aggregates and per industrial facility and the level of data is very variable depending of the compound.
RAINS emissions	http://www.iiasa.ac.at/web-apps/tap/RainsWeb/	The Regional Air Pollution INformation and Simulation (RAINS)-model provides a consistent framework for the analysis of reduction strategies for air pollutants. The model considers emissions of sulfur dioxide (SO2), nitrogen oxides (NOx), ammonia (NH3), volatile organic compounds (VOC) and particulate matter (PM). Geographical coverage is Europe.	Air only, includes emission factors also
CEPMEIP Database – Emissions	http://www.air.sk/tno/cepmeip/emissions.php	The Co-coordinated European Programme on Particulate Matter Emission Inventories, Projections and Guidance (CEPMEIP) is part of the activities aimed at supporting national experts in reporting particulate matter emission inventories to the EMEP programme. Information for emissions of TSP, PM10 and PM2.5 for European countries in year 2005. Same data can be obtained also from WebDab (EMEP database). Includes also emission factors for particles categorized based on the source and fuel.	Air only, also emission factors in http://www.air.sk/tno/cepmeip/em_factors.php
EDGAR	http://www.mnp.nl/edgar/	Provides global emission inventories of direct and indirect greenhouse gases from anthropogenic sources including halocarbons and aerosols both on a per country and region basis as well as on a grid. Gases included are CO2, CH4, N2O and HFCs, PFCs and SF6 and the precursor gases CO, NOx, NMVOC and SO2.	Air only

Name	Source	Description	Other comments
Greenhouse Gas Inventory Data	http://ghg.unfccc.int/	National annual greenhouse gas inventories for EU countries for Carbon dioxide, Methane, Nitrous oxide, Perfluorocarbons, Hydrofluorocarbons and Sulphur hexafluoride. The data contain the most recently submitted information, covering the period from 1990 to 2004. At the moment only predefined tables are available, searchable database is under development. Emissions are also available by source categories.	Air only
National emission statistics	http://www.naei.org.uk/emissions/emissions.php	Emission inventory in UK level for various pollutants (POPs, non-metals and metals) and for various years. Also categorized by a source.	Air only, and in UK level.
REZZO	http://www.chmi.cz/uoco/isko/groce/gr06e/adatz.html	The Air Quality Information System collects and generally provides access to data gathered within major ambient air pollution monitoring networks in Czech Republic. Contains information on particles, VOC, PAHs, PCBs, PCDD/Fs, heavy metals etc. for several years.	Only in Czech Republic level
SPECIATE	http://www.epa.gov/ttn/chief/software/speciate/	SPECIATE is the EPA's repository of total organic compound (TOC) and particulate matter (PM) speciation profiles of air pollution sources. Among the many uses of speciation data, these source profiles are used to: 1) create speciated emissions inventories for regional haze, particulate matter (PM2.5), and ozone (O3) air quality modelling; 2) estimate hazardous and toxic air pollutant emissions from total PM and TOC primary emissions; 3) provide input to chemical mass balance (CMB) receptor models; and, 4) verify profiles derived from ambient measurements using multivariate receptor models (e.g., factor analysis and positive matrix factorization). SPECIATE includes a total of 4,080 PM and TOC profiles.	Emission profiles
WebFIRE	http://cfpub.epa.gov/oarweb/index.cfm?action=fire.main	The WebFIRE application provides fast and complete access to the EPA's air emissions factors information. AP42 supplements are also included in the WebFIRE.	Emission factors
Emission Factors Database	http://www.naei.org.uk/emissions/index.php	Emission factors in UK level for various sources in year 2000. For year 2005 emissions factors for road transport are available for 1,3-butadiene, Benzene, Carbon Dioxide as C , Carbon Monoxide, Methane, Nitrogen Oxides as NO2, Nitrous Oxide, Non Methane VOC, PM10 and Sulphur Dioxide.	UK level only, Emission factors
Material Emission Database for 90 Target VOCS	http://irc.nrc-cnrc.gc.ca/pubs/fulltext/nrcc48314/nrcc48314.pdf	Emission factors for 90 VOCs for 69 building material.	pdf file, emission factors
AP42	http://www.epa.gov/ttn/chief/ap42/index.html	Emission factors in tables categorized for sources of various field.	pdf file, emission factors

Annex 8. Summary table for media concentration databases

Name	Source	Description	Other comments
Outdoor Air			
AirBase	http://air-climate.eionet.europa.eu/databases/AirBase/index_html	AirBase is maintained by the European Topic Centre for Air and Climate Change A total of 34 countries (until 2004) have reported air quality data to this monitoring network, including all from the European Union with 1320 sites across Europe. Most common pollutants reported are CO, NOx (NO and NO2), ozone, PM10, PM2.5, SO2 and TSP, with a minor number of countries also reporting on metals (As, Cd, Cr, Cu, Fe, Hg, Mn, Ni, Pb, Zn) and various organic compounds. Data can be presented as statistics, raw data or meta-information. The statistics and raw data are shown either as a table or in a graph (where one can choose between daily or hourly values). Statistical values indicate annual mean, maximum, and the 50, 95 and 98 percentile values	Level of information is dependable of the year and country
EMEP measurement data	http://www.nilu.no/projects/ccc/emepdata.html	Includes measured data from 36 European countries. Measured pollutants include Acidifying and eutrophying compounds, ozone, heavy metals, POPs, particulate matter (Joint EMEP, GAW-WDCA and CREATE database) and VOCs.	Measured components and time frame of measurements varies between cases.
Indoor Air			
EXPOLIS measurement data	http://www.ktl.fi/expolis/index.php?id=19	PM and VOC concentrations measured in years 1996-1997 in Helsinki (Finland), Athens (Greece), Basel (Switzerland), Grenoble (France), Milan (Italy), Prague (Czech) and Oxford (UK).	In Access format

Name	Source	Description	Other comments
Water			
GEMStat database	http://www.gemstat.org/	The GEMStat database provides access to data on groundwater and surface water quality collected by the GEMS/Water Global Network. This Global Network comprises 1400 monitoring stations in 80 countries and incorporates 2 000 000 separate records of over 100 parameters. Monitoring results are collated and submitted to GEMS/Water by National Focus Points (NFPs), themselves appointed and financed by member countries. Includes information on nutrients, ions, metals, microbiology and organic contaminants.	Level of information varies between countries. No data for Czech or Slovakia
Waterbase	http://dataservice.eea.europa.eu/dataservice/available2.asp?type=findkeyword&theme=waterbase	Waterbase is the name of a grouping of European Environment Agency (EEA) databases on status and quality of Europe's rivers, lakes, groundwater bodies and transitional, coastal and marine waters, as well as the quantity of Europe's water resources. Includes information for pesticides, organic matter and nutrients.	Available as raw data, but not relevant information for EnviRisk
Soil and sediment			
EMEP-MSCE	http://www.msceast.org/pops/pop_index.html	Modelled concentrations of POPs and heavy metals in soils on national and hemispheric scale. Concentration maps are provided in national level, but detailed numerical values have to be requested separately. Several reports on EMEP project are provided in the web page.	

Name	Source	Description	Other comments
Food			
GEMSfood	http://sight.who.int/newsearch.asp?cid=131&user=GEMSuser&pass=GEMSu	Established in 1976, GEMS/Food operates through a network of WHO Collaborating Centers and other participating institutions located in over 70 countries around the world. The purpose of GEMS/Food is to collect health-oriented population-based monitoring data on levels and trends of contaminants in food and their significance for health and trade, including a number of pesticide residues.	Includes PCB information for Slovakia
National Food Residue Database (NFRD)	http://nfrd.teagasc.ie/	The National Food Residue Database (NFRD) contains data on chemical residues and contaminants in foods in Ireland. The data is taken from annual residue monitoring programmes and from individual residues studies and surveys. The scope of the data includes: veterinary drugs, prohibited substances, pesticides, heavy metals, dioxins and PCBs, mycotoxins, nitrates and PAHs.	Data only for Ireland
Annual EU-wide Pesticide Residues Monitoring Report	Annual EU-wide Pesticide Residues Monitoring Report	In the EU coordinated programme, eight commodities (apples, tomatoes, lettuce, strawberries, leek, orange juice, head cabbage and rye/oats) are analysed for 47 pesticides. Latest report is for 2004. Overall, 13953 samples were analysed in this programme. The 2004 report covers the situation with regard to pesticide residues monitoring in the participating Member States of the EU and the three EEA States Norway, Iceland, and Liechtenstein. In 2004, data from the eight new Member States Cyprus, Czech Republic, Hungary, Lithuania, Malta, Poland, Slovakia and Slovenia were included in the report for the first time.	Pdf-report

Annex 9. Dispersion models

Name	Source	Description
CALPUFF	http://www.src.com/calpuff/calpuff1.htm	CALPUFF is a multi-layer, multi-species, non-steady state puff dispersion model which can simulate the effects of time- and space-varying meteorological conditions on pollutant transport, transformation, and removal. CALPUFF consists of three main components: CALMET, which is a diagnostic 3-dimensional meteorological model, CALPUFF, an air quality dispersion model and CALPOST, a post processing package. CALPUFF can handle point sources (constant or variable emissions), line sources (constant emissions), volume sources (constant or variable emissions with 1-hour time constant) and area sources.
AERMOD	http://www.epa.gov/scram001/dispersion_prefrec.htm#aermod	AERMOD is a steady-state plume model that incorporates air dispersion based on planetary boundary layer turbulence structure and scaling concepts, including treatment of both surface and elevated sources, and both simple and complex terrain. There are two input data processors that are regulatory components of the AERMOD modelling system: AERMET, a meteorological data preprocessor that incorporates air dispersion based on planetary boundary layer turbulence structure and scaling concepts, and AERMAP, a terrain data preprocessor that incorporates complex terrain using USGS Digital Elevation Data.
AURORA	http://www.vito.be/english/environment/environmentalstudy9d.htm	The AURORA model consists of several modules. The emission generator of AURORA calculates hourly pollutant emissions at the desired resolution, based on available emission data, and proxy data to allow for proper downscaling of coarse data. Vehicle emissions can be generated by coupling the MIMOSA road traffic emission model to the emission generator. The actual Chemistry Transport Model then uses the hourly meteorological input data and emission data to predict the dynamic behaviour of air pollutants (both gaseous and particulate) in the model region. This results in hourly three-dimensional concentration and two-dimensional deposition fields for all species of interest. Available on request for research purposes.
CAMx	http://www.camx.com/	CAMx is an Eulerian photochemical dispersion model that allows for integrated "one-atmosphere" assessments of gaseous and particulate air pollution (ozone, PM2.5, PM10, air toxics) over many scales ranging from sub-urban to continental. It is designed to unify all of the technical features required of "state-of-the-science" air quality models into a single system that is computationally efficient, easy to use, and publicly available. CAMx can be provided environmental input fields from any meteorological model (e.g., MM5, RAMS, and WRF) and emission inputs from any emissions processor (SMOKE, CONCEPT, EPS, EMS).

Name	Source	Description
UDM-FMI, CAR-FMI and EXPAND	http://pandora.meng.auth.gr/mds/showlong.php?id=103&MTG_Session=741185074ecea6e247fdaf18d2e535e1 http://pandora.meng.auth.gr/mds/showlong.php?id=121	For the assessments of air pollutant (NO_2, NO, O_3, $PM_{2.5}$, CO, and SO_2) concentrations in urban areas, a more extensive modelling system has been developed for evaluating traffic flows, emissions from stationary and vehicular sources, and atmospheric dispersion of pollution in an urban area. The dispersion modelling is based on combined application of the Urban Dispersion Modelling system (UDM-FMI) and the road network dispersion model (CAR-FMI), developed at FMI. The modelling system has been extended to contain a mathematical model for determination of human exposure to ambient air pollution in an urban area (EXPAND). These models are available within research co-operation

Annex 10. Time-microenvironment activity models

Name	Source	Description
MENTOR/SHEDS (The Modelling Environment for Total Risk studies/Stochastic Human Exposure and Dose Simulation)	Georgopoulos PG et al. Journal of Exposure Analysis and Environmental Epidemiology, (2005) 15, 439-457	These models estimate population exposure and dose by calculating ambient outdoor concentrations and subsequent in-microenvironment concentrations, characterizing populations by demographics and their associated time-activity patterns and inhalation rates, and in some cases using biologically-based modelling to estimate target tissue dose. The model is essentially a joint application of concentration, exposure and dosimetry models and databases. Mass balance and indoor source emission factors are used to estimate indoor concentrations from both indoor and outdoor sources. Outdoor concentrations may be derived from measurement or dispersion modelling. Time-activity is based on diary days (not distributional). Model is stochastic
STEMS (The Space-Time Exposure Modeling System)	Gulliver J and DJ Briggs. Environmental Research (2005) 97(1), 10-25.	STEMS models a time series of exposure from a specific source (or sources) to a specific individual across his/her movement paths and locations over a specific time span. For input data STEMS requires air pollution source and/or concentration data of high space and time resolution (See Dispersion Models fact sheet), and respective path and location data (e.g. from GPS) of the individual(s) whose exposure is/are being modelled. It is possible to model also indoor exposures to air pollutants of outdoor origin (See Ventilation/dilution Modelling fact sheet). It is also possible to run STEMS in a probabilistic modelling mode using the activities, paths and locations of simulated individuals. A disadvantage, however, is that running STEMS for an extended time and large number of individuals – representing a population – is a quite data intensive process.
EXPOLIS stochastic exposure modelling framework	Kruize H, et al. Journal of Exposure Analysis and Environmental Epidemiology (2003) 13 (2): 87-99.	Probabilistic application using Latin hypercube sampling of a simple microenvironment model was used to estimate population exposures to PM10 in the Dutch population and PM2.5 exposure distributions in four European cities. Model was developed using Microsoft Excel with the @Risk add-on. The model is best for 24-hour or more averaging times. Input data were measured indoors and outdoors at home and indoors at work with participant time activity data to model personal exposure from the EXPOLIS study. Both time activity and concentration distributions were developed.

Annex 11. Probabilistic intake models

Name	Source	Description
SHEDS models	Zartarian, V. G., H. Ozkaynak, et al. Environ Health Perspect (2000), 108(6): 505-14	Available for various applications in different media, such as particulate matter and pesticides; also part of MENTOR/SHEDS toolbox for source-to-dose modelling; dermal and non-dietary exposure models developed for home pesticide use and arsenic in playground equipment for children.
CONSEXPO	http://www.rivm.nl/en/healthanddisease/productsafety/Main.jsp	Developed by RIVM, the Dutch National Institute for Public Health and the Environment, CONSEXPO is a model that allows for estimation of exposure or intake for several classes of consumer products and various use scenarios. The model is available in both deterministic and stochastic versions.

Annex 12. Multimedia and Food Chain Models

Name	Source	Description
WATSON	Bachmann, 2006	WATSON facilitates the coverage of exposures towards hazardous substances, i.e. heavy metals, through ingestion of various food items in a spatially-resolved pan-European setting by following the Impact Pathway Approach (IPA). The overall method relies on a coupled set of environmental fate models for air on the one hand and for soil and (fresh) water on the other, the latter described with the help of a spatially-resolved climatological box model similar to Mackay level III/IV models (Mackay, 1991). The estimation of ingestion-related exposures builds on the site-specific risk assessment approach recommended by the US-EPA for hazardous waste combustion facilities (United States - Environmental Protection Agency, 1998), thereby striving for representative rather than for protective estimates. The exposure assessment follows administrative units taking the availability of food and population data into account. Trade is considered as an extension of the (natural) environmental fate.
IMPACT 2002	Pennington et al., 2005; Jolliet et al., 2003; Pelichet, 2003 http://www.sph.umich.edu/riskcenter/jolliet/impact2002+.htm	A delineation of the atmosphere according to a grid is suggested which is in line with many existing air quality models for larger scales (Pekar et al., 1999; Green et al., 2000; Bey et al., 2001; Ilyin et al., 2001) and with global water balance models (e.g. Vörösmarty et al., 1998). While the sea environment also follows the grid delineation for air, the terrestrial environment is spatially differentiated in IMPACT 2002 according to watersheds. For human health, different exposure pathways are aggregated into the so-called Intake Fraction (Bennett et al., 2002) which assesses the portion of an emission that a population will be finally exposed to. The effects on human health due to the estimated exposure are assessed following the Disability Adjusted Life Years (DALY) concept (Murray and Lopez, 1996a, 1996b).
TRIM (Total Risk Integrated Methodology)	United States - Environmental Protection Agency, 1999a, 1999b, 2002a, 2002b http://www.epa.gov/ttn/fera/trim_fate.html	The TRIM design offers a rather flexible framework for the assessment of so-called hazardous and criteria air pollutants, examples for the latter are particulate matter (PM), ozone, carbon monoxide, nitrogen oxides, sulphur dioxide, and lead. The flexibility is realized, for instance, by the capability of using different environmental fate models that may be based on first-order or higher order algorithms. While aiming at multimedia capabilities, the modular design may even allow the use of single medium models, i.e. Gaussian plume models for air. In addition to providing exposure estimates relevant to ecological risk assessment, TRIM generates media concentrations relevant to human ingestion exposures that can be used as input to the ingestion component of the Exposure-Event module. Human exposures are evaluated by tracking either randomly selected individuals that represent an area\'s population or population groups referred to as "cohorts" and their inhalation and ingestion through time and space.

Name	**Source**	**Description**
CalTOX	http://eetd.lbl.gov/ie/ERA/caltox/index.html	CalTOX has been developed as a set of spreadsheet models and spreadsheet data sets to assist in assessing human exposures from continuous releases to multiple environmental media, i.e. air, soil, and water. It has also been used for waste classification and for setting soil clean-up levels at uncontrolled hazardous wastes sites. The modelling components of CalTOX include a multimedia transport and transformation model, multi-pathway exposure scenario models, and add-ins to quantify and evaluate uncertainty and variability.
EUSES2	http://ecb.jrc.it/euses/	EUSES is a risk assessment model, which includes module for exposure assessment. Other modules included are input, emission, distribution, effect, risk characterization and output module. Calculations can be made in personal, local, regional and continental levels. Inhalation, dermal and ingestion routes are considered and also consumer and occupational exposures can be calculated. Requires free registration.
Dynabox	Heijungs, 2000 http://www.leidenuniv.nl/cml/ssp/publications/wp99005.pdf	

Annex 13. Regression models

Name	Source	Description
MLR (Multiple Linear Regression)	Espigares et al. 2003	Levels of THMs in water seem to correlate directly with levels of combined residual chlorine and nitrates, and inversely with the level of free residual chlorine. Statistical analysis with multiple linear regression was conducted to determine the best-fitting models. The models chosen incorporate between two and four independent variables and include chemical oxygen demand, nitrites, and Ammonia. These indicators, which are commonly determined during the water treatment process, demonstrate the strongest correlation with the levels of trihalomethanes in water and offer great utility as an accessible method for THM detection and control.
Linear regression	Harris et al. 2002	Purpose of the study was to define what factors affect to the level of exposure for pesticides among professional turf applicators. Level of three pesticides in urine was collected from the test persons. The group also filled out questionnaires to acquire information on all known variables that could potentially increase or decrease pesticide exposure relative to the amount handled. Linear regression was used to assess the relationship between the concentrations of the substances in urine and the questionnaire data.

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P.O. Box 100, N-2027 Kjeller, Norway
Associated with CIENS and the Environmental Research Alliance of Norway
ISO certified according to NS-EN ISO 9001

REPORT SERIES SCIENTIFIC REPORT	REPORT NO. OR 30/2009	ISBN: 978-82-425-2120-0 (printed) 978-82-425-2122-4 (electronic) ISSN: 0807-7207	
DATE	SIGN.	NO. OF PAGES 53	PRICE NOK 150.-
TITLE EnviRisk Review of databases, modelling methods and tools for exposure assessment		PROJECT LEADER Alena Bartonova NILU PROJECT NO. U-106177	
AUTHOR(S) [1] Arja Asikainen, Miranda Loh, Matti Jantunen [2] Karen Bruusgaard, Hai-Ying Liu, Alena Bartonova 1) Norwegian Institute for Air Research 2) National Institute for Health and Welfare (THL), Finland		CLASSIFICATION * A CONTRACT REF. FP6, Project No. 044232	
REPORT PREPARED FOR European Commission			
KEYWORDS Databases	Exposure assessment	Modelling methods, modelling tools	

ABSTRACT
This study reviewed all available databases and modelling tools for exposure assessment in the areas relevant for the EC EHAP and ENHIS-2. For databases, we reviewed data for general exposure factors (e.g. time activity, ingestion, housing, land use, physiological and population size related data), emission data (e.g. air, water, soil and sediment, emission factors and emission profiles) and data for media concentrations (outdoor air, indoor air, water, soil and sediment, food). For exposure assessment methods and modelling tools, we separated it into: (i) sources and media of exposure; (ii) exposure and intake modelling; (iii) modelling environmental concentration; and (iv) model descriptions by category.

** Classification* *A* *Unclassified (can be ordered from NILU)*
B *Restricted distribution*
C *Classified (not to be distributed)*

REFERENCE: U-106177
DATE: October 2009
ISBN: 978-82-425-2120-0 (printed)
978-82-425-2122-4 (electronic)

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